VIII International Conference on Computational Methods for Coupled Problems in Science and Engineering

COUPLED PROBLEMS 2019

3-5 June 2019 in Sitges, Spain

Eugenio Oñate, Manolis Papadrakakis and Bernhard A. Schrefler (Eds.)
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PREFACE

This volume contains the Technical Programme of the papers accepted for presentation at the VIII International Conference on Computational Methods for Coupled Problems in Science and Engineering, COUPLED PROBLEMS 2019 (3 – 5 June 2019, Sitges, Barcelona, Spain).

The previous five editions of this conference were held on the islands of Santorini (Greece) on 25-28 May 2005, Ibiza (Spain) on 21-23 May 2007, Ischia (Italy) on 8-11 June 2009, Kos (Greece) on 20-22 June 2011, Ibiza (Spain) on June 17 – 19 June 2013, San Servolo, Venice, Italy on May 18 - 20 2015 and Rhodes Island, Greece on June 12-14 June 2017.

The objectives of COUPLED PROBLEMS 2019 are to present and discuss state of the art, mathematical models, numerical methods and computational techniques for solving coupling problems of multidisciplinary character in science and engineering. The conference goal is to make a step forward in the formulation and solution of real life problems with a multidisciplinary vision, accounting for all the complex couplings involved in the physical description of the problem.

The conference is one of the Thematic Conferences of the European Community on Computational Methods in Applied Sciences (ECCOMAS) and a Special Interest Conference of the International Association for Computational Mechanics (IACM).

The conference is jointly organized by the International Centre for Numerical Methods in Engineering (CIMNE) of the Technical University of Catalonia (UPC), the National Technical University of Athens (Greece), and the Department of Civil, Environmental and Architectural Engineering (DICEA), of the University of Padova (Italy).

The organizers would like to thank the authors for submitting their contributions and for their respect of the deadlines. Special thanks go to the colleagues who contributed to the organization of the 33 Invited Sessions in the fields of the Conference, and to the colleagues of international prestige that accepted the invitation to address a Plenary Lecture.

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SUPPORTING ORGANIZATIONS

The conference organizers acknowledge the support of the following organizations:

- International Centre for Numerical Methods in Engineering (CIMNE), Spain
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- Department of Civil, Environmental and Architectural Engineering (DICEA) of the University of Padova, Italy
- European Community on Computational Methods in Applied Sciences (ECCOMAS)
- International Association for Computational Mechanics (IACM)
- Universitat Politècnica de Catalunya (UPC)
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LECTURES
COUPLING FEM AND CFD SOLVERS FOR CONTINUOUS CASTING PROCESS SIMULATION USING PRECICE

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Key words: thermo-mechanical coupling, FVM, FEM, casting

Abstract. The numerical investigation of continuous casting requires more than just one simulation technique. In continuous casting, liquid metal is continuously poured into a mould while the starting head is slowly moved downwards, which results in a growing metal ingot. Though, the ingot’s outer surface is solidified after the mould, its inside core is still a mixture of liquid and mushy phases. This mixture of physical states requires different numerical schemes to describe the constitutive behaviour and relation. While the liquid region is described in the Eulerian approach, the solid is well described in the Lagrangian approach. Commonly the finite volume method is chosen for the Eulerian and the finite element method for the Lagrangian perspective. Consequently, it is logical to combine a CFD solver with a FEM solver for an ideal numerical representation of the continuous casting process. The coupling of two different solvers communicating in two different programming languages - in the present work OpenFOAM and LS-DYNA - is not an easy task. However, preCICE enables the coupling of the different solvers with a minimum of intrusive functions.

The present work deals with the first step towards the coupled simulation routine for the continuous casting process. A first basic simulation of a simple plate was setup consisting of OpenFOAM for the Eulerian approach and LS-DYNA for the Lagrangian approach. OpenFOAM calculates the temperature field due to time-dependent boundary conditions, while the mechanical LS-DYNA solver calculates resulting strains and stresses considering thermal strain. The aim of this simulation was to develop and test the preCICE adapter for LS-DYNA, as the adapter for OpenFOAM is already available and ready to use. The mapping techniques of preCICE did manage to achieve good energy conservation results. The first results showed a good correlation especially in the middle of the domain. The difference at the plates’ ends between the two different methods defined the next steps for the coupling.
1 INTRODUCTION

As pointed out in [1] the attitude of modern society is changing. Sustainability and energy efficiency became more important throughout the different industries. These changes also had a big impact on metal casting. Although metal casting processes are well established over a long period of time, the casting industry is facing new challenges according to the change in society as described in [2], leading to the need for continuous process improvement and its prominent role in today’s industries.

The improvement of well established processes is in general more difficult. They demand for an in-depth knowledge about the process and the full understanding of its phenomena. In [3] the importance of numerical models is described. They are generally capable of simulating the details of the phenomena and mechanisms involved in the processes. The continuous casting process is no exception. Its virtual representation can help to solve the arised challenges.

The continuous casting process is a very complex process, especially from the viewpoint of a numerical simulation. According to [4], the numerical model has to consider thermal, mechanical, electromagnetic, hydrodynamic and free boundary phenomena. All of these phenomena are strongly dependent on the chosen material and its properties. Besides the influence of the phenomena, the material properties greatly influence the casting process and its parameters. Especially the casting of high strength aluminium alloys is critical due to the limited ductility and the resulting risk of hot tearing or cold cracking as outlined in [5].

1.1 State of the art

The requirements, constraints and boundary conditions of a simulation model specify the ideal numerical method. Each method has its strength and weaknesses. Especially for a process involving a lot of different phenomena it is normal that a variety of solution methods exist, as different physical aspects are addressed and challenged.

In [6] the role of coupling different length scales as well as the interaction between the fluid flow and solidification phenomena is addressed. Furthermore, it is outlined that a strong and complex coupling between the physical phenomena at different scales is crucial for a correct description of the process by means of numerical simulations.

In [7] the need for the simulation of flow related phenomena and the simulation of stress and deformation is described. A simulation method is proposed to simulate the solidification while considering elastic stresses implemented in the Finite Volume Method (FVM) based solver OpenFOAM.

In [5], a simulation model for the continuous casting process has been developed based on the Finite Element Method (FEM) solver ALSIM5. The goal of this approach was to receive in-depth understanding of the thermo-mechanical thermo-mechanical processes in the ingot during the casting process. Hereby, the time-dependent boundary conditions have been defined to consider thermal field effects. The heat flow due to convective heat
transfer is apparently not solved within ALSIM5. A criterion for cold cracking has been proposed to predict failure mechanisms in the process and to improve the production efficiency of high strength aluminium alloys. Another approach is documented in [4], where the continuous casting process is simulated in a simplified manner with a sole FEM solver, where convective heat transfer and resulting heat flow are neglected.

1.2 Motivation

Continuous casting involves many different physical phenomena. These phenomena will mostly inquire different solver formulations as well as different software products. In addition, it is often desired to use already in-house available software products. Hence, the coupling of the different physical domains and involved solvers is of great interest to develop a reliable and agile simulation model.

This paper presents a solution for the coupling of a FVM based CFD solver and a FEM based structural solver by means of preCICE [8]. The FVM based CFD solver is ideal for the simulation of the fluid flow and the resulting temperature field considering convective and conductive heat transfer. The FEM based structural solver is capable of simulating deformations of structures, hence resulting strain and stress fields.

In section two a first pilot study will be presented together with the physical and numerical setup. Afterwards, in section 3 the results of the first pilot study are shown before those are being discussed in section 4. The final outlook will deal with the next steps for the setup of a continuous casting process simulation based on a coupled FVM based CFD solver and a FEM based structural solver.

2 SETUP

A strongly simplified setup is defined aligned with the requirements of a continuous casting simulation. It serves as a first pilot study for coupling the commercial FE Code LS-DYNA (R9.3.0) with a CFD solver via the coupling library preCICE (v1.3.0). Since, the main objective of this work is the development and implementation of a preCICE adapter in LS-DYNA, it was necessary to test the adapter for its functionality. To do so, the second participant should have an established and tested adapter. OpenFOAM (v5.0) is chosen as CFD solver and second participant in the coupling, as this adapter is already available [9]. More specifically, OpenFOAM’s laplacianFoam is chosen for solving the heat equation. In the current version of the OpenFOAM adapter, the exchange of the temperature fields is restricted to patches. Patches are restricted to surfaces and so they are excluding data mapping within volume elements [9]. Therefore, the geometrical setup is defined such, that it can be meshed with a single volume or element in the thickness direction. In this way, the definition of patches provides comparable data as the volumetric definition would provide for the chosen test setup. Furthermore, the deformations will be kept small since displacements are not mapped from LS-DYNA to OpenFOAM in this
investigation. Nevertheless, the elastic behaviour of the material should be observable, resulting in elastic stresses.

For ease of complexity, the geometry is defined as a rectangular, thin walled plate with the dimensions $L_x$, $L_y$ and $L_z$ (see figure 1). The plate is fixed against motion in $x$-direction on both ends. In addition, the two points $A$ and $B$ are fully constrained to prevent rigid body motion. A transient, structural mechanical analysis is applied to the plate considering thermal expansion with the material density $\rho$, Young’s modulus $E$, Poisson’s ratio $\nu$ and the linear thermal expansion coefficient $\alpha_T$. The thermal diffusivity $\alpha$ is determined by $\alpha = \lambda/(\rho c_p)$ with the thermal conductivity $\lambda$ and the specific heat capacity $c_p$ (see table 1).

<table>
<thead>
<tr>
<th>Parameter</th>
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The plate is initialised with the temperature $T_{\text{init}}$. An adiabatic Neumann condition is applied for the heat equation as $\left(\frac{\partial}{\partial x}T(x=0,t)\right) = 0$ on the left wall at $x=0$. At $x=L_x$ the wall temperature increases over time. This time dependent boundary condition describes as $T(x=L_x,t) = T_{\text{init}} + t/t_{\text{tot}} \cdot \Delta T$ with the temperature increase $\Delta T$ over the total simulation time $t_{\text{tot}}$ (see table 1).

The domain is discretised with different meshes (see table 2). Mesh 1 is denoted as the reference mesh. This is also applied for a standalone thermomechanical LS-DYNA simulation. The variation of meshes in the OpenFOAM simulations results in non-conforming meshes with respect to the reference mesh used by LS-DYNA. In LS-DYNA the element formulation $e\text{form 1}$ is applied. The OpenFOAM discretisation schemes are the default for the laplacianFoam solver.

The total simulation time $t_{\text{tot}}$ is discretised using a fixed time step $\Delta t$ with an implicit Euler time stepping scheme for both solvers. The fixed time step was chosen to simplify the programming of the preCICE adapter for LS-DYNA. Although the time step management would theoretically be possible with preCICE, it demands for more access and
intrusive interfacing which is not guaranteed to work. Therefore, an adaptive time step was excluded in the first phase of adapter development.

The preCICE configuration file defines the main parameters for the coupling. In this present case, the calculation of the mapping matrix is done at the very beginning of the simulation. The data is transferred in a two-way coupling from OpenFOAM to LS-DYNA and vice versa in a consistent way. Though, the data transferred from LS-DYNA to OpenFOAM are currently only dummy data with $T_{(Sink)} = 0$.

While in LS-DYNA the temperature data is stored on the nodes (corners of an element), the data storage in OpenFOAM depends on the coupling settings. In this case, data is stored on the faceCentres, as option faceNodes did not work correctly with the used OpenFOAM adapter. Followingly, the vertices for data transfer do never conform. As a consequence, the choice for the mapping algorithm and its settings was quite impor-

Table 2: Overview of the different, used mesh parameters

<table>
<thead>
<tr>
<th>Simulation</th>
<th>elem. type</th>
<th>discr. in x</th>
<th>discr. in y</th>
<th>discr. in z</th>
<th>tot. elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>LS-DYNA mesh</td>
<td>hex</td>
<td>30</td>
<td>10</td>
<td>1</td>
<td>300</td>
</tr>
<tr>
<td>OpenFOAM mesh 1</td>
<td>hex</td>
<td>30</td>
<td>10</td>
<td>1</td>
<td>300</td>
</tr>
<tr>
<td>OpenFOAM mesh 2</td>
<td>hex</td>
<td>75</td>
<td>25</td>
<td>1</td>
<td>1875</td>
</tr>
<tr>
<td>OpenFOAM mesh 3</td>
<td>tet</td>
<td>30</td>
<td>10</td>
<td>1</td>
<td>3275</td>
</tr>
<tr>
<td>OpenFOAM mesh 4</td>
<td>tet</td>
<td>75</td>
<td>25</td>
<td>1</td>
<td>37591</td>
</tr>
</tbody>
</table>
tant. preCICE has to extrapolate data from the OpenFoam points to the LS-DYNA nodes. Thin plate splines are applied for spatial mapping, as they have provided the best mapping results. A thermo-mechanical simulation was set up for the development of the preCICE adapter for LS-DYNA to compare and validate the results of the coupled solvers. In the following, this thermo-mechanical simulation is referred to as the reference solution.

3 RESULTS

Figure 2 shows the final contour plots for the temperature (3a) and the von Mises (2b) equivalent stress of the thermo-mechanical reference simulation in LS-DYNA. The contour plot of the temperature shows the temperature field increasing from 299 K to 493 K. The absence of externally applied forces means that the von Mises equivalent stress ranging from 40 MPa to 103 MPa are induced by the thermal strains. So, it is necessary to validate the temperature field between the original OpenFOAM values and the received LS-DYNA values versus the thermo-mechanical solution within LS-DYNA.

![Contour plots at $t = t_{tot}$ for the thermo-mechanical calculation with LS-DYNA](image)

Figure 2: Contour plots at $t = t_{tot}$ for the thermo-mechanical calculation with LS-DYNA.

Figure 3 shows the temperature curves for the different simulations and compares the thermo-mechanical LS-DYNA calculation. However, the absolute values are not of great interest only the the difference to the original temperature field. Thereby the temperature has been normalised. $\Theta$ corresponds to the normalised temperature difference as $\Theta = (T - T_{init})/\Delta T$. While figure 3a shows the complete temperature curve along the interface, figure 3b and figure 3c are detailed to $0 \leq x \leq 0.1$ and to $0.95 \leq x \leq 1.0$, respectively. The overall view shows a good correlation between the reference curve and the results of the coupled simulations. With the detailed views it can be seen, that the temperatures of the coupled simulations are overestimating at $x = 0$ and underestimating at $x = L$. 
Table 3 shows the energy conservation during data transfer. Therefore, the total thermal energy in OpenFOAM ($E_{OF}$) and LS-DYNA ($E_{LS}$), respectively, was calculated. In addition, the total error between $E_{OF}$ and $E_{LS}$ was calculated with respect to the total thermal energy in OpenFOAM. The thermal energy $E_{OF}$ shows a slight difference between the hex and tet meshes. The thermal energies between the coarse and fine meshes are very close. The energies $E_{LS}$ are always very close to the original energies $E_{OF}$, as the total errors show with values between $10^{-4}$ and $10^{-6}$.

**Table 3: Energy conservation**

<table>
<thead>
<tr>
<th>simulation</th>
<th>$E_{OF}$</th>
<th>$E_{LS}$</th>
<th>total error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0260831</td>
<td>0.0260832</td>
<td>$3.8 \cdot 10^{-6}$</td>
</tr>
<tr>
<td>2</td>
<td>0.0260833</td>
<td>0.0260869</td>
<td>$1.4 \cdot 10^{-4}$</td>
</tr>
<tr>
<td>3</td>
<td>0.0261217</td>
<td>0.0261191</td>
<td>$-1.0 \cdot 10^{-4}$</td>
</tr>
<tr>
<td>4</td>
<td>0.0261257</td>
<td>0.0261224</td>
<td>$1.3 \cdot 10^{-4}$</td>
</tr>
</tbody>
</table>

4 DISCUSSION

The main goal of the presented simulations and results was to develop a first draft of a preCICE adapter for LS-DYNA and show the applicability of preCICE for future process simulations. The comparison of the normalised temperature curves at $t = t_{end}$ shows a very good agreement with a very small total error between $10^{-4}$ and $10^{-6}$. The detailed view at the beginning and the end of the interface for $x = 0$ and $x = L$ shows deviations of about 3% with the chosen mapping setup. With the OpenFOAM data points at the face centres and the LS-DYNA data points on the nodes (corners of the elements) the temperature values in the LS-DYNA on the left and right boundary area of the geometry are extrapolated. The general mapping was sufficiently precise, apart from the missing mapping inside of the exemplary geometry. The error for the total energy of the OpenFOAM is negligible compared to the LS-DYNA calculation.

5 OUTLOOK

The described work presents a first step towards a continuous casting process simulation consisting of a FEM based structural solver coupled to a FVM based CFD solver to increase the predictability of the temperature field. In the future, it is necessary to gradually increase the complexity in order to be able to describe the continuous casting process. Hereby, it is planned to introduce fluid flow inside the liquid metal in order to calculate the convection driven temperature field. Afterwards, the phase change from the liquid metal to the solid material has to be implemented.
The available OpenFOAM adapter does not include volume mapping, the simulation setup was chosen as an interface (surface) mapping or a quasi-2D problem, which is no option for future process simulation. In the future, the final setup of the simulation has to be a volume mapping.

These steps can be done based on the presented setup. However, the setup also has to be extended to a two-way coupling, to consider the displacement and its consequences on to the cooling behaviour.

ACKNOWLEDGEMENTS

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REFERENCES


Figure 3: Temperature for the quasi-2D conduction case with $LS$ corresponding to the results of the mechanical solver LS-DYNA, $OF$ corresponding to the thermal solver OpenFOAM and $tm$ corresponding to the reference solution.
FLUID STRUCTURE INTERACTION MODELLING ON FLAPPING WINGS

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Key words: Computational Fluid Dynamics, Fluid Structure Interaction, FSI, Open-Source, Flapping Wings

Abstract. Flapping wings display complex flows which can be used to generate large lift forces. Flexibility in wings is widely used by natural flyers to increase the aerodynamic performance. The influence of wing flexibility on the flow can be computed using numerical analysis with Fluid Structure Interaction (FSI).

The influence of inertial, elastic and aerodynamic forces is quantified using a 2D wing. A sinusoidal flapping motion is imposed on the leading edge of the vertical wing. The inertial force on the wing dominates for high mass ratios and the wing deflection is rather independent of the flow. For a low mass ratio, the wing deformation scales with the increasing elasticity. The maximum lift and lowest drag were found for the wing with large flexibility and low mass so the passive deformation by aerodynamic forces creates a favourable shape for lift production.

Flexible translating and revolving wings at an angle of attack of 45 degrees show that chordwise flexibility decreases both lift and drag, however the lift over drag ratio is increased. The flow around both wings forms a coherent structure with a Root Vortex (RV), Tip Vortex (TV), Leading Edge Vortex (LEV) and Trailing Edge Vortex (TEV). The LEV on the revolving wing is stable for approximately up to half the span because vorticity is transported outward in the vortex core. The flowfield and LEV breakdown are consistent with experimental data of the same wing. The translating wing builds up circulation but the LEV detaches quickly near the centre of the wing. Chordwise bending reduces the angle of attack which decreases the distance to the core of the shed LEVs.
1 INTRODUCTION

Over the past years increased interest in Micro Air Vehicles (MAVs) has lead to an increase in research towards flapping wing aerodynamics. This research is often based on natural flyers as these display remarkable capabilities in force production, manoeuvrability and efficiency. Currently, these capabilities are unmatched by man-made flyers. The aerodynamic phenomena found on flapping wing are different from the classic airfoil theory that is used at higher Reynolds numbers. Unsteady phenomena play a large role in the force production by flapping wings. The Wagner effect, added mass effect, clap and fling effect, Kramer effect, wake capture effect, tip vortex contribution and a stable LEV. The latter effect was first recognised in 1996 and is often the most prominent feature for lift generation in flapping wing aerodynamics [10]. It is seen on wings moving at a high angle of attack which feature dynamic stall [20]. A vortex is formed over the leading edge which can remain stably attached to the wing surface and creates a low pressure area inherent to the vortex with a large suction force on the wing. The suction force acts perpendicular to the wing surface and is dominant in lift production. The high suction force leads to a maximum in the lift coefficient for $45^\circ$ angle of attack [17, 22, 18].

The motion of flapping wings is determined by an acceleration phase and a phase of rectilinear motion. Both translating and revolving wings at high angles of attack are capable of developing a LEV at the acceleration phase, but only for revolving wings the LEV can remain stably attached to the wing surface [15]. For translating wings a vortex streak is formed which resembles the von Kármán vortex street behind a cylinder. Early research postulated that the LEV stability in revolving wings was caused by outboard vorticity transport [10]. Subsequent researches evaluate the influence of the various apparent rotational effects on the LEV, and reach the conclusion that mainly the Coriolis force is responsible for the stability of the LEV [15, 13, 12]. The relative influence of the Coriolis force is related to the degree of translating versus rotating motion, expressed in the Rossby number. The rotational effects scale inversely with the Rossby number on the wing, and the LEV stability is deteriorates for higher Rossby numbers.

Apart from a different flapping motions, natural flyers exhibit flexible wings. Birds and bats actively deform their wings, while most insects rely on passive wing deformation [21]. Experimental research showed that the application of flexibility on a simple revolving wing leads to smaller lift but decreases the drag likewise [30]. Numerical research on 2D and 3D flapping wings showed that the wing efficiency for a given angle of attack can be increased by the application of flexible wings. The dynamic behaviour of the wing is categorised by the mass and frequency ratio, which determine the relative importance of the inertial, elastic and aerodynamic force on the wing. Flapping wing with a low mass ratio reach the largest lift over drag (L/D) for a frequency ratio near $FR = 1/3$ [27, 8, 16]. Heavier wings create an advanced pitching motion.

More recently, experiments towards the influence of flexibility on flapping wings was performed using tomographic PIV [26]. In this work a revolving wing was tested for three
wings with a varying elasticity. The lift and drag decreased for the added flexibility, but an increase in L/D ratio was noted. The flowfield showed similar structures with more coherency with increasing flexibility. Furthermore, the LEV of the flexible cases was more compact and showed higher levels of vorticity transport through the LEV core. Breakdown of the LEV is seen for all three wings around midspan after the wing revolved for approximately 40°.

Numerical modelling of the wing using a FSI method can be used to gain more insight in the fundamental interaction that takes place between the structure and the fluid. Several commercial methods exist for the modelling of FSI coupled simulations, however, on the open-source side a smaller variety is available. The most used open source CFD code, openFOAM does not include standard methods of creating a FSI simulation [1]. Recent progress by on a generic OpenFOAM adapter has opened the door for a new approach [7]. Coupling of the simulation is performed using the multi-physics coupling library preCICE [24]. The adapter was extended to support Fluid structure interaction modelling [19]. The method was validated along the Cylinder with a Flap benchmarking case [23]. In this paper the influence of flexibility in flapping wings is investigated using the newly developed FSI method. The following section treats the influence of flexibility on 2D flapping wing, where the influence of the wing mass and elasticity on the force coefficients is derived.

2 2D Flapping wing

In this section a simple hovering flapping wing in a 2D domain is considered, at the low Reynolds number of 150 [29]. The mass and stiffness of the wing are varied to change the relative importance of the aerodynamic, elastic and inertial forces which act on the wing. The structure for this case shows large, nonlinear deformations, therefore the case is solved in an implicit FSI simulation using the newly developed FSI method [19].

2.1 Model description

The flow around the wing is characterised by several non-dimensional numbers which can be obtained by combining the structure and fluid parameters. Figure 1 shows the wing with the kinematic parameters and with the surrounding mesh. The chord (c) and thickness (h) influence both the fluid and the structure side. The angle of attack is defined with respect to the horizontal direction x.

The wing kinematics are purely defined by the translation $x_0$ and angle of attack $\alpha$ of the wing at the leading edge. In the current set-up no phase differences between the translation and pitching of the wing are considered. The wing kinematics are determined by the following equations:

$$x_0(t) = \frac{A_0}{2} \cos(2\pi ft), \quad \alpha(t) = \alpha_0 + \beta \sin(2\pi ft).$$  (1)

Following from the wing movement the non-dimensional time can be defined: $\tau = t/T,$
with $T$ the period of the flapping motion: $T = 1/f$. The non-dimensional numbers are the Reynolds number, non-dimensional stroke amplitude, mass and frequency ratio:

$$Re = \frac{\pi A_0 f c}{\nu_f}, \quad A^* = \frac{A_0}{c}, \quad (2)$$

$$m^* = \frac{\rho_s h}{\rho_f c}, \quad FR^* = \frac{f}{f_n}. \quad (3)$$

where $f_n$ is the frequency of the first bending eigenmode of the wing. The frequency ratio ($FR$) is a measure for the flexibility of the wing with respect to the fluid forces and is used to define the relative importance of elastic and inertial forces. Previous research has shown that there is an optimum in the frequency ratio such that the wing has the highest efficiency [27, 16, 8]. The mass ratio ($m^*$) defines the ratio between the aerodynamic forces and the inertial force. For a simple flapping wing with no active pitching the drag increases for higher mass ratios [16]. The forces generated by the airflow typically bend the wing into a shape with a lowered angle of attack, reducing the frontal area and thus the drag. The parameters used to set up the simulation are given in table 1. The relation between the fluid and structural component are determined using the expressions in equation 4

$$\rho_s = \frac{m^* \rho_f c}{h}, \quad E = \frac{12 \rho_s}{h^2} \left( \frac{c}{k_n} \right)^4 \left( \frac{2\pi f}{FR} \right)^2, \quad (4)$$

where $k_n$ is a constant for a given bending eigenfrequency.

Table 1: Set-up for the flexible flapping wing

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c$ [m]</td>
<td>$1 \cdot 10^{-2}$</td>
</tr>
<tr>
<td>$h$ [m]</td>
<td>$5 \cdot 10^{-4}$</td>
</tr>
<tr>
<td>$\nu_f$ [m$^2$s$^{-1}$]</td>
<td>$5 \cdot 10^{-5}$</td>
</tr>
<tr>
<td>$\rho_f$ [kg m$^{-3}$]</td>
<td>10</td>
</tr>
<tr>
<td>$f$ [s$^{-1}$]</td>
<td>1.910</td>
</tr>
</tbody>
</table>

Table 2: Structural parameters for the flexible wings

<table>
<thead>
<tr>
<th>$m^*$ [-]</th>
<th>$\rho_f$ [kg m$^{-3}$]</th>
<th>$E$ [kg m$^{-1}$s$^{-2}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>FR = 1/6</td>
<td>FR = 1/4</td>
<td>FR = 1/3</td>
</tr>
<tr>
<td>1</td>
<td>200</td>
<td>3.295-10$^4$</td>
</tr>
<tr>
<td>5</td>
<td>1,000</td>
<td>1.647-10$^5$</td>
</tr>
<tr>
<td>25</td>
<td>5,000</td>
<td>8.235-10$^5$</td>
</tr>
</tbody>
</table>

The flexible definition of parameters easily allows for the choice of different settings. The mass ratio can be increased to increase the relative effect of inertial over aerodynamic forces. Three different mass ratios are tested as shown in table 2. In flapping wing analogy, the lowest mass ratio is comparable with a dragonfly wing, the $m^* = 5$ wing is close to a moths wing [9]. For the highest mass ratio the wing deformation is largely determined by the inertial forces [16].
2.2 Mesh sensitivity study

For the mesh sensitivity study a rigid wing is selected. $A_0 = 2.5c$ and $\beta = \pi/8$ in equation 1 define the sweeping and rotation of the wing. A small pitching angle is used to assert some asymmetry in vertical direction to the flowfield and to generate a finite average lift. An $O$-grid is shaped around the wing and extruded for 40 chord lengths to form a circular domain. A large domain is required to avoid large recirculation of shed vortices which create chaotic behaviour. A free inflow/outflow and zero pressure is applied on the outer boundary. The mesh surrounding the wing is shown in figure 1 for the coarsest grid.

Under the sweeping and rotational motion the mesh is deformed by solving the laplacian equation for the mesh displacement. To limit deformation and preserve the mesh quality the leading and trailing edge were rounded. The shape of the leading edge is of relative low importance for the overall flowfield, so the round-off is not expected to have a serious impact on the flow simulation [25]. Furthermore, the mesh cells are grown perpendicular with respect to the wing surface. It was found that this reduced the chance of large skewness or even cell collapse.

The force coefficients are evaluated for three meshes of increasing refinement. The coarse mesh has 4,968 elements. The normal and fine mesh feature respectively 19,440 and 77,760 elements. The wing surface is refined with respectively 54, 108 and 216 cells, which leads to an average mesh spacing of approximately $0.02c$ for the coarsest mesh. This is comparable to the mesh spacing used in similar research [29].

Figure 2 shows the phase-averaged lift and drag over the wing for 6 flapping periods.
The drag is defined as the force opposite to the direction of travel, so the drag vector changes direction during supination and pronation. The range in which the lift and drag occurred over this range of periods is shaded. From $\tau = 0$ to $\tau = 0.5$ the wing is in upstroke. While the wing kinematics imposed to the wing movement are completely symmetric, the lift and drag show very different graphs for the up- and downstroke. This means that the flow is determined to a large extend by the shed vortices of the previous motion.

The total average value for the lift and drag (shown in table 3) shows good correlation for the average lift and drag.

Taking the finest mesh as the most accurate solution, both the coarse mesh and the normal mesh fall within the range of the average force value plus or minus the average maximum deviation. Over the range of the motions over 6 periods, it is clear that the average lift and drag of the coarse mesh fall within the possible values for the normal mesh and fine mesh.

The mesh deformation method described earlier performs significantly better with coarser meshes. It is less prone to collapse under large rotation and deformation. Since the behaviour of the coarse mesh shows good correlation with the fine mesh, it is selected to investigate the effect of different mass and frequency ratios.
2.3 Results

Flexibility is added to the wing according to the parameters given in table 2. Furthermore a rigid wing with the same kinematics is tested to obtain the limiting case of \( FR = 0 \). The wing kinematics are defined by a pure sweeping motion: \( A_0 = 2.5c \) and \( \beta = 0 \). This entails that the wing can only obtain an angle of attack by structural bending. The effect of the mass ratio on the tip displacement and force coefficients is shown in figure 4 for four wings: Rigid, and \( m^* = [1, 5, 25] \) with a frequency ratio of \( FR = 1/3 \). The first eigenfrequency is noted for all three wings as the oscillation with a value three times the flapping frequency.

![Figure 4: Influence of the mass ratio \( m^* \) on the (top) tail x- and y displacement and (bottom) lift and drag coefficient over two flapping periods. - Rigid, \( m^* = 1 \), \( m^* = 5 \), \( m^* = 25 \)](image)

The tail deflection with respect to the rigid position shows that the wing with the smallest mass ratio has a phase delay with respect to the two heavy wings. Furthermore the deflection of the wing is much larger, with a maximum horizontal deflection of approx-
imately 0.7 chordlength. The delay and larger amplitude of the deflection means that the light wing creates a lower angle of attack during both the up- and downstroke. In both these strokes a large portion of lift is created, whereas the drag is comparable or smaller to the other wings. Large asymmetry is caused because the shedding behaviour between both strokes is different, as will be treated later.

Small differences can be seen between the $m^* = 5$ and $m^* = 25$ wing but these are far less pronounced than the differences with the lightest wing. For both these wings the deflection is nearly symmetrical between up- and downstroke, while the aerodynamic forces are not. As soon as the wing decelerates during midstroke, the deflection in x-direction changes sign. During both the middle part of the up- and downstroke the $m^* = 5$ wing maintains a higher deflection, which is caused by a LEV which stays closely attached to the wing. The low pressure favours a larger lift and drag creation during this phase of high translational velocity. During the latter part of the stroke a small portion of thrust is created by the wing because of the advanced rotation.

In figure 4 the lift and drag profile for the wing with $m^* = 1$ shows irregular behaviour at the point of large displacement. The discontinuous force coefficients are caused by large fluctuations in the pressure field between timesteps. This represents the limits of the current mesh deformation method.

![Figure 5](image-url)

**Figure 5:** Average (left) lift and (middle) drag coefficient, and (right) lift over drag ratio for different mass ratios. (top) FSI simulations with $m^* = 0.5$, $m^* = 1$, $m^* = 5$ and $m^* = 25$. (bottom) the reference case with $m^* = 1$, $m^* = 5$ and $m^* = 25$ [16]. Note the scale difference on the x-axis between the top and bottom figures. For both the FSI simulations and the reference data the forces are averaged over 15 periods. The flowfield of points 1, 2 and 3 is shown in figure 6.
The effect of a higher stiffness by changing the frequency ratio (FR) causes the elastic effect to dominate the wing movement in the latter part of the stroke. During the acceleration part of the stroke, the wing is deflected by the wings’ mass (inertial force). The aerodynamic forces can help to maintain this deflection during the latter part of the stroke and prolong a lower angle of attack. This effect is most pronounced for the most flexible wings. A larger deflection causes a lower angle of attack and decreases the frontal area. The drag history shows a clear that the drag is reduced for a large portion of the stroke for more flexible wings. However, the advanced rotation by the stiffer wings create a small portion of thrust, as also seen for the rigid wing. This lacks for the most flexible wings.

Figure 5 displays the average lift and drag coefficient, and lift over drag ratio for all the tested wings over 15 flapping periods. A wing with an even lower mass ratio of $m^* = 0.5$ is incorporated for two additional mass ratios, which indicates the limit of the mesh deformation method. Furthermore, reference data is shown on the bottom row for same wing geometry and kinematics, where a wing was tested up to frequency ratios of 0.8 [16].

For the tested range of flapping frequencies any flexibility increases the lift over the wing. The wing bending creates a lower angle of attack which points the residual fore more towards the lift direction. Furthermore, a clear relation can be distinguished between the mass ratio and the lift. Lower mass ratios lead to a higher lift for this range of the frequency ratio. This result is also seen for the reference data. The relative higher importance of the aerodynamic forces with respect to the inertial forces helps in maintaining a lower angle of attack throughout the latter part of the stroke. The highest lift coefficient is obtained for the $m^* = 1$ and $FR = 1/3$ wing with a value of $C_L = 1.076$. It appears that the delayed rotation of the wing for low mass ratios helps in decreasing the drag on the wing by reducing its frontal area. The advanced rotation by the heavier wings initially increases the drag. The peak for the $m^* = 5$ wing at a frequency ratio of $FR = 1/3$ is featured in both the reference data and the simulated data. This point is interesting since it shows a different behaviour for the wings with $m^* = [5, 25]$ and $FR = 1/3$. Up to this point the lift and drag of these two wings were very similar.

For this frequency range a straightforward relation is seen between the lift to drag ratio. A more flexible wing leads to higher ratios. Also the lightest wings create higher lift over drag ratios by means of a high lift creation. This is in good agreement the reference data which shows the same trend for this range of frequency ratios [16]. In figure 6 the vorticity flowfield around three wings is shown for one flapping motion. The vorticity is normalised according to: $\omega^* = \omega \frac{U}{c}$. The left column indicates the wing in which the inertial force is dominant: $m^* = 25$, $FR = 1/3$, named hereby wing 1. The middle figure shows the wing 2 with dominance of the elastic forces: $m^* = 1$, $FR = 1/6$. The latter column shows the wing 3 for which the three forces are more balanced. This wing features the highest lift and lift over drag ratio in the tested range.
All three cases show a similar shedding of the vortices. In the beginning of the period ($\tau = 0.1$), the LEV of the previous stroke remains close to the wing surface and is convected both above and below the wing after stroke reversal. The wake capturing causes rapid buildup of vorticity on the leading edge, but the newly formed LEV cannot stay attached closely to the wing ($\tau = 0.3$). At stroke reversal ($\tau = 0.5$), the LEV catches up with the wing and it is shed under the wing and forms a counter rotating vortex pair with the previous TEV. The shed vortex pair has a larger downward component for wing 3 compared to the other wings. This indicates that it is more efficient in inducing downward momentum in the flow, while the other wings create a larger horizontal momentum.

Without the wake capturing, the formation of a new LEV takes longer, and around ($\tau = 0.7$) a compact core can be seen around the LE which has grown to a large LEV with significant force contribution near the end of stroke.

Figure 6: Non-dimensional in-plane vorticity (left) $m^* = 25$ and $FR = 1/3$. (middle) $m^* = 1$ and $FR = 1/6$. (right) $m^* = 1$ and $FR = 1/3$. A representative period is taken and the time instance is scaled to the time.
The effect of the mass ratio is most evident by the phase of the flapping motion. Neglecting the amplitude of the deflection, the shape of the wing 3 is often similar to that of wing 1 in for $\tau - 0.2$, which indicates a phase delay of $1/5^{th}$ of a period.

Comparing the effect of the wing frequency ratio shows that the vortical structure of the flows are very similar. Also the wing displacement shows smaller effect of the phase delay. Only at $\tau = 0.9$ wing 2 is clearly already near $90^\circ$ angle of attack, while wing 3 still has a much lower value. The main difference in flowfield is caused by the lower angles of attack of the flexible wing. This helps pointing the resulting force in the direction of the lift vector, while reducing the drag at the same time. For wing 1 the upstroke has a larger deflection and is responsible for the major part of lift production. This effect is much less pronounced for wing 2, since its shape is more determined by elastic forces.

3 CONCLUSIONS

The section above treats the influence of different degrees of stiffness and mass of a flapping 2D wing. The newly developed FSI method is able to capture well the relative importance of the various forces that occur on the flapping wing [19]. A simple translation motion is prescribed without any pitching. The stiffness and mass of the wing determine the relative effect of the inertial and elastic forces and can be related to the aerodynamic forces by defining the frequency ratio ($FR$) and mass ratio ($m^*$).

A large mass ratio renders the fluid forces insignificant due to high inertial forces. The wing deformation is determined by the wing kinematics and hardly by the influence of the flowfield. As soon as the wing starts to decelerate during midstroke the wing deflection is reversed shortly after. A light wing shows a deflection which causes lowered angle of attack during almost the entire stroke because the aerodynamic forces help to sustain the angle of attack. The advanced rotation of the higher mass ratio wings is not beneficial for the production of lift. For the investigated range of flapping frequencies, a lower mass ratio always leads to a higher lift and lift over drag ratio. The influence of the frequency ratio is more predictable. The deflection is lower for stiffer wings which creates lower lift and higher drag. The more rigid wings show a slight advance in pitching behaviour.

The horizontal flapping motion creates an asymmetric flowfield between the up- and downstroke which was present for every combination of the mass ratio and frequency for the tested cases. The wings with a relative large influence from the aerodynamic forces to be are influenced by the asymmetry in the flowfield and show a difference in deflection between the up- and downstroke. Especially for the wing with $m^* = 1$ and $FR = 1/3$ this difference is pronounced. Wings dominated by either elastic or inertial forces are less affected by the flowfield and show more symmetric deflection of the trailing edge.

The results regarding the influence of the mass and frequency ratio obtained in this section are in good agreement with comparable research [16]. Therefore the FSI module is able to simulate the relative importance of the various forces in flapping wing aerodynamics.
References


FRAMEWORK FOR FLUID-STRUCTURE INTERACTION SIMULATIONS WITH UZEN AND PRECICE: SIMULATIONS PROCEDURE AND VALIDATION

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Key words: FSI, load transfer, time coupling, panel flutter

Abstract.
The paper illustrates a new framework developed to face with Fluid Structure Interaction phenomena in a partitioned approach. The CIRA multi-block structured flow solver[1] for unsteady RANS equations, UZEN, was updated and tightly coupled with an open-source FEM code CalculiX[2]. The solvers are glued in space and time through an open source library, preCICE[3] to deliver exchanging data. preCICE manages the communications, loads mapping and time coupling.

Motivation of the work is the simulation of unsteady aerodynamic problems strongly dependent upon structural behaviour, like flexible aircraft, rotor-craft, counter-rotating rotors, etc.

As validation tests, the results of 2D and 3D panel flutter response at supersonic velocity are illustrated. The results are compared in terms of Limit Cycle Oscillation amplitude and frequency of panel flutter with data available in literature.

1 INTRODUCTION
In the present work, a multi-block structured flow solver[4] for unsteady RANS equations has been coupled with a structural solver within the software environment managed by the open source library preCICE [3], in order to perform fluid-structure interaction simulations.
preCICE (Precise Code Interaction Coupling Environment) is a coupling library for partitioned multi-physics simulations. The software offers methods for transient equation coupling, communication means, and data mapping schemes.

An adapter that delivers exchanging data from CFD solver to preCICE library has been developed, that translates data from CFD to the interfaces, and receives data from FEM solver through preCICE. The loads transfer, or space coupling, is afforded within the library with different techniques, such as Nearest-Neighbour or RBF; the time coupling and convergence check are also managed by the schemes available in the library.

Motivation of the work is the simulation of unsteady aerodynamic problems strongly dependent from structural behaviour, like flexible aircraft, rotor-craft, counter-rotating rotors, or in the framework of airplane weight minimization, where flow induced vibrations influence stability and durability of aircraft\[5, 6\].

Structural solver, already interfaced within the preCICE framework, is the open source FEM code Calculix\[7\].

The choice of the preCICE framework was driven by several reasons: the open source environment (no costs and limitations stemming from licences), possibility of testing both explicit and implicit fluid-structure interaction, several interpolation and exchange methods for forces and deformations already available and implemented. Finally the library has been developed with the aim of allowing efficient usage of massively parallel computing architectures\[8\]. At the same time, the FEM solver, Calculix, is already coupled with an official adapter. The package is able to perform linear and non-linear analysis of static and dynamic problems.

As far as we know, this is the only CFD system based upon structured multi-block meshes fully integrated with a structural dynamic solver for unsteady simulations with dynamic meshes.

To validate the FSI framework, 2D and 3D inviscid panel flutter at supersonic speed is investigated. The problem of instability of plates in gas flow has been studied and reported in literature. In supersonic flow, the instability has the oscillatory nature known as flutter, that can be distinguished in coupled or single-mode flutter\[9\]. Several time-domain simulations of non-linear panel flutter were performed from transonic to supersonic flows by several authors \[10, 11, 9, 12, 13\]. From their results at supersonic Mach number flows we should expect high frequency Limit Cycle Oscillations (LCO).

Since it was discovered, inter alia in the 60s at NASA on the Atlas-Centaur and Saturn V rocket, considerable effort was spent to investigate the impact on panel flutter of several structural and aerodynamic parameters. Due to the great cost and complexity involved in supersonic wind tunnel tests, panel flutter has always been studied mainly via mathematical and numerical modelling. Focusing on the aerodynamics side of numerical approach (i.e. the kind of solvers coupled to structural ones to model the aeroelastic phenomena), in the decade going from 50s to 70s theoretical studies have considered different aerodynamic modelling: from the linear piston-theory, a quasi-steady relation between pressure and panel deflection valid for high supersonic Mach numbers in Von Karman’s plate the-
ory to the unsteady linearized potential flow theory, and to the unsteady 'shear flow' theory developed by Dowell\cite{14} that takes into account the viscous effects in the boundary layer on the aeroelastic behavior.

Recent works have introduced FEM and CFD solvers to investigate panel flutter in high subsonic and low supersonic flows. Euler equations and FEM were coupled to study non-linear Karman plate equations \cite{10}, Navier-Stokes equations to take into account the unsteady viscous laminar boundary layer were introduced in flutter studies by Gordinier and Visbal \cite{11} for the solution of non-linear Karman plate equations again. Hashimoto \cite{12} involved RANS computations to take into account the effects of a turbulent boundary layer, confirming that the boundary layer has a stabilizing effect on the flutter. Also Alder \cite{15} focused on the effects of the turbulent boundary layer defining the stability limits and post flutter characteristics of a 2D and 3D simply supported panel.

Recently, Hejranfar\cite{16} employed a second-order central-difference cell-vertex finite volume method to study 2D panel flutter in inviscid compressible flow: unsteady Euler equations governing fluid flows in the arbitrary Lagrangian-Eulerian form and the large deformation of the solid structure is considered to be governed by the Cauchy equations formulated in the total Lagrangian form. In his study, on the FEM solver side, the panel is modeled with plane strain element, where also the thickness is modeled in order to compute the stress distribution.

In this paper the results of two and three-dimensional analyses of panel flutter are shown, after presenting the two solvers and the way they are coupled by means of preCICE library. The 2D panel flutter analysis is suited to set up the numerical approaches to face with the problem, verifying time and space convergence of the solutions. Finally, the results of the flutter of square and rectangular 3D plates are compared with literature data.

2 Aerodynamic Solver

ZEN is a multi-block structured flow solver developed at CIRA for the U-RANS equations with classical ALE formulation\cite{17, 1}. The spatial discretization is based upon cell-centred finite volumes discretization, with second and fourth order artificial dissipation. The unsteady computations are carried out by using an implicit second order backward difference method together with dual time stepping toward steady state for each physical time step.

CIRA has recently developed a system for flow simulation\cite{4} which allows the non-conformal block to block coupling (i.e. sliding mesh) and dynamic mesh on block base (i.e. some specific blocks in the flow field can be deformed and updated at each time step). Mesh is updated outside the flow solver, which makes possible to iterate with other systems to compute, in a segregated approach, structural deformation, body dynamics and possibly other physical phenomena. Dynamic meshes are implemented by following the 3 step backward implicit time scheme in such a way to satisfy the discrete geometrical conservation law (DGCL\cite{6}). The updated mesh is reloaded at each time step, which
allows to post-process surface deformations due to structural dynamics and, possibly, body dynamics outside the flow solver. It is possible to apply dynamic mesh modifications only in some blocks, to save computational time. The code is adapted to face with FSI problem: in detail, to allows a strong-coupling, the current time step calculations can be repeated (and the updated mesh reloaded), when required, under control of external routines that check for suitable convergence criteria. This will described in details in the following sections.

The flow simulation system communicates by delivering local forces on specific mesh surfaces, as specified in a set-up file, and it is capable to re-mesh the flow domain starting from a set of updated geometric entities like surfaces, curves and vertices, by following specific directives. Geometric entities can be specified or modified by control points.

The adapter code developed for ZEN code is designed as a stand alone software that synchronizes communications with preCICE library, sending and receiving data to and from interface grids. It will be described in the following sections.

3 Structural Solver

CalculiX is a free/open-source (GPL) Finite Element package, developed at the MTU Aero Engines, currently coupled with preCICE with an official adapter in order to face with Fluid-Structure Interaction (structure part), Conjugate Heat Transfer (solid part). Through its adapter CalculiX can write displacement, temperature, heat flux, sink temperature, heat transfer coefficient and can read force, temperature, heat Flux, sink Temperature, heat transfer coefficient. According to the type of analysis, different solvers are available: linear and non-linear, implicit and explicit solver (CCX), written by Guido Dhondt[7, 2]. Those solvers are implemented in C and Fortran modules.

The implicit solver uses incomplete Cholesky pre-conditioning and the iterative solver by Rank and Ruecker [7], which is based on the algorithms by Schwarz [2]. The equation of motion is integrated in time using the $\alpha$-method developed by Hilber, Hughes and Taylor[7]. This implicit scheme is unconditionally stable and second-order accurate when the $\alpha$ parameter lies in the interval [-1/3,0], in order to controls the high frequency dissipation: $\alpha=0$ corresponds to the classical Newmark method inducing no dissipation at all, while $\alpha=-1/3$ corresponds to maximum dissipation[2].

In this work, Calculix is employed to carry out non-linear analysis of structural dynamic problems. A ready-to use adapter able to communicate through preCICE is already available[18].

4 FLUID - STRUCTURE COUPLING: preCICE

This section describes the way CFD and FEM solvers are coupled in a partitioned approach. The aim is to achieve convergence towards solution in every time step by executing each solver independently.

In the context of a partitioned approach, crucial aspects are the load and deformations
transfer over the interfaces shared by the different computational domains, and the time coupling of the different solutions, in order to ensure convergence at each time iteration. Momentum and energy exchanged between the two sub-systems have to be conserved, otherwise the spurious work introduced leads to instabilities divergence of the solution. The introduction or removal of spurious energy by the interface scheme may affect the overall stability properties of the aeroelastic system [19]. Hence, the time synchronization and the transfer of information at interface for non-matching space discretization influence the stability of the algorithm.

The coupling between the two solvers is managed by the open-source preCICE library. The library treats the numerical methods for equation’s coupling among the different solvers involved in the multi-physics simulations.

From the structural solver side, the architecture illustrated by Rush[3] is adopted, i.e. the Calculix solver has its adapter that exchanges data with CFD solver through preCICE library. From the CFD solver side, a black-box adapter coupled with a bash script that is able to manage the timing processes and the ZEN-interface with preCICE was developed.

The adapter interface developed in this framework is designed as a stand-alone code, not fully integrated within the CFD solver. Only the communication toward the FEM direction is managed by preCICE: this is configured with a point-to-point based on TCP/IP socket. The communications between CFD and preCICE direction, are based on file-transfer.

4.1 Time-coupling

A coupling scheme describes the logical execution order of two participants in the partitioned approach it is possible to distinguish between a weakly (explicit) and fully coupled (implicit) schemes: the former solves the fluid and solid sub-domains in a staggered fashion without convergence or residual checks, and the stability of this procedure is dependent on density ratio (structure vs fluid), temporal discretization precision order, fluid velocity and flow compressibility[20]. The latter approach foresees that both solvers are executed multiple times until convergence criteria are satisfied at the end of each time step. To this family belong the Block Gauss-Seidel (BGS), the Newton and quasi-Newton strategies.

In the preCICE library either explicit and implicit coupling schemes are available, with the possibility to apply different convergence criteria.

Furthermore, either serial or parallel executions can be selected. Serial refers to the staggered execution of one participant after the other. Parallel refers to the simultaneous execution of both participants.

The strong coupling approaches transform the coupling conditions into Fixed Point Formulation or Equation (FPE). The kind of FPE used determines the execution sequence of the two solvers. One is the staggered execution (see Figure 1), while two parallel approaches introduced by preCICE developers are showed in figure 2, both allowing for the simultaneous execution of fluid and structure solver.
A key role in time coupling is played by the post-processing technique to be applied at data exchanged between the segregated solvers. A pure implicit coupling without post-processing corresponds to a simple fixed-point iteration, which still has the same stability issues as an explicit coupling. A postprocessing techniques is needed in order to stabilize and accelerate the fixed-point iteration.

In preCICE, three different types of post-processing can be configured: constant (constant under-relaxation), Aitken (adaptive under-relaxation), and various quasi-Newton variants (IQN-ILS also known as Anderson acceleration, IQN-IMVJ or generalized Broyden).

4.2 Load Transfer

In the frame of partitioned approach, the meshes of the different solvers are not conforming at the fluid structure domain interface: they differ in the refinement and gaps and or overlap can also be present. Then a projection of the variables valued with the different solvers at interface should be implemented.

Several authors treat those approaches, showing pro’s and con’s[21, 22, 23, 24, 25, 26, 27]. There are several criteria which such a data exchange or coupling method ideally should satisfy. The most important are: (i) global conservation of energy over the interface, (ii) global conservation of loads over the interface, (iii) accuracy, (iv) conservation of the accuracy order of the coupled solvers and (v) efficiency, which is defined as a ratio.
between accuracy and computational costs.

According to the main hypotheses on which the transfer operator is built, it is possible to follow a conservative or consistent approach: in the former, the energy is conserved when transferring displacement, pressure and viscous forces over the interface, and it is based on the global conservation of Virtual Work over the interface. In the consistent approach, the constant displacement and constant pressure are exactly interpolated over the interface. In this case the energy conservation is not guaranteed, however can be shown that the error in work transferred can be reduced refining the meshes[23].

A number of methods able to transfer data from grid to grid are available, they are classified in groups: Point-to-Point, Point-to-element and Virtual Surface Method.

In this paper, focus is given on Radial Basis Function (RBF) method, belongs the class of point-to-point schemes, also known as multivariate transfer technique, they are widely adopted in the frame of FSI([28, 29, 30, 31, 24]. Those are mesh-less methods allow to couple structural and fluid domains by reducing them to pure point information. A clear advantage of this technique is the fact that the information about discretization schemes and geometrical typologies are not required.

The value of $f$ at a generic location $x$, is obtained as a weighted sum of radial basis functions $\phi(|x - x_{C_j}|)$ based on the Euclidean distance between the control points position $x_j$ and $x$:

$$f(x) = \sum_{j=1}^{N_c} \gamma_j \phi(|x - x_{C_j}|) + q(x)$$

(1)

The interpolation condition is also imposed at the control points:

$$f(x_{C_j}) = f_{C_j} \quad \text{for} \quad j = 1, \ldots, N_c$$

(2)

in order to guarantee the positive definiteness of the RBF problem, the following condition

$$\sum_{j=1}^{N_c} \gamma_j p(x_{C_j}) = 0$$

(3)

should hold for any polynomial $p$ with degree less or equal than the degree of $q$.

The basis functions investigated in this work, are Thin Plate Spline and Gaussian spline:

- Thin Plate (TPS):
  $$\phi(|x|) = |x|^2 \log |x|$$
  (4)

- Gaussian Spline:
  $$\phi(|x|) = \exp^{-a|x|^2}$$
  (5)

where $a$ is a shape parameter.
Radial Basis Functions guarantee a consistent interpolation, but energy is not preserved when loads are transferred over the interface. On the other hand, by adopting a conservative interpolations, the consistency is lost[23]. Moreover, the basis functions need a tuning for the proper setting of the shape parameters.

4.3 CFD ZEN INTERFACE

The CFD ZEN code is coupled with the FEM solver Calculix through the preCICE library. From the FEM side, CalculiX exchanges data with preCICE through a devoted interface[3, 8, 18]. In this section the way the ZEN solver exchanges data with preCICE is described.

The adapter is designed in a less intrusive way, from the point of view of the ZEN solver, since the adapter is totally self-standing and very few coding was made within the solver.

Figure 3 illustrates conceptually how the FSI analysis starts and how data are exchanged during the calculation between the ZEN CFD solver and the ZEN adapter: the latter sends data to preCICE.

The ZEN adapter is coded in cpp language. It is designed to share the CFD variables (i.e. the non-dimensional loads), available after each time step, with the preCICE library.

The simulation starts by launching a shell script that manages the library initialization step. The initialization sets up communications between the adapters to preCICE (from both sides), in order to assign labels, allocate pointers and memory for deforming grids nodes. Moreover, the interface reads information about the face numbering for the exchange of local loads, those have to match the structural mesh.

As the CFD code solves non-dimensional equations, reference dimensions are required in order transform local and global forces, i.e. free-stream static pressure and static temperature, time step and scale length. When launched, the CFD adapter employs the information about free-stream values, to calculate the dimensional loads.

In order to explain how the FSI simulation works, it is convenient to describe first how the CFD solver ZEN performs a flow simulation with dynamic meshes. When a flow simulation with dynamic meshes is running, ZEN requires an updated mesh at each new time step, together with a flag that informs the flow solver whether the time step is completed or the updated mesh has to replace the current one without advancing in time. The latter case happens when implicit coupling occurs and iterative loops are executed with other models. Handling the mesh updating outside the flow solver has several advantages. Among them it allows different models to interact with the configuration geometry (like structural dynamics, body dynamics, configuration changes driven by time laws or any kind of control systems, and so on) and it makes possible to check convergence on both aerodynamic forces and configuration shape by using procedures external to the flow solver. Figure 4 highlights the main tasks performed during a time step. The ZEN flow solver reads a GRID file and writes output files containing (non dimensional) local and global aerodynamic forces, then it waits for an updated GRID. Meanwhile the ZEN
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Figure 3: Global chart

The adapter reads the aerodynamic forces, computes dimensional loads and sends them to the FEM solver CalculiX through preCICE library. The FEM solver computes displacements, preCICE routines checks loads and displacements for convergence and returns displacements to the adapter, together with information whether to advance in time or to repeat the computation to improve residuals. The adapter writes output files containing the updated shape of configuration surfaces, required to make a new GRID, and the FSI.LOOP flag to inform ZEN about the time step convergence. As the updated surfaces are ready, the procedure to update the dynamic grid produces an updated GRID. The CFD solver checks whether to advance the time step or repeat it by reading the FSI.LOOP flag, then it reads the updated GRID and computes aerodynamic forces again. In figure 4 is also shown how another model which requires aerodynamic forces and computes configuration movements could fit into the procedure, by communicating information to the procedure to update the GRID. More details about the tasks are given in the next paragraph.

5 RESULTS

In this section the output of the 2D panel flutter investigation will be shown, aimed to explore the preCICE capability and to find a better tuning to obtain reliable results in an efficient way. The investigation has regarded the load transfer methods, time-coupling and post-processing scheme, and convergence threshold. Finally, 3D panel flutter results are compared with literature data.

5.1 Numerical Settings

In order to set the numerical methods discussed in previous sections, preCICE can be configured at runtime via an xml file (precice-config.xml), where the solvers, the fluid and solid interfaces exchanging data, the kind of data (i.e. scalars, vectors) are defined and
The nature of the problem under investigation requires a strongly coupled approach, as noted also from [11], hence an implicit coupling was chosen. To stabilize and accelerate the fixed-point iteration several post-processing schemes were tested, such as Aitken and the two Quasi Newton variants: IQN-ILS also known as Anderson acceleration, IQN-IMVJ or generalized Broyden.

For implicit coupling scheme, preCICE employs a convergence measure that can be relative or absolute. Here a relative convergence threshold values for displacements and forces is adopted. The FEM solution is taken as reference: all data relative to FEM are post-processed and the convergence is valued on forces and displacement elaborated from the FEM side. The effects of threshold are investigated for forces and displacement ranging from $10^{-3}$ to $10^{-6}$ for both displacement and forces.

Other parameters in the coupling schemes and postprocessing have to be set, such as starting relaxation parameters applied to delivered forces and or displacements, maximum number of iterations and extrapolation order. The maximum number of sub-iterations within an implicit coupling loop was set to 30.

On fluid side, in order to compare the results with other authors without the uncertainties stemming from boundary layer thickness and turbulence model effects, the flow is solved with Euler equations.

Even if the non-linear FEM solver allows subcycling within each iteration by changing the time step size to achieve convergence of loads, the current Calculix adapter cannot
manage sub-cycling. Hence the user-defined initial time step is not changed.

5.2 2D Panel Flutter

Here we investigate how the amplitude and the frequency of the LCO changes, according to the critical dynamic pressure, \( \lambda \), defined as \( \lambda^* = \frac{\rho_\infty u_\infty^2 a^3}{D} \), where \( D \) is the plate stiffness, \( \frac{Eh^3}{12(1-\nu^2)} \). Hence, by changing the Young modulus of the plate, we have obtained a set of \( \lambda \) values at which the analysis are carried out. The mass ratio, \( \mu \), calculated as \( \mu = \frac{\rho_\infty a}{\rho_m h} \), is kept constant during the simulations and equal to 0.1. The thickness ratio, \( h/a \) is equal to 0.002. Free stream Mach number is set to \( M_\infty = 1.2 \), furthermore pressure and static temperature are fixed and equal to 25000 Pa and 223 K. The panel is pinned at ends, the length is \( a = 0.5 \) (m) with uniform thickness \( h = 1.00 \times 10^{-3} \) m.

The CFD grid, shown in Figure 5, is made of a single block with three different grid density that will be tested to verify their influence on the LCO calculations showed in the following. The coarser grid, L1, has 105x80 cells, the medium grid L2, 169x80 cells and the finest grid, L3, has 297x80 cells. The flexible interface surface that defines the panel is hence sampled respectively with 64, 128 and 256 cells.

The FEM model of the panel is made of quadratic plane-strain elements with 8 nodes, that would be able to model an infinite panel in the cross-wise direction, in fact, as stated by Calculix\[2\] manual, they are used to model a slice of a very long structure.

For 2D calculations, the FEM element chosen is a second order Plain - Strain one (CPE8, see in [2]).

![Figure 5: CFD grid](image)

Dependency on spatial resolution and time step, from CFD side, is evaluated by considering as a term of comparison the maximum vertical panel displacement, localized at 75\% of plate length, normalized with panel thickness, \( w/h \), that identifies the normalized
Figure 6: solutions at different time-step size

LCO amplitude. The physical time step of the CFD solver is varied from 0.1 to 0.01 (plus 0.005 for L2 grid), while the grid density changes according to the discretization of the panel, from 64 to 256 CFD grid points.

Figure 6 (a) resume the spatial and temporal study, taking in account both the effects of time and grid refinement and showing the maximum displacement of the point at 0.75a versus timestep sampling, for L1, L2 and L3 grid levels: the maximum displacement decreases as timestep is reduced, and slightly increases with grid level refinement.

Figure 6 (b) is referred to the LCO frequencies. The range of frequencies is within 5% with respect to the finest timestep frequency solution on L2 grid level.

In the following, the solution with timestep 0.025 is considered the reference, in order to compare CIRA results with those available in literature.

Figure 7 shows the flowfield pressure coefficient contours in the expansion phase $\phi = 90$, in which are noticeable expansion fans at leading and trailing edges; and compression phase, $\phi = 270$, with presence of shock waves on leading and trailing edges. In this phase the panel showed a deformation in the form of its first natural mode.

In figure 8 are shown both the deformation an the relative pressure coefficient distribution in the expansion and compression stages.

The two solvers start together the integration from free-stream values, and an initial vertical displacement is assigned to the flat panel, equal to $\delta w = w_0 \sin^2 \left( \frac{\pi x}{L} \right)$ where $w_0$, is a constant suitable to produce an initial perturbation. The choice of the modulus of this perturbations influence the time needed to reach the oscillating period of the panel. Even if it can be convenient to simulate the minimum transient time to reach LCO, the modulus of displacements has an influence on the LCO amplitude, as stated by [9]. Figure 9 shows the effects of modulus $w_0$ on the final LCO.
The higher \( w_0 \), the shorter time needed to reach a stable LCO. This is not the only effect since the modulus of \( w/h \) maximum displacement at 75% of panel length starts to change, up to reach a value of 1.556 with the highest initial perturbation.

Figure 10 shows the time-history, the phase portrait and the spectrum of a point at 75% of panel length, for increasing \( \lambda \). The LCO becomes wider as the \( \lambda \) grows, but the other noticeable phenomena is that it becomes non-symmetric with larger \( \lambda \). Such phenomena was evidenced also by Shishaeva[9], even if the analysis was relative to increasing Mach number. The progressive switch from symmetric to non-symmetric LCO is due to the appearance of the second mode, whose frequency yields increase of plate velocity: the flutter is changing from non-resonant to resonant LCO[9]. This is evident the phase-velocity portrait: in the Figure 10 a, it is slightly non-elliptic due to the triple-harmonic, evidenced on the relative frequency spectra on the right. As pressure grows, the 2nd mode amplitude grows as well because to the internal resonance, the velocity increases on phase-velocity portraits, and the relative importance of the 2nd peak of frequency also increases, as it is shown in the spectra on the right.

The results are compared in terms of flutter amplitude and frequency with some data available in literature: figure 16 (a) shows that the maximum displacement foreseen at 0.75a panel point is aligned with recent works that are based on coupling of inviscid CFD codes on fluid side, in the case of pinned panel. Compared to Alder[15], the instability of post-flutter is anticipated to lower \( \lambda \). Figure 16 (b) is relative to LCO frequency: in this case the trend is similar to other data, even if a shift toward higher frequencies can be noted.

After that physical results have been shown, some numerical considerations about the time coupling techniques follow. The average number of coupling iterations, \( k \), shown
Figure 8: Panel shape and Pressure Coefficient during flutter at $M = 1.2$, $\lambda = 100$

Figure 9: Effect of $w_0$ modulus on panel flutter LCO. DTF = 0.025, level L2 grid

in table 1, are relative to results obtained employing a parallel-implicit coupling with Aitken adaptive relaxation, chosen as post-processing technique, that should stabilize and accelerate the fixed point iteration.

From table 1 can be summarized that, by reducing the timestep, the average amount of sub-iterations decreases, and, when a finer CFD grid is employed, the sub-iterations
Figure 10: LCO, Phase portrait and Spectra of reference point at 0.75a, M=1.2, for different $\lambda$, pinned plate.
needed to reach convergence increases.

The time-coupling methods and post-processing techniques are investigated in the following, in order to verify whether they have an influence on computational costs and/or the quality of the solutions. The post-processing techniques compared are Aitken and the two Quasi Newton variants, IQN-ILS and IQN-IMVJ. Aitken was tested also in the staggered coupling, since it is known from literature that it performs better than in parallel coupling.

Table 2 shows that IQN-ILS performs better of other settings in terms of computational costs.

Not reported in the table is also an analysis carried out with a Staggered explicit coupling, and Aitken post-processing. As expected, this analysis diverges, after 450 timesteps.

Other numerical aspects influence the average number of coupling iterations. First of all, the average number of iterations grows by decreasing the measure of convergence tolerance on the data exchanged by the coupled solvers. When an implicit parallel coupling

<table>
<thead>
<tr>
<th>DTF/Grid Lev.</th>
<th>L1</th>
<th>L2</th>
<th>L3</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.005</td>
<td>-</td>
<td>4.02</td>
<td>-</td>
</tr>
<tr>
<td>0.01</td>
<td>3.97</td>
<td>4.84</td>
<td>-</td>
</tr>
<tr>
<td>0.025</td>
<td>4.00</td>
<td>5.25</td>
<td>-</td>
</tr>
<tr>
<td>0.05</td>
<td>6.16</td>
<td>6.25</td>
<td>6.57</td>
</tr>
<tr>
<td>0.075</td>
<td>7.64</td>
<td>7.74</td>
<td>-</td>
</tr>
<tr>
<td>0.1</td>
<td>11.35</td>
<td>11.86</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 1: Average number of coupling iterations for different DTF and Grid Level
is adopted, as in those runs, the relative tolerance of forces and displacement is checked for the convergence within the time-step.

From the table 3 can be noted that, as expected, when the tolerance is small, the iterations needed increases.

Other parameter that depends on the post-processing coupling and that can influence the results, is the initial value of the relaxation factor (common to Aitken and Quasi Newton methods): a larger value of $\omega$ (0.1) has produced a longer convergence history than smaller values (i.e. $\omega = 0.01$).

In the two Quasi Newton variants, a relevant factor is the timestep-reused parameter, that limits the previous iterations used to generate the data basis for Jacobian estimation. To set this, some preliminary evaluations were needed.

### 5.3 3D Panel Flutter

The 3D panel test constitutes a more significant test case for the validation of the FSI environment.

The FEM model of a square panel, $a/b = 1$, is a 20x20x2 solid elements ($C3D20R$). The CFD grid has 64x64 cells on panel, and 112x112x80 in stream-wise, span-wise and normal direction respectively. Furthermore, a rectangular plate $a/b = 0.5$ is also analysed at the same conditions. The square plate results are relative to clamped and pinned boundary conditions (all four edge), while the rectangular plate is clamped at all four edges.

The free-stream flow conditions and the structural plate properties are the same as the 2D simulations: Mach 1.2 and $\lambda = 250, 300$ and 350.

Figure 12 (a) and (b) show the surface pressure contours for square and rectangular plate, respectively, at maximum upward deflection. Both are symmetric with respect to the centerline at $y/b = 0$.

A sequence of compression, expansion and finally a shock wave can be noted in both cases, with larger gradient in the $a/b = 0.5$ case.

Figure 13 (a) and (b) show, for square and rectangular plate respectively, the normalized displacements, $w/h$, on the panel at $\lambda = 300$, when it is at the maximum upward deflection. The results are symmetric with respect to the centerline. The peak of the deflection is found at about $x/a = 0.66$: those results are comparable to the ones shown in [11] for the case of the squared plate.

<table>
<thead>
<tr>
<th>Coupling</th>
<th>k</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stag-Impl Aitken</td>
<td>4.05</td>
</tr>
<tr>
<td>Par-Impl Aitken</td>
<td>6.25</td>
</tr>
<tr>
<td>Par-Impl IQN-ILS</td>
<td>3.27</td>
</tr>
<tr>
<td>Par-Impl IQN-IMVJ</td>
<td>4.83</td>
</tr>
</tbody>
</table>

**Table 2**: Average number of coupling iterations per coupling type (DTF=0.05, L2 grid; point at $x=0.75a$.)
Table 3: Average number of coupling iterations: tolerance effects (DTF=0.05, L2 grid; point at x=0.75a.)

<table>
<thead>
<tr>
<th>ε_{forces};ε_{displacements}</th>
<th>k</th>
</tr>
</thead>
<tbody>
<tr>
<td>1e-3;1e-3</td>
<td>2.94</td>
</tr>
<tr>
<td>1e-4;1e-4</td>
<td>4.60</td>
</tr>
<tr>
<td>1e-5;1e-3</td>
<td>3.27</td>
</tr>
<tr>
<td>1e-5;1e-5</td>
<td>7.16</td>
</tr>
<tr>
<td>1e-6;1e-6</td>
<td>15.76</td>
</tr>
</tbody>
</table>

Figure 12: Surface pressure contours for (M = 1.2, λ = 300) at maximum upward deflection

Figure 14 and 15 show the time history, phase portrait and frequency for the 3D panel at λ = 300, with a/b = 1 and a/b = 0.5, respectively. The reference point considered is the same of previous figures at 0.75 of x/a: the three dimensional effects are evident in phase portraits: when a/b = 0.5 the portrait is quite similar to the 2D results shows in fig. 10.

Figures 16 (a) and (b) show the LCO amplitude and frequency versus dynamic pressure of a point at y = 0.5b and x = 0.75a of the square plate, with clamped and pinned edges. The calculations here performed show good agreement with literature, especially at high pressure levels. The fundamental linear frequency for a 3D panel is valued by ω₀ = π²(1 + AR²)√D/ρsₚₜₚₜₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚₚportion of the document.

Finally, some considerations from the numerical point of view. In the 3D simulations, the Par-Impl IQN-ILS time coupling is chosen. The average number of coupling iterations for the square plate is k = 3.1, while for the rectangular plate k = 2.9. A difference between the two cases is the average amount of iterations that the CFD solver has to run in order to reach convergence in the time step: it is lower for the case with a/b = 1.0 (72)
than for the case $a/b = 0.5$ (99).

6 CONCLUSIONS

This report has described the development and validation of a new framework able to face with FSI problems. Partitioned approach is followed to take advantage of already existing codes: in house CFD solver, and open source FEM. An adapter was developed, by using the preCICE library, that ‘glues’ the CFD code with FEM solver, Calculix. Classical FSI problem of 2D and 3D panel flutter at supersonic speed have been simulated with strongly-coupled partitioned approach and the results are compared with available literature showing good agreement.

REFERENCES


Figure 14: LCO, phase portrait and spectra of point at 0.75a, 0.5b, \( \lambda = 300 \), \( a/b = 1 \), clamped edges


Figure 15: LCO, phase portrait and spectra of point at 0.75a,0.5b, $\lambda = 300$, $a/b = 0.5$, clamped edges

Figure 16: Limit-cycle versus dynamic pressure for 3D panel flutter, $M = 1.2$


A HYBRID MULTIPHASE MODEL BASED ON LATTICE BOLTZMANN METHOD DIRECT SIMULATIONS

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Key words: Wet granular materials, multiphase flow, Lattice Boltzmann, porous media, pore-network, pore-scale

Abstract.

By means of the multicomponent Shan-Chen lattice Boltzmann method (LBM), we investigate the multiphase flow through porous media. Despite the excellent accuracy of the LBM, large domains result in unaffordable computational expenses. The Hybrid model developed in this study is based on a pore-network (PN) approach that enhances a decomposition of the granular assembly into small subsets (pore throats). Lattice Boltzmann simulations are performed for each pore throat to determine the hydrodynamic properties (entry capillary pressure, primary drainage curve, liquid morphology, etc) at the microscale. The local properties obtained with LBM are incorporated at the network to solve the larger-scale problem. This strategy leads to a significant decrease of the computation time at the sample-scale compared to a fully resolved method. Fluid morphology and phase distribution are evaluated during the drainage of a small granular assembly using the Hybrid model (PN-LBM). Results are contrasted with those obtained in a fully resolved simulation (LBM). The agreement between the two models illustrates the capability of the Hybrid method, which combines the efficiency of the PN approach and the accuracy of the LBM at the pore scale.

1 INTRODUCTION

Fluid flow has a strong impact on the mechanical behavior of partially saturated granular systems. The hydromechanical response of partially saturated granular material has been studied by means of the Discrete Element Method (DEM) [1, 2]. Such works were restricted to low liquid content to ensure the pendular regime, where liquid is retained in the form of bridges between particles. When the liquid content is increased, pendular
bridges coalesce forming complex liquid morphologies. At this point, the pendular regime is replaced by the funicular regime. Less attention has been devoted to examine the mechanism of wet materials during the funicular regime. Nowadays, three-dimensional images from X-ray tomography are a useful and common tool to characterize the fluid morphology in the porous medium [3]. Despite these recent advances, very few attempts have been carried out to obtain the details of the liquid distribution within the porous media [4, 5].

Several modeling techniques can be adopted to reproduce the fluid displacement within the porous media. *Macro-scale models* are based on continuum descriptions of flow. These models incorporate the local fluctuations induced by the microscopic interactions between the fluids ensuring mass conservation. In spite of the low computational cost, macro-scale continuum models rely on empirical relations and information about constitutive properties is required. *Micro-scale continuum models* are fully resolved methods capable to simulate multiphase flow through complex geometries and do not rely on empirical relations. Even though these models have been proven successful to reproduce the physical phenomena at the different scales, they are computationally much more demanding. Lattice Boltzmann method (LBM) [6], volume of fluid (VOF) method [7] or Lagrangian mesh-free methods [8] are examples of micro-scale continuum models employed in the analysis of multiphase flow through porous media. Finally, *pore-scale models* manage to reduce the high complexity of porous morphology by a discretization of the pore bodies and pore throats.

The multiscale method presented in this article is inspired in the pore-scale approach referred as ”two-phase pore-scale finite volume-discrete element method” (2PFV-DEM) [9]. In this method, fluid displacement is controlled by the entry capillary pressure ($p_{e}$). When the capillary pressure ($p_{e}$) exceeds the entry capillary pressure ($p_{e} > p_{c}$), the non-wetting phase passes through a narrow throat invading a pore body. $p_{c}$ can be approximated by the Incircle method [10], the Mayer-Stowe-Princen (MS-P) method [9], or direct fluid simulations. The present Hybrid model follows the pore-scale decomposition scheme proposed by [11] and relies on LBM simulations to determine the main hydrostatic properties ($p_{c}$, liquid morphology, capillary pressure - saturation curves).

2 NUMERICAL METHODS

2.1 Lattice Boltzmann Method

A multicomponent multiphase Shan-Chen LB model [12] is implemented using the open source library of Palabos. The motion of a fluid is described by the lattice Boltzmann equation:

$$
\begin{align*}
&f^{\omega}_{k}(x_{k} + e_{k} \Delta t, t + \Delta t) - f^{\omega}_{k}(x_{k}, t) = -\frac{\Delta t}{\tau^{\omega}}(f^{\omega}_{k}(x_{k}, t) - f^{\omega, eq}_{k}(x_{k}, t))
\end{align*}
$$

(1)

where the superscript \(\omega\) denotes the \(\omega\)th fluid, \(\tau^{\omega}\) is the rate of relaxation towards local equilibrium, \(f^{\omega, eq}_{k}\) is the equilibrium distribution function, \(\Delta t\) is the time increment,
\( e_k \) are the discrete velocities which depend on the velocity model, in this work, D3Q19 (three-dimensional space and 19 velocities) model is adopted, and \( k \) varies from 0 to \( Q - 1 \) representing the directions in the lattice. The left-hand side of Eq. 1 corresponds to the streaming step, which describes the motion of the fluid particles between nodes, whereas the right-hand side stands for the collision step based on the Bhatnagar-Gross-Krook (BGK) approximation. The collision operator represents the evolution of the system towards the equilibrium.

The macroscopic density and momentum variables are recovered from the distribution functions:

\[
\rho^\omega = \sum_k f_k^\omega \\
\rho^\omega u^\omega = \sum_k f_k^\omega e_k
\]

In order to ensure a system of immisible fluids, a repulsive force between the fluid phases is introduced. According to \cite{12}, the non-local force responsible for the fluid-fluid interaction can be expressed as:

\[
F^\omega(x) = -\Psi(x) \sum_{\bar{\omega}} G_{\sigma \bar{\omega}} \sum_k \Psi_k(x + e_k)e_k
\]

where \( \Psi_k \) is the interparticle potential that induces phase separation and \( G_{\sigma \bar{\omega}} \) is the interaction strength between components \( \omega, \bar{\omega} \).

Finally, the non-ideal equation of state can be expressed as:

\[
p = c_s^2(\rho_\omega + \rho_{\bar{\omega}}) + c_s^2 G \rho_\omega \rho_{\bar{\omega}}
\]

where \( \rho_\omega \) and \( \rho_{\bar{\omega}} \) are the densities of the fluids at a certain position and \( c_s \) is the speed of sound.

### 2.2 PN-LBM Hybrid model

#### 2.2.1 Pore-space decomposition

The pore-scale network employed in the present Hybrid method is based on the 2PFV-DEM scheme developed by \cite{9}, which combines a three-dimensional triangulation method and DEM to model the hydro-mechanical behavior of unsaturated deformable granular materials. The triangulation of the pore space leads to a tetrahedral mesh whose vertices coincide with the centers of the spheres. Each tetrahedral element defines a pore body and four pore throats (see tetrahedral facets in figure 1a). A 2D schematic diagram is included in figure 1b to illustrate the discretization of the void space. This technique is particularly convenient to describe the topology of the pore throats.
2.2.2 Fluid displacement

The fluid front displacement and the possible combinations of fluid in the porous media are mainly controlled by the entry capillary pressure. Following the work of [13], the displacement of the non-wetting phase is directly linked to the capillary pressure. The interface curvature increases as the capillary pressure builds up following Laplace-Young equation. When the local capillary pressure is larger than the entry capillary pressure, the interface front becomes unstable and the non-wetting phase passes through the pore throat invading the pore body. According to [14], the analysis of the capillary pressure and meniscus shape requires solving the Laplace-Young equation, a nonlinear, second-order, partial differential equation which, can be numerically solved for very few 3-spheres configurations. Due to this limitation, it seems reasonable to consider other approaches that can predict the entry capillary pressure and liquid morphology.

The pore space is decomposed into a series of throat-domains following a regular triangulation (see figure 2). The decomposition leads to a list of pore throats that are solved independently. LBM simulation are performed for each pore throat to estimate the primary drainage curve, the entry capillary pressure and liquid morphology. The computation domain is a triangular-shaped prism defined by three solid walls orthogonal to the pore throat. Each of these solid boundaries passes through two of the spheres centers (two vertex of the triangle defined by the 3 spheres centers). The reader is directed
to figure 2 for a more comprehensive review. The domain is enclosed by two triangles at the top and bottom of the prism representing the inlet and outlet sections of the LBM simulations.

Figure 3: a) Fluid-fluid interface deforming due to increments of capillary pressure. b) Vertical view of the interface at the moment of the pore throat invasion. c) Wetting phase is accumulated in the corners while in the center non-wetting phase fills the pore throat. d) Capillary pressure - Saturation curve for the pore throat. Three snapshots displaying vertical and horizontal slices of the simulation evidence the liquid morphology before, during and after the pore invasion.

Figure 3d shows the evolution of a typical subset. In this case, the pore throat is formed by three equal-sized spheres in contact. The density of the nodes located in the inlet and outlet sections is adjusted to gradually increase the capillary pressure. Such increment induces the displacement of the interface (see figures 2c and figure 3).

The evolution of normalized capillary pressure \( p^*_c = \frac{2p_c R}{\gamma} \), where \( \gamma \) is the surface tension, \( R \) is the radius of the spheres and \( p_c \) is the capillary pressure) during the invasion is related to the change of volume of the wetting phase in figure 3d. Dimensionless volume is defined as: \( V^* = \frac{V(t)}{4 \pi R^3} \), where \( V(t) \) is the volume at time \( t \).

The entry capillary pressure \( p^e_c \) is defined as the maximum value reached by \( p_c \) during the invasion process. When the capillary pressure reaches the entry capillary pressure \( (p_c = p^e_c) \), the non-wetting phase penetrates into the pore body (see figure 3). Immediately after the invasion, the interface meniscus expands leading to a reduction of the capillary...
pressure. This procedure is repeated for all the pore throats of the sample. Thus, \( p_c^e \) is determined for all the subdomains and incorporated into the global problem handled by the pore-network.

3 RESULTS

3.1 Flow through a 40 spheres granular assembly

This section presents the results of a drainage process in a 40 sphere granular assembly. A fully resolved LBM simulation has been performed and assumed as reference data. Then, results are compared with the Hybrid model.

3.1.1 Numerical setup

A random sphere pack is created by the open-source code YADE [16]. A cubic box of 10 mm x 10 mm x 10 mm is defined in which 40 polydisperse spheres are packed. The mean sphere radius is 1.26 mm. The following assumptions are made during the numerical simulations:

- Negligible gravitational forces.
- Static solid skeleton.
- Drainage is evaluated under quasistatic flow.
- Perfect wetting of the solid by the wetting phase.
- Disconnected regions remain saturated by a fixed amount of wetting phase.

Figure 4: Distribution of the wetting phase after the drainage simulation of a 40 sphere packing. The wetting phase is trapped in some areas of the sample as pendular bridges or liquid clusters.

Initially, the granular assembly is completely saturated (see figure 5a - Full LBM). A porous membrane is located at the bottom of the sample in order to prevent the non-wetting phase to reach the outlet and ensure a complete drainage. The displacement of
the interface is conducted by a fixed flow controlled by a pressure difference between the non-wetting reservoir (top of the sample) and the wetting reservoir (bottom of the granular assembly). The interface flows towards the bottom driven by the pressure gradient invading the largest pores at first, then, the non-wetting phase progressively occupies the pore spaces of the sample. Capillary pressure is increased and recorded until all the nodes above the porous plate are filled with the non-wetting phase (see figure 5d - Full LBM). At this moment, the remaining wetting phase is trapped in the granular assembly in form of liquid clusters. Figure 4 evidences the presence of pendular bridges and trimers (liquid cluster formed between three grains) in the sphere packing after the drainage.

![Figure 5](image)

**Figure 5**: Comparison of the invasion path between the full LBM simulation (translucent interface) and Hybrid model (wetting phase depicted in blue).

### 3.1.2 Invasion paths

The aim of the present section is to characterize the invasion path of the non-wetting phase through the porous media. Figure 5 captures the non-wetting pathways for different time steps for each method. The full LBM interface is shown as translucent blue isosurface and the wetting phase is depicted in blue for the Hybrid model in figure 5. We remark the ability of Hybrid model to predict the first preferential path (identical intrusion are observed in figures 5b and 5c). As the drainage proceeds, the non-wetting phase keeps occupying the sample leaving behind some disconnected liquid clusters (see figure 5d). Even though wetting phase trapped in the assembly is well represented with the Hybrid method, figure 5d suggests that there is a certain phase mismatch between the models in some regions.
It is worth mentioning that the CPU time for a complete drainage corresponds to 29.6 days for the full LBM. On the other hand, by using the Hybrid model, the computational cost is reduced down to 11.2 days.

4 CONCLUSIONS

Compared to a fully resolved method (in this work: LBM), the Hybrid model presented in this article provides more efficient results in terms of computation time. Results show that Hybrid method is able to mimic the interface displacement during the drainage of pore space with excellent accuracy.

This technique would probably have a stronger impact on a larger problem with thousands of pore throats. In parallel simulations with relatively small computational domains, the execution speed is multiplied by a factor two doubling the number of cores. Large-scale problems that require the exploitation of massively parallel systems are frequently accompanied by a drop in efficiency. In the Hybrid method, however, the scalability is optimal. Due to the fact that each pore throat (small domains) are assigned to a single core, efficiency does not depend on the size of the granular assembly. Besides, some regions of the sample can be excluded from the simulation (empty pores and isolated clusters with no flux).

REFERENCES


OPTIMIZATION OF THE HYPERTHERMIA TREATMENT OF A SKIN TUMOR CONTAINING NANOPARTICLES

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Key words: bioheat transfer, finite volume, thermal damage, Arrhenius model, optimization

Abstract. This paper deals with the optimization of the hyperthermia treatment of skin cancer, with gold nanoshells loaded in the tumor. The physical problem involves a one-dimensional bioheat transfer problem, coupled to a radiation problem for the laser propagation within a multi-layered medium that includes several tissues. The corresponding bioheat transfer problem is governed by Pennes' equation, while the laser radiation propagation in the tissues is modelled with the diffusion δ-P1 approximation. The solution of the direct problem was obtained by finite volumes and verified with an analytic solution, as well as with the Matlab function pdepe. The thermal decomposition in the tissues was modelled with an Arrhenius equation, while the objective function was given by a quadratic form involving the difference between the predicted and the desired spatial variation of the thermal damage at a specific final time. Both the Levenberg-Marquardt and the Particle Swarm methods were implemented and provided similar results for the two design variables of interest in this work: the volume fraction of nanoparticles within the tumor and the laser power, by considering a fixed duration of 10 minutes for the treatment. The results obtained in this work also show that more than one treatment session is required for the total eradication of the tumor.

1 INTRODUCTION

The hyperthermia treatment of cancer has recently regained the attention of the scientific community due to developments in nanotechnology. In fact, several works can be found in the literature related to the use of nanoparticles in tumors, in order to increase the localized absorption of energy by cancerous cells and to decrease the thermal damage to surrounding healthy cells [1-6]. Different external non-intrusive energy sources have been reported for the hyperthermia treatment of cancer, like lasers in the near-infrared range, radio-frequency antennas, etc. [3,7]. Similarly, different kinds of nanoparticles have been used, such as those made of iron oxides [8]. In particular, noble metal nanoparticles can be designed in terms of their shapes and sizes to increase the plasmon resonance in a specific wavelength range, in order
to improve the energy absorption [9].

Heat transfer in tissues, induced by hyperthermia, is a complex combination of various phenomena as metabolic heat generation, blood perfusion, convection, and heat conduction, which makes it difficult to model. However, numerical simulations are necessary to provide accurate results about this process, with lower cost, time and manual work than experimental manipulations. Mathematical models describing heat transfer were developed with some approximations that limit the computational time, as the bio-heat transfer equation of Pennes [10], the P1 approximation [11], a diffusion approximation of light transport, and the Arrhenius equation for thermal damage [12].

As any cancer treatment, hyperthermia requires a priori planning, specific for each patient, based on the prediction of a thermal damage to the cells. Although the localized heat absorption is enhanced by the injection of nanoparticles, its efficiency needs to be improved by modifying some hyperthermia parameters to destroy cancerous cells while avoiding the damage of healthy cells [13].

The present work focuses on the optimization of the laser emissive power and the nanoparticles concentration for the hyperthermia treatment of a skin cancer, with the Levenberg-Marquardt and Particle Swarm algorithms. The subcutaneous tumor, assumed to be surrounded by healthy tissues and containing gold nanoshells, is irradiated by an external collimated laser for 10 minutes. A one-dimensional coupled radiation – bio-heat transfer equation is used to formulate the physical problem, and then solved with the finite volume method.

2 PHYSICAL PROBLEM AND MATHEMATICAL FORMULATION

In the problem examined here, the skin tissue is irradiated by an external collimated laser radiation for a duration of 10 minutes. The laser beam is perpendicular to the tissue and uniform, with a continuous and constant optical intensity, thereby the problem is considered one-dimensional. The skin is modelled as a superposition of five layers, each one homogeneous with constant thermal and optical properties, namely: epidermis, tumor (loaded with nanoparticles), papillary dermis, reticular dermis and fat.

2.1 Simple model

In order to choose the solution method for the problem detailed above, a simple model will first be studied, comparing the results of the different methods with the analytical solution. This model is a one-dimensional diffusion problem with an additional constant heat source, in a homogeneous medium with constant thermal properties. Convective boundary conditions are applied on both sides, and the initial temperature is considered constant, as it is given below:

\[
\begin{align*}
\rho c_p \frac{\partial T(x, t)}{\partial t} &= k \frac{\partial^2 T(x, t)}{\partial x^2} + Q \quad 0 < x < d, \quad t > 0 \\
-k \frac{\partial T(x, t)}{\partial x} + h_q T(x, t) &= h_q T_b \quad x = 0, \quad t > 0 \\
k \frac{\partial T(x, t)}{\partial x} + h_q T(x, t) &= h_d T_b \quad x = d, \quad t > 0 \\
T(x, t) &= T_0 \quad 0 < x < d, \quad t = 0
\end{align*}
\]
where \( \rho \) is the density of the tissue, \( c_p \) is the specific heat, \( k \) is the thermal conductivity, \( Q \) the heat source, \( h_0 \) and \( h_d \) the heat transfer coefficients, \( T_\infty \) and \( T_b \) the boundary temperatures, \( T_0 \) the initial temperature and \( d \) the domain length.

These equations are then solved analytically, decomposing the temperature in two terms: a homogeneous solution \( T_h \), and a particular solution \( T_p \):

\[
T(x, t) = T_h(x, t) + T_p(x)
\]

The particular solution is not time-dependent and can be written as a quadratic function of the position as it is given below:

\[
T_p(x) = -\frac{Q x^2}{k} + A x + B
\]

\[
A = \left( h_d(T_b - T_\infty) + Q d \left( 1 + \frac{h_d d}{2k} \right) \right) \left( k + h_d d + \frac{h_d k}{h_0} \right) ; \quad B = T_\infty + \frac{k}{h_0} A
\]

The homogeneous solution is obtained by separation of variables according to [14]:

\[
T_h(x, t) = \sum_{m=1}^{\infty} \frac{1}{N(\beta_m)} e^{-\beta_m^2 t} X(\beta_m, x) \int_0^d \left( T_0 - T_p(x) \right) X(\beta_m, x) dx
\]

\[
\frac{1}{N(\beta_m)} = 2 \left[ \beta_m^2 + \frac{h_0^2}{k^2} \right] \left( d + h_d \left( \beta_m^2 + \frac{h_0^2}{k^2} \right) \right) + \frac{h_0^2}{k} \left( \beta_m^2 + \frac{h_0^2}{k} \right)^{-1}
\]

\[
X(\beta_m, x) = \beta_m \cos \beta_m x + \frac{h_0}{k} \sin \beta_m x
\]

The \( \beta_m \) eigenvalues are given by the roots of the equation below:

\[
\tan \beta_m d = \frac{\beta_m (h_0 + h_d)}{\beta_m - h_0 h_d} \quad \beta_m^2 - h_0 \frac{h_d}{k} = 0 \quad 0 < x < d, \quad t > 0
\]

In this way, it is possible to determine the solution of the simple model and select the solution method that will be used to solve the bioheat transfer problem.

### 2.2 Bioheat transfer formulation

The mathematical formulation of the bio-heat transfer problem in this work is described by Pennes’ model [10]:

\[
\rho(x)c_p(x) \frac{\partial T(x, t)}{\partial x} = \frac{\partial}{\partial x} \left( k(x) \frac{\partial T(x, t)}{\partial x} \right) + \rho_b c_{p,b} \omega_b(x) (T_b - T(x, t)) + Q_{\text{met}}(x) + Q_{\text{laser}}(x)
\]

where \( \rho_b \) is the blood density, \( c_{p,b} \) is the blood specific heat, \( \omega_b \) is the blood perfusion rate, \( T_b \) is the blood temperature, \( Q_{\text{met}} \) is the metabolic heat source and \( Q_{\text{laser}} \) is the laser heat source, given by equation (2).

The interfaces between the different layers are assumed to be in ideal thermal contact. The temperature of the irradiated interface is considered constant and equal to \( T_0 \), while a convective boundary condition is applied on the interface with deeper tissues, characterized by a heat
transfer coefficient \( h_d \) and a surrounding temperature \( T_0 \). The initial temperature is considered uniform and equal to \( T_0 \). The initial and boundary conditions are then given by:

\[
\begin{align*}
T(x, t) &= T_0 , \quad x = 0 , \quad t > 0 \\
k(x) \frac{\partial T(x, t)}{\partial x} + h_d T(x, t) &= h_d T_0 , \quad x = d , \quad t > 0 \\
T(x, t) &= T_0 , \quad 0 < x < d , \quad t = 0
\end{align*}
\] (5.b, 5.c, 5.d)

2.3 Laser heat source term

The laser heat source is computed from the tissue absorption coefficient \( K \) and the total fluence rate composed of a primary collimated component \( \Phi_p \) and a secondary diffuse component \( \Phi_s \) [5], as given by the equation below:

\[
Q_{laser}(x) = K(x)[\Phi_p(x) + \Phi_s(x)]
\] (6)

The Beer-Lambert’s law is used to determine the collimated component. It is given by:

\[
\Phi_p(x) = I_{w,i}e^{-\beta_i(x-x_{w,i})}
\] (7.a)

where \( I_{w,i} \) is the fluence rate at the irradiated surface of each layer \( i \), \( \beta_i \) is the attenuation coefficient and \( x_{w,i} \) is the position of the interface between layers \( i \) and \( i-1 \). For the first layer, we have:

\[
I_{w,1} = I_0 (1 - R_{sc})
\] (7.b)

with \( I_0 \) the optical intensity of the laser beam and \( R_{sc} \) the specular reflection coefficient at the external surface, which is a function of the tissue refractive index \( n_t \):

\[
R_{sc} = \left(\frac{n_t - 1}{n_t + 1}\right)^2
\] (8)

The diffuse component of the total fluence rate is obtained by applying the diffusion \( \delta \)-P1 approximation [11] given by:

\[
\begin{align*}
\frac{d}{dx} \left( -D(x) \frac{d\Phi_s(x)}{dx} + \frac{\sigma_s'(x)g'(x)}{\beta_{tr}(x)} \Phi_p(x) \right) + K(x)\Phi_s(x) &= \sigma_s'(x)\Phi_p(x) , \quad 0 < x < d \\
-D(x) \frac{d\Phi_s(x)}{dx} + \frac{\sigma_s'(x)g'(x)}{\beta_{tr}(x)} \Phi_p(x) &= \sigma_s'(x)g'(x) \Phi_s(x) , \quad x = 0 \\
D(x) \frac{d\Phi_s(x)}{dx} + \frac{\sigma_s'(x)g'(x)}{\beta_{tr}(x)} \Phi_p(x) &= \sigma_s'(x)g'(x) \Phi_s(x) , \quad x = d
\end{align*}
\] (9.a, 9.b, 9.c)

with

\[
D = \frac{1}{3\beta_{tr}} ; \quad \beta_{tr} = K + \sigma_s(1 - g) ; \quad \sigma_s' = (1 - g^2)\sigma_s ; \quad g' = g/(1 + g)
\] (10.a, b, c, d)

\[
A_1 = (1 + R_f)/(1 - R_f) ; \quad A_2 = (1 + R_t)/(1 - R_t)
\] (10.e, f)

\[
R_t = \omega_{tr}/\left[(1 + \sqrt{1 - \omega_{tr}})\left(1 + 2\sqrt{1 - \omega_{tr}}\right)\right]
\] (10.g)

where \( g \) is the anisotropy factor, \( \sigma_s \) is the scattering coefficient, \( R_f \) is the Fresnel specular reflection coefficient, \( R_t \) is the reflection coefficient of the internal boundary and \( \omega_{tr} \) is the transport albedo.
2.4 Thermal damage model

In order to optimize the hyperthermia treatment, it is first necessary to define the thermal decomposition of the irradiated tissue. The Arrhenius model is used to describe the thermal damage in this work in terms of a dimensionless damage parameter $\Omega$ [12]:

$$\Omega(x) = \int_0^t A e^{-\frac{E_a}{RT(x)}} dt$$  \hspace{1cm} (11.a)

where $A$ is the frequency factor, $E_a$ is an energy barrier, $R$ is the ideal gas constant and $T$ is the temperature. The Arrhenius parameters $A$ and $E_a$ that characterize the process can be determined experimentally. Moreover, as the finite volume method will be used to solve the problem, the thermal damage will be written in the discrete form as it is given below, the index $i$ designing the position and $n$ the time:

$$\Omega^{n+1}_i = \Omega^n_i + A e^{-\frac{E_a}{R T_i}} \Delta t$$  \hspace{1cm} (11.b)

The goals of the optimization are to maximize the destruction of the tumor and minimize the damage of the surrounding healthy cells. A target damage parameter $\Omega^*$ is thus defined with a linear evolution in time, to reach a final thermal damage of $\Omega^* = 1$ in the tumor, which corresponds to the necrosis of the tissue, and 0 in the other layers. The objective function is then written as in the equation below, considering the optimization of two parameters of the hyperthermia treatment: the optical intensity of the laser $I_0$ and the concentration of nanoparticles $f_v$.

$$\min S^*(I_0, f_v) = \int_0^t \int_0^d [\Omega(x, t, I_0, f_v) - \Omega^*(x, t)]^2 dx dt$$  \hspace{1cm} (12.a)

The discrete form of this objective function for use with the finite volume method and optimization algorithms is written as:

$$\min S^*(I_0, f_v) = \sum_{k=1}^{IN} [\Omega_k(I_0, f_v) - \Omega_k^*]^2 , \quad \Omega_k = \Omega^n_i$$  \hspace{1cm} (12.b)

where $IN$ is the number of finite volumes multiplied by the number of time steps

3 RESULTS AND DISCUSSIONS

3.1 Code Verification

The simple model presented by equations (1.a-d) is solved for a unidimensional medium with a thickness of 100mm and the thermal and optical properties of human fat [15]. The initial temperature is considered equal to 37°C, while the left boundary is characterized by a surrounding medium temperature $T_\infty=22.5°C$ and a convective heat transfer coefficient $h_0=10W/m^2K$. For the right boundary, the convective heat transfer coefficient is $h_d=50W/m^2K$ and the temperature of the surrounding medium exchanging heat with the surface is equal to 40°C. This medium is submitted to an external constant radiation which results in a volumetric heat source rate of 100W/m$^3$. 
In order to compute the analytical solution of this problem, the Newton-Raphson method is used for finding the $\beta_m$ eigenvalues.

Figure 1 presents the analytically computed temperature distribution after 1000s, as well as the temperatures obtained with the *pdepe* function of MATLAB, and the ones determined with the finite volume method by an explicit discretization of the equations.

![Temperature distribution for the simple model at t=1000s](image)

The results obtained with the finite volume method perfectly agree with the analytical solution at the graph scale. However, the *pdepe* function, a MATLAB solver for partial differential equations, computes a temperature distribution quite different from the analytical one, especially near the convective boundaries.

As the Pennes’ bioheat transfer equation is more complex than the model used for the verification, the finite volume method, which is more accurate than the *pdepe* function, will be used to simulate the temperature and thermal damage for the hyperthermia treatment.

### 3.2 Temperature and thermal damage modelling for the skin cancer

The geometry of the skin considered in this work is divided in five layers with a total thickness of 3.6mm, as represented by Figure 2. The initial temperature is considered equal to 37°C, which is also the blood temperature, $T_b$. The temperature of the irradiated boundary is constant and equal to $T_0$, while the right boundary presents a convective heat transfer coefficient $h_d=50\,\text{W/m}^2\text{K}$ [2].
The blood density and specific heat are respectively equal to 1060 kg/m³ and 3770 J/kgK, while the thermal and optical properties of the other tissues are listed in Table 1 [15-17].

**Table 1: Tissue properties [15-17]**

<table>
<thead>
<tr>
<th></th>
<th>Epidermis</th>
<th>Tumor</th>
<th>Papillary dermis</th>
<th>Reticular Dermis</th>
<th>Fat</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$ (kg/m³)</td>
<td>1200</td>
<td>1030</td>
<td>1200</td>
<td>1200</td>
<td>1000</td>
</tr>
<tr>
<td>$c_p$ (J/kg K)</td>
<td>3589</td>
<td>3582</td>
<td>3300</td>
<td>3300</td>
<td>3674</td>
</tr>
<tr>
<td>$k$ (W/m K)</td>
<td>0.235</td>
<td>0.558</td>
<td>0.445</td>
<td>0.445</td>
<td>0.185</td>
</tr>
<tr>
<td>$Q_{mer}$ (W/m²)</td>
<td>0</td>
<td>3680</td>
<td>368.1</td>
<td>368.1</td>
<td>368.4</td>
</tr>
<tr>
<td>$\omega_b$ (s⁻¹)</td>
<td>0</td>
<td>0.0063</td>
<td>0.0002</td>
<td>0.0013</td>
<td>0.0001</td>
</tr>
<tr>
<td>$K$ (m⁻¹)</td>
<td>800</td>
<td>50</td>
<td>15</td>
<td>15</td>
<td>2.6</td>
</tr>
<tr>
<td>$\sigma_s$ (m⁻¹)</td>
<td>17500</td>
<td>6000</td>
<td>17500</td>
<td>17500</td>
<td>12000</td>
</tr>
</tbody>
</table>

The first and second layers, which correspond to the epidermis and the tumor, respectively, are supposed to contain gold nanoshells, thus increasing their absorption of the laser radiation. The absorption and scattering coefficients of these tissues are then obtained with the following equations [2]:

$$K' = K + 0.75 f_v \frac{Q_a}{a}$$  \hspace{1cm} (13.a)

$$\sigma'_s = \sigma_s + 0.75 f_v \frac{Q_s}{a}$$  \hspace{1cm} (13.b)

where $Q_a = 7.828$ and $Q_s = 1.144$ are efficiency factors, $a$ is the radius of the nanoparticles assumed equal to 20 nm and $f_v$ is the volumetric fraction of nanoparticles, assumed here as $2 \times 10^6$ [2].

The skin, which presents a refractive index $n_t = 1.4$ and an anisotropy factor $g = 0.9$, is irradiated from the left by a laser with a constant optical intensity of 20 kW/m² [2]. The diffuse component of the fluence rate is determined using the method of successive over-relaxation for solving the δ-P1 approximation, assuming the coefficient $A_1$ equal to zero.
The finite volume method with explicit scheme is then implemented and used to obtain the results presented in the figure 2, showing the effects of the nanoparticles injection on the temperature distribution (figure 2a) and fluence rate and volumetric heat source (figure 2b).

As can be seen in Figure 2a, the temperature distribution presents a peak at 41.7°C after 10s in the tumor region, between 0.3 and 0.4 mm, with the tissue embedded with gold nanoshells. For the tissue without nanoparticles, the maximum temperature is reached in the papillary dermis, which increases the risk of damaging healthy cells rather than cancerous cells. Figure 2b highlights the radiation absorption in the skin containing nanoparticles, where a strong attenuation of the total fluence rate is observed, as well as a higher volumetric heat source in the tumor.

For the thermal damage modelling, Arrhenius parameters are taken from the experimental results of [18] for the belly skin, where the activation energy $E_a$ is considered equal to $3.935 \times 10^5$ J/mol and the frequency factor $A$ has the value of $1.151 \times 10^6$ s$^{-1}$. Equation (11.b) is then applied to compute the thermal damage parameter from the temperature obtained with the finite volume method, assuming the initial thermal damage equal to zero.

Figure 3a shows the values of the thermal damage parameter in the different layers. We notice that the thermal damage follows the evolution of the temperature presented by figure 2a, with a peak at the end of the tumor region and a strong attenuation in the dermis and fat. It can be observed in figure 3b that the thermal damage increases over time, which corresponds to the Arrhenius model. However, the maximum value is only $4.4 \times 10^{-4}$ after 10s, while the thermal damage parameter must reach the value of 1 to obtain the necrosis of the tumor. That is why it is necessary to apply the hyperthermia treatment on a longer duration and modify its characteristics within an optimization procedure, as described next.
3.3 Optimization of the thermal damage

For the optimization of the hyperthermia treatment, the final time is fixed and equal to 10 minutes, while two parameters are modified to find the minimum of the objective function: the laser optical intensity $I_0$ and the nanoparticles volumetric fraction $f_v$. The optical and thermal properties of the different layers of the skin, the Arrhenius constants and the laser and nanoparticles characteristics remain the same as for the example in the previous section.

The thermal damage computed with equation (11.b) is compared with the ideal one through the objective function. The ideal thermal damage parameter is considered to follow a linear evolution in time starting from 0 to reach 1 in the tumor and stay at 0 in the healthy cells. A shape parameter has been added to this ideal thermal damage function to smooth the distribution in the boundaries of the tumor so that it is more similar to the real one.

Two different optimization algorithms are applied to the problem, namely: the Levenberg-Marquardt method, a nonlinear least squares minimizer, and the Particle Swarm Optimization (PSO) algorithm, a population based stochastic optimization technique, implemented with a population size of 50. The table below presents the results of the algorithms obtained using an Intel Pentium 3665U @ 1.70 GHz, in a 64-bit system, with 4 Gb of RAM. Two objective functions are studied: one includes the thermal damage for all time steps during the treatment, while the other consider only the thermal damage at the final time, that is, 10 minutes, which correspond to the maximum value of the thermal damage since it increases in time.

Figure 3: Evolution of the thermal damage parameter in the skin (a) as a function of the position ($t=10s$) (b) as a function of time ($x=0.375\text{mm, tumor}$)
Table 2: Results of the optimization algorithms

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Objective Function</th>
<th>Computational Time</th>
<th>Stopping Criteria</th>
<th>$f_i$</th>
<th>$I_0$ (W/m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Levenberg-Marquardt</td>
<td>All time</td>
<td>28533 s</td>
<td>Step size $10^{-30}$</td>
<td>8.08$x10^{-5}$</td>
<td>66116</td>
</tr>
<tr>
<td></td>
<td>Final time</td>
<td>3838 s</td>
<td>Step size $10^{-50}$</td>
<td>8.48$x10^{-5}$</td>
<td>66328</td>
</tr>
<tr>
<td>Particle Swarm</td>
<td>All time</td>
<td>98782 s</td>
<td>50 iterations</td>
<td>8.23$x10^{-5}$</td>
<td>66572</td>
</tr>
<tr>
<td></td>
<td>Final time</td>
<td>128199 s</td>
<td>100 iterations</td>
<td>8.48$x10^{-5}$</td>
<td>66328</td>
</tr>
</tbody>
</table>

As can be seen in Table 2, the two algorithms give identical results for the optimization of the objective function at final time, with a higher computational time for the implemented PSO method. The stopping criteria for the all-time evaluation of the objective function are considered lower than for the final time evaluation, due to a higher computational time: the step size tolerance is $10^{-30}$ instead of $10^{-50}$ for the Levenberg-Marquardt algorithm, and the maximal number of iterations is 50 instead of 100 for the PSO. For this reason and the possible deviations of the real and ideal thermal damages in time, the resulting parameters are slightly different from the ones of the final thermal damage optimizations. By any way, the optimized values $f_i$ of $I_0$ and are consistent for all cases considered.

Figure 4 presents the temperature and thermal damage distributions computed with $f_i = 8.48\times10^{-5}$ and $I_0 = 66328$ W/m², the parameters resulting from the final thermal damage optimization.

![Figure 4](image-url)  

Figure 4: Distribution after 10min of the optimized hyperthermia treatment on the skin of: (a) temperature (b) thermal damage

The temperature presents a peak of 46.8°C in the tumor region, around 0.2mm, where the thermal damage parameter reaches a maximum value of 0.4, next to the left boundary of the tumor.
However, the optimized thermal damage is still lower than the ideal one after 10 minutes of exposure and the cancerous tissue is not fully destroyed with one single session of the hyperthermia treatment. A second session is therefore needed to increase the thermal damage in the tumor, while maintaining reasonable temperatures. For this second session, the skin was assumed to cool down and return to $T_0$ between the two applications. The hyperthermia treatment is then applied with the same optimal conditions for 10 minutes, with the initial thermal damage of the second session considered equal to the final thermal damage of the first session. As can be seen in Figure 5, a second session of the hyperthermia treatment with the same optimal parameters of the first session doubles the thermal damage of the skin, with a peak at 0.8, which still remains in the tumor region.

**Figure 5:** Thermal damage distribution in the skin after a second application of the 10min hyperthermia treatment

4 CONCLUSIONS

From this simulation, it can be concluded that the Levenberg-Marquardt and PSO algorithms can be used for the optimization of the hyperthermia treatment. It was also shown that, with a fixed exposure duration of 10 minutes, at least a second session of the hyperthermia treatment is necessary to inflict a thermal damage to the tumor that approaches the tissue necrosis. On the other hand, the optimization of parameters like the beam size, the time of exposure or a non-constant laser emissive power may also be relevant to provide a more suitable treatment.

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REFERENCES


ENERGY HARVESTING FROM SLOW ROTATIONAL MOTION

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Key words: Energy Harvesting, Electromechanics, Co-Simulation

Abstract. An electromechanical rotating energy harvester design is presented. The Energy Harvester is devoted to extract energy from a rotating flange in an agricultural machinery designed for ploughing and laying seeds. The harvested energy is used to supply a motion sensor that sends wireless signals to a console controlling the process. The device is structured as an axial electromechanical generator with excitation provided by permanent magnets. As no contact with stationary parts is allowed, an inertial reference is provided by a pendulum. Integrated design of electromechanical generator and pendulum is performed and results in terms of maximum harvested power are provided.

1 INTRODUCTION

Energy Harvesting (EH) is a technique to extract power dispersed in the environment providing power to detached and secluded apparels, like sensors, whose electrical supply would not be possible by regular wirings. This issue is becoming more and more important by the widespread use of sensors in the Internet Of Things where many devices are thought to dialogue with others to form a network both for sensing and for control purposes [1], [2]. An example of the application of this concept to the harvesting of energy from human motion is reported in [4]. The previous reference also gives a good overview of the reasons why the design of a EH has to be treated as a coupled phenomenon simulating the whole chain of power conversion from the primal one to the desired outcome, usually expressed in terms of electrical energy.

Several primal sources of energy can be found like light, electromagnetic radiation, temperature difference etc. In electromechanics harvesting the source of motion is a relative movement of some parts that can be unidirectional, as in the case of mechanical vibrations, or rotational. In the last case usually an electromagnetic structure shaped like an electrical machine can be used, as for instance in [3].
In the present work the design of a EH connected to the rotating parts of an agricultural machinery designed for ploughing and laying seeds is pursued. The application gets its rationale by the fact that ploughing disks get often stuck in obstacles and if they are blocked the whole process of ploughing and seeding can be disrupted. As a consequence there is a need to sense state of motion of these disks. As a modern machine can have tens of this disks, a central control of the process is sought by sending the state of motion of each disk to a central control unit. The EH is then devoted to the supply of a wireless transmitting device able to send a signal to the central unit.

The design of the EH has the requirement that no modifications should be made to the existing structure: the EH should be an add-on to the disk without requiring any change or machining to the existing disk. As a result the device will have to be attached on the external surface of the disk ball bearing. As the add-on must not have any other connections with the moving parts, a new standing reference has to be created in a limited space.

Another trouble in the conceptual design of this apparel is due to the relative slow motion of the ploughing disk. The electrical power requirements are set by the supply of wireless transmitter able to communicate the motion status of the wheel to a central unit located in the cockpit of the machine, this constraint will be the main target of the design.

The work performed is presented in the following structure: in first section the main geometrical and functional specifications will be presented, in second section the design of the electromechanical parts is outlined, in the third section the definition of the counterweight shape and mass is highlighted while in the last section the model of the whole structure is finally described. Eventually some conclusions on the design process are drawn.

2 TECHNICAL SPECIFICATION OF THE ENERGY HARVESTER

The EH to be designed has to be attached on the exterior part of the ball bearing of the ploughing disk, whose dimensions are reported in figure (1). The region where the EH can be located is highlighted in the same figure and regards the external part of the disk that is rotating. The radial encumbrance of the EH is limited between the internal radius $R_1 = 29.5$ mm and the external one $R_2 = 45.5$ mm, while the axial maximum dimension is of $h = 27$ mm. No connections to other parts of the structure are allowed so that the external part of the EH will be rotating solidly with the disk. The limits on the power generated by the EH are given by the designer of the blue-tooth transmitter that, due to the distance involved in the whole machine, is requiring an average value of 0.3 W to guarantee for the efficient communication with the central unit.
3 DESIGN OF THE MAGNETIC STRUCTURE

Due to the limits on the geometric dimensions of the device, it is not possible to resort to a classical radial flux machine, due to the hindrance of the coil ends. The choice is then that of an axial flux machine where an array of permanent magnets faces a set of coils where electromagnetic flux is linked. The relative slow rotational speed of the ploughing disk is another challenge to the design. In fact the disk is rotating at approximately 140 rpm leading to a value of angular velocity of $\omega = 14.62$ rad/s. In order to increase the rate of change of linked flux to raise a decent value of voltage, a quite large number of magnetic pole-pairs has to be used. After a study involving permanent magnet dimensions and number of turns on the coil, the number of pole-pairs was set to $N_p = 7$ using a number of $N_{mag} = 14$ magnets with reversing polarity, as sketched in figure (2). By neglecting the presence of ferromagnetic parts in the surrounding, the value of magnetic linked flux with the coils can be performed by means of analytical formulas of permanent magnets. Magnetic vector potential is calculated and thus its circulation gives the value of the linked flux. The linked flux as calculated for the whole set of coils is reported in figure (3). The electric speed of the flux variation is obtained by:

$$\omega_{el} = \frac{N_{mag}}{2} \omega$$  \hspace{1cm} (1)

By considering the first harmonic of the linked flux and $\lambda_{max}$ its maximum value, the estimation of the value of the maximum electro-motive force obtained is obtained as:
Elvio Bonisoli and Maurizio Repetto

Figure 2: Schematic structure of the magnetic part of the EH: red and blue cylinders are permanent magnets with opposite polarity while circular turns are placed facing them, dimensions in m.

\[ e_{\text{max}} = \frac{N_{\text{mag}}}{2}\omega_{el}N_{\text{turn}}\lambda_{\text{max}} = \frac{N_{\text{mag}}^2}{2}\omega N_{\text{turn}}\lambda_{\text{max}} \]  \hspace{1cm} (2)

By taking into account the maximum geometric dimensions and considering a winding made of a copper wire with diameter \( D_{\text{wire}} = 0.108 \text{ mm} \), the number of turns is \( N_{\text{turn}} = 1232 \) which leads to a value of maximum voltage \( e_{\text{max}} = 35.6 \text{ V} \). The dimensions of the coils and the number of turns allow to compute the value of electrical resistance of the whole set of coils of \( R = 535 \text{ } \Omega \) and a self inductance of \( L = 0.22 \text{ H} \).

The induced voltage value is then applied as an independent source to a load circuit whose resistance is equal, due to the maximum power transfer theorem in linear circuits to the one of the coil. By the analysis of the circuit so defined the average value of power transferred to the load resistance is equal to \( P = 0.56 \text{ W} \). This value is considered sufficiently higher than the requested one (0.3 W) so that it could accommodate also the needed power electronics for the voltage conditioning and supply of the transmitter.

4 DESIGN OF THE MECHANICAL STRUCTURE

The previously described magnetic structure can generate the desired power only in presence of a relative velocity between the magnets, fixed to the rotating disk, and the coils. As the coils cannot be linked to a static structure, an out of axis mass acting as a pendulum is connected to the coils. The effect of this mass is to contrast the torque that is created between magnets and coils and that is responsible for the electrical power generation. A sketch of the system is presented in figure (4). The dynamics of the system should ensure that the pendulum is able to counteract the electromagnetical torque exerted by the coils.

In order to optimize the encumbrance and the effect of the mass of the pendulum, it is realised by a ABS structure enclosing three masses made of lead. The geometric structure
of the system is shown in figure (5). The overall constructive vision is reported in figures (6) and (7). The geometric parameters of the three masses structures are carefully chosen in order to maximise the effect of the eccentricity, that is of the moment of inertia. Once this process is completed, a dynamic model of the system is defined by:

\[ I_0 \ddot{\theta} + c_m (\dot{\theta} - \dot{\theta}_{\text{inp}}) + mgl \sin(\theta) = T_{\text{em}} (\theta) \]  

(3)

where:

- \( \theta \) and \( \dot{\theta} \) are respectively the angular position and the angular speed of the pendulum;
- \( \dot{\theta}_{\text{inp}} \) is the rotational speed of the disk and of the magnets;
- \( I_0 \) is the momentum of inertia of the all rotating parts (coils+pendulum);
- \( c_m \) is a coefficient that takes into account mechanical friction between the parts;
- \( m \) is the pendulum mass, \( g \) the acceleration of gravity and \( l \) the distance between the mass center of gravity and the rotation axis of the system;
- \( T_{\text{em}} \) is the electromagnetic force that is dependent on the relative position and velocity between coils and magnets and on the circuit response.

\[ T_{\text{em}} = \frac{P_{\text{el}}}{\omega} = \frac{e \cdot i}{\dot{\theta}} = -\frac{d\lambda(\theta(t))}{dt} \cdot i = -\frac{d\lambda}{d\theta} \frac{d\theta}{dt} \cdot i = -\frac{d\lambda}{d\theta} i \]  

(4)

In turn the current \( i \) is obtained by the solution of the ohmic-inductive circuit.
The dynamic model is implemented in a Simulink model and its output is obtained for an input velocity that starts from zero and reaches the steady state speed of 140 rpm in an interval of 5 s.

The analysis showed that the pendulum is able to keep a position that in average is different from zero, so that there is relative motion between the magnets and the coils. Nevertheless, the position of the pendulum it is not fixed but it is subject to a ripple as this is the result of the electro-motive force that is dependent on the angular position $\theta$ and on the partially reactive circuit, as it is shown in figure (8). The model gives also the results for the electric variables current voltage and instantaneous power. The values are shown in figure (9). Both voltage values due to the electromagnetic induction ($V_0 = -d\lambda/dt$) and at the load terminals ($V_{in}$) are shown.

5 CONCLUSIONS

The work presented regards the design of an energy harvester taking energy from the motion of a rotating disk. Both geometrical and electrical constraints make the design challenging and requires the definition of an integrated electro-mechanical model to assess the device performances.

Even if the design of the system is quite classical, the magnetic structure and the corresponding mechanical shape of the pendulum required ad-hoc procedures that has shown the feasibility of the harvester.

Prototyping would be anyhow necessary to validate the quality of the design choices made.
Figure 5: Realisation of the pendulum by three lead masses joined within a plastic structure.

REFERENCES


Figure 6: Rendering of the whole structure in a plain view.

Figure 7: Rendering of the whole structure in a three-dimensional view.
Figure 8: Time behaviour of the angular position and velocity as a response to a ramp disk velocity saturated at 140 rpm.

Figure 9: Time behaviour of the electric variables as a response to a ramp disk velocity saturated at 140 rpm.
PIEZOELECTRIC FINITE BEAM ELEMENT WITH FGM CORE FOR MECHATRONIC APPLICATIONS

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Key words: Finite Element Method, Piezoelectric Analysis, Functionally Graded Material

Abstract. The paper deals with finite beam element with piezoelectric layers and functionally graded material of core. In the paper homogenization of FGM material properties and homogenization of core and piezoelectric layers is presented. In the process of homogenization direct integration method and multilayer method is used. The concept of transfer functions and transfer constants is used for computation of individual submatrices. Functionality of new FGM finite beam with piezoelectric layers is presented by numerical experiments. Static, harmonic and full transient piezoelectric analysis of FGM beams with piezolayers is presented.

1 MOTIVATION

Modern mechatronic systems are focusing on minimizing size, active vibration control and low energy consumption [1]. To improve performance of mechatronic systems, new materials and technologies are developed - one of them, which found broad application usage is Functionally graded material (FGM). Connection of FGM with piezoelectric materials [2] is very attractive combination of material composition, which can improve functionality of the system.

2 PIEZOELECTRIC CONSTITUTIVE EQUATIONS

Piezoelectric constitutive equations describe the relationship between mechanical and electrical quantities [2, 3]. This relationship is derived in tensor notation, but for practical usage it can be rewritten into matrices notation.
The constitutive equations can be expressed by strain tensor components $\varepsilon_{kl}$ and vector components of electric field intensity $E_k$ and has a form

\[
\sigma_{ij} = c_{ijkl}^{E} \varepsilon_{kl} - e_{ijk} E_k
\]
\[
D_i = e_{ikl} \varepsilon_{kl} + \varepsilon_{ik} E_k
\]

where $\sigma_{ij}$ are mechanical stress tensor components, $D_i$ are components of electric displacement vector, $c_{ijkl}^{E}$ are components of stiffness tensor under constant electric intensity, $\varepsilon_{ik}$ are components of permittivity tensor under constant mechanical stress and $e_{ijk}$ are components of piezoelectric modulus tensor.

If we use symmetric properties of individual tensor in constitutive tensor equations, we can rewrite constitutive equations into matrix notation \[4\]. Then equations (1) and (2) have a form

\[
\sigma_p = c_{pq}^{E} \varepsilon_q - e_{pk} E_k
\]
\[
D_i = e_{iq} \varepsilon_q + \varepsilon_{ik} E_k
\]

$D_i$ and $E_k$ are vectors with three components, $\sigma_q$ and $\varepsilon_q$ are vectors with six components, matrices $s_{pq}^{E}$ and $c_{pq}^{E}$ have dimension $6 \times 6$, matrices $d_{iq}$ and $e_{pk}$ have dimension $3 \times 6$ and matrix $\varepsilon_{ik}$ has dimension $3 \times 3$.

3 FGM BEAM WITH PIEZOELECTRIC LAYERS

Straight sandwich beam with core made from functionally graded material (FGM) and top and bottom layers made from piezoelectric material with constant material properties is shown in Fig. 1.

Cross-section of FGM core has height $h_{FGM}$ and depth $b$, one piezoelectric layer has height $h_p$ and depth $b$. Cross-section area of FGM core is $A_{FGM}$ and area moment of inertia is $I_{FGM}$. Cross-section area of one piezoelectric layer is $A_p$ and area moment of inertia is $I_p$. Length of beam element is $L$. 

![Figure 1: FGM beam with piezoelectric layers](image-url)
3.1 FEM equations for piezoelectric beams with FGM core

2D beam element with piezoelectric layers and FGM core with mechanical and electrical degrees of freedom is shown in Fig. 2.

FEM equations for beam element with piezoelectric layers and FGM core for transient analysis have classical form

$$\begin{bmatrix} M_{ee} & 0 \\ 0 & 0 \end{bmatrix} \dddot{u}^e + \begin{bmatrix} C_{ee} & 0 \\ 0 & 0 \end{bmatrix} \ddot{\phi}^e + \begin{bmatrix} K_{ee} & K_{e\phi} \\ K_{\phi e} & K_{\phi\phi} \end{bmatrix} \begin{bmatrix} u^e \\ \phi^e \end{bmatrix} = \begin{bmatrix} F^e \\ Q^e \end{bmatrix}$$

(5)

Vector of nodal unknowns is defined as

$$\begin{bmatrix} u^e \\ \phi^e \end{bmatrix} = \begin{bmatrix} u_i \\ v_i \\ \varphi_i \\ u_j \\ v_j \\ \varphi_j \\ \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{bmatrix}^T$$

(6)

and vector of nodal loads is defined as

$$\begin{bmatrix} F^e \\ Q^e \end{bmatrix} = \begin{bmatrix} F_{xi} \\ F_{yi} \\ M_i \\ F_{xj} \\ F_{yj} \\ M_j \\ Q_1 \\ Q_2 \\ Q_3 \\ Q_4 \end{bmatrix}^T$$

(7)

where $Q_1$, $Q_2$, $Q_3$ and $Q_4$ are electric charge on electrodes 1, 2, 3 and 4, respectively.

Individual submatrices are defined by concept of transfer functions and transfer constants and the input parameters for their computation are homogenized material properties in polynomial form. Derivation of individual submatrices is described in [5].

3.2 Homogenization of material properties

Material properties of beam core, which is made from functionally graded material, is defined by:

- volume fractions of fibres $v_f(x, y)$ and by volume fractions of matrix $v_m(x, y)$
- Young’s modulus of fibres $E_f(x, y)$ and Young’s modulus of matrix $E_m(x, y)$
Both parameters – volume fractions and Young’s moduli, can vary in longitudinal and transversal directions of beam, i.e. in directions $x$ and $y$. Effective Young’s modulus of FGM core can be calculated as

$$E_{FGM}(x, y) = v_f(x, y)E_f(x, y) + v_m(x, y)E_m(x, y)$$ (8)

Homogenized material properties of FGM core must be calculated separately for axial loading and separately for bending. Homogenized Young’s modulus for axial loading is defined by equation

$$E_{HN}^{FGM}(x) = \frac{\int_{-h_{FGM}/2}^{h_{FGM}/2} bE_{FGM}(x, y)dy}{A_{FGM}}$$ (9)

Homogenized Young’s modulus for bending is defined by equation

$$E_{HM}^{FGM}(x) = \frac{\int_{-h_{FGM}/2}^{h_{FGM}/2} by^2E_{FGM}(x, y)dy}{I_{FGM}}$$ (10)

Both homogenized Young’s moduli are only function of longitudinal direction $x$.

The last step in the process of homogenization of material properties of beam is homogenization of FGM core and piezoelectric layers. Young’s moduli for axial loading and bending of whole beam can be calculated using these two equations

$$E_{HN}^{}(x) = \frac{A_{FGM}}{A}E_{HN}^{FGM}(x) + \frac{2A_p}{A}E_p$$ (11)

$$E_{HM}^{}(x) = \frac{I_{FGM}}{I}E_{HM}^{FGM}(x) + \frac{2I_p}{I}E_p$$ (12)

where $A$ and $I$ is cross-sectional area and area moment of inertial of whole beam cross-section.

4 NUMERICAL EXAMPLE

The effectiveness of new piezoelectric beam element is shown on simple example, where piezoelectric beam is fixed at left end (point $i$) and right end is free (point $j$) – see Fig. 3.

Geometry parameters of beam are as follows:

- the length of beam: $L = 100$ mm
- height of FGM core: $h_{FGM} = 10$ mm
- height of piezolayer: $h_p = 1$ mm
- depth of cross-section: $b = 10$ mm
Figure 3: Simple cantilever made of FGM with piezoelectric layers

Beam core is made from FGM material – see chapter 4.1. Upper and bottom layers of the beam are made of piezoelectric material PZT5A. PZT5A is orthotropic material and has following material properties (direction of poling has index 3 – axis $y$ in Fig. 3):

- mechanical properties:
  - Young’s moduli: $E_1 = 61$ GPa, $E_2 = 61$ GPa, $E_3 = 53, 2$ GPa
  - Poisson numbers: $\mu_{12} = 0.35$, $\mu_{13} = 0.38$, $\mu_{23} = 0.38$
  - shear moduli: $G_{12} = 22.6$ GPa, $G_{13} = 21.1$ GPa, $G_{23} = 21.1$ GPa
  - density: 7750 kg/m$^3$

- piezoelectric properties: $d_{31} = -171 \times 10^{-12}$ C/N, $d_{33} = 374 \times 10^{-12}$ C/N, $d_{15} = 584 \times 10^{-12}$ C/N, $d_{24} = 584 \times 10^{-12}$ C/N

- relative permittivity: $\epsilon_{11}^\sigma = 1728.8$, $\epsilon_{22}^\sigma = 1728.8$, $\epsilon_{33}^\sigma = 1694.9$

4.1 Computing of homogenized properties

Properties of FGM core are defined by volume fractions of fibre and matrix and by variation of their Young’s moduli. Variation of volume fraction of fibre $v_f(x, y)$ and variation of volume fraction of matrix $v_m(x, y)$ were chosen as planar variation (in coordinates $x$ and $y$) – see Fig. 4, mathematically they are represented by following functions

$$v_f(x, y) = 1.33333 \times 10^8 x^3 y^2 - 1333.33x^3 - 2. \times 10^7 x^2 y^2 + 200 x^2 + 40000 y^2 \quad [\cdot] \quad (13)$$

$$v_m(x, y) = 1 - v_f(x, y) \quad [\cdot] \quad (14)$$

Variation of Young’s moduli of fibre and matrix was chosen as linear function longitudinal coordinate $x$ and can be expressed as

$$E_f(x) = 400 - 1000x \quad [\text{GPa}] \quad (15)$$

$$E_m(x) = 255 - 950x \quad [\text{GPa}] \quad (16)$$
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Figure 4: Variation of volume fraction of fibre $v_f(x, y)$ and matrix $v_m(x, y)$

$$E_f(x), E_m(x)$$

0.00 0.02 0.04 0.06 0.08 0.10
150
200
250
300
350
400
$x[m]$

$E [GPa]$

The variation of $E_f(x)$ and $E_m(x)$ is shown in Fig. 5 Left. Variation of effective Young’s modulus $E_{FGM}(x, y)$ is defined by equation (8) and for our example has form

$$E_{FGM}(x, y) = -6.66666 \times 10^9 x^4 y^2 + 66666.7 x^4 + 2.03333 \times 10^{10} x^3 y^2 -$$
$$- 20333.3 x^3 - 2.9 \times 10^9 x^2 y^2 + 29000 x^2 - 2. \times 10^6 x y^2 -$$
$$- 950. x + 5.8 \times 10^6 y^2 + 255. [GPa]$$  

(17)

This variation of effective Young’s modulus is shown in Fig. 5 Right. Homogenized Young’s moduli for axial and bending loading of FGM core can be calculated by equations (9) and (10) – $E_{HN}^{FGM}(x)$ and $E_{HM}^{FGM}(x)$. homogenized Young’s moduli of whole beam can

Figure 5: Left – defined variation of $E_f(x)$ and $E_m(x)$, Right – computed variation of effective Young’s modulus $E_{FGM}(x, y)$

The variation of $E_f(x)$ and $E_m(x)$ is shown in Fig. 5 Left. Variation of effective Young’s modulus $E_{FGM}(x, y)$ is defined by equation (8) and for our example has form

$$E_{FGM}(x, y) = -6.66666 \times 10^9 x^4 y^2 + 66666.7 x^4 + 2.03333 \times 10^{10} x^3 y^2 -$$
$$- 20333.3 x^3 - 2.9 \times 10^9 x^2 y^2 + 29000 x^2 - 2. \times 10^6 x y^2 -$$
$$- 950. x + 5.8 \times 10^6 y^2 + 255. [GPa]$$  

This variation of effective Young’s modulus is shown in Fig. 5 Right. Homogenized Young’s moduli for axial and bending loading of FGM core can be calculated by equations (9) and (10) – $E_{HN}^{FGM}(x)$ and $E_{HM}^{FGM}(x)$. homogenized Young’s moduli of whole beam can
be calculated by (11) and (12) and they have form

\[
E^{HN}(x) = 11111.1x^4 - 33888.9x^3 + 4833.33x^2 - 966.667x + 303.333 \text{ [GPa]}
\] (18)

\[
E^{HM}(x) = -33333.3x^4 + 101667.x^3 - 14500.x^2 - 980.x + 342 \text{ [GPa]}
\] (19)

Homogenized Young’s moduli for axial and bending loading are shown in Fig. 6.

4.2 Static analysis

Fig. 3 shows simple cantilever made of FGM with piezoelectric layers, which is loaded by transversal force \( F = 100 \text{ N} \) at free end – point \( j \). Electrodes on top and bottom piezoelectric layers are short circuited. The goal of analysis is to investigate static responds of structure on prescribed loading and compare the results with different number of elements.

Because the analysis is static and piezoelectric layers are short circuited (\( \phi^e = 0 \)), final FEM equations for deformation and electric charge have form

\[
K_{uu} u = F \quad K_{\phi u} u = Q
\]

The static analysis of system was performed by FGM beam element with piezoelectric layers. The analysis was performed by 1, 2, 4 and 10 elements – see Fig. 7 Left.

Deformed shape of beam is shown in Fig. 7 Right. Displacement in \( y \) direction of free end is \(-114.4 \mu\text{m}\). Electric charge on top electrodes for FEM models with different number of elements are summarized in Table 1.

As we can see from obtained results, new FGM beam element with piezoelectric layers is very accurate and effective in static analysis, because variation of material properties of FGM core of beam is directly incorporated into stiffness matrix.
4.3 Harmonic analysis

Investigated FGM beam with piezoelectric layers was loaded by harmonic force $F$ at the free end (point $j$ – see Fig. 3) with amplitude 100 N with different angular frequency $\omega$. In performed harmonic analysis two different electric boundary conditions are considered:

- short circuit ($\phi^e = 0$)
- open circuit ($Q^e = 0$)

electrode FEM equations for short circuit has form:

$$M_{uu} \ddot{u} + C_{uu} \dot{u} + K_{uu} u = F \quad K_{\phi u} u = Q$$

FEM equations for open circuit has form:

$$K_{\phi u} u + K_{\phi \phi} \phi = 0 \quad M_{uu} \ddot{u} + C_{uu} \dot{u} + K_{uu} u + K_{u \phi} \phi = F$$

**Table 1**: Electric charge on individual electrodes

<table>
<thead>
<tr>
<th>Number of elements</th>
<th>1</th>
<th>2</th>
<th>4</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q_{\text{elem 1}}$ [C]</td>
<td>$1.0263 \times 10^{-6}$</td>
<td>$7.2525 \times 10^{-7}$</td>
<td>$4.0460 \times 10^{-7}$</td>
<td>$1.7154 \times 10^{-7}$</td>
</tr>
<tr>
<td>$Q_{\text{elem 2}}$ [C]</td>
<td>$3.0110 \times 10^{-7}$</td>
<td>$3.2065 \times 10^{-7}$</td>
<td>$1.5861 \times 10^{-7}$</td>
<td>$1.4560 \times 10^{-7}$</td>
</tr>
<tr>
<td>$Q_{\text{elem 3}}$ [C]</td>
<td>$2.1883 \times 10^{-7}$</td>
<td>$8.2276 \times 10^{-8}$</td>
<td>$1.3204 \times 10^{-7}$</td>
<td>$1.1746 \times 10^{-7}$</td>
</tr>
<tr>
<td>$Q_{\text{elem 4}}$ [C]</td>
<td>$1.0137 \times 10^{-7}$</td>
<td>$8.3309 \times 10^{-8}$</td>
<td>$6.2864 \times 10^{-8}$</td>
<td>$3.9732 \times 10^{-8}$</td>
</tr>
<tr>
<td>$Q_{\text{elem 5}}$ [C]</td>
<td>$1.3829 \times 10^{-8}$</td>
<td>$1.0263 \times 10^{-6}$</td>
<td>$1.0263 \times 10^{-6}$</td>
<td>$1.0263 \times 10^{-6}$</td>
</tr>
<tr>
<td>$Q_{\text{SUM}}$ [C]</td>
<td>$1.0263 \times 10^{-6}$</td>
<td>$1.0263 \times 10^{-6}$</td>
<td>$1.0263 \times 10^{-6}$</td>
<td>$1.0263 \times 10^{-6}$</td>
</tr>
</tbody>
</table>
Harmonic analysis is performed with two different damping conditions:

- without damping
- with Rayleigh damping – the mass proportional Rayleigh damping coefficient is \(2 \times 10^{-5}\) and the stiffness proportional Rayleigh damping coefficient is \(2 \times 10^{-5}\)

Amplitude of \(y\) displacement of free end as function of angular frequency \(\omega\) for all investigated damping and electric conditions are shown in Fig. 8. As we can see from Fig. 8, amplitude-frequency characteristic for open circuit is shift to right – eigenfrequencies of the beam with open circuit are higher.

![Figure 8: Amplitude-frequency characteristics: Left – without damping, Right – with damping](image)

### 4.4 Transient analysis

Also transient analysis of investigated FGM beam with piezoelectric layers was performed. Electrodes on top and bottom piezoelectric layers are short circuited. The goal of analysis is to investigate free vibration of structure with considering Rayleigh damping – see Harmonic analysis. FEM equations for displacements and electric charge for transient analysis and for short circuit have form

\[
M_{uu} \ddot{u} + C_{uu} \dot{u} + K_{uu} u = F \quad K_{\phi u} u = Q
\]

Initial conditions:

- initial displacement of nodes – initial deformation of system is defined by static analysis – see chapter 4.2
- initial velocity of nodes – all nodes have zero initial velocity

The transient analysis of system was performed by Newmark integration scheme. Total simulation time was 0.01 s and number of equidistant substeps was 100. 1D model of system was discretized by 10 elements – see Fig. 7 Left. Displacement of selected nodes in direction \(y\) as function of time are shown in Fig. 9 Left. Time variations of electric charge in top electrode on selected elements are shown in Fig. 9 Right.
5 CONCLUSIONS

The paper presents beam finite element with piezoelectric layers, where core of the beam can be made of FGM materials. Such combination of materials is very attractive for mechatronic applications, because material composition of FGM core can be optimized for design stress state and deformation can be controlled by voltages on electrodes.

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REFERENCES


COMPUTATIONAL MODELLING OF GAS FOCUSED THIN LIQUID SHEETS

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Key words: Microfluidics, Liquid Sheets, Multiphase System, Surface Tension Driven Flow

Abstract. Formation of liquid sheets has been demonstrated as a critical capability needed in many different research fields. Many different types of liquid sheets have been produced experimentally, its thickness ranging from few tens of nanometres to few micrometres. Due to the small size of such systems, where physical parameters such as thickness, velocity and temperature are difficult to measure, a need for numerical simulation of liquid sheets arises. In this paper we demonstrate such capability with sheets that can be used in experiments with synchrotrons, X-ray free electron lasers or lab sources. A modified gas dynamic virtual nozzle (GDVN) design is used in order to generate micrometre thin sheets. The system is characterised by a strongly coupled problem between the focusing gas flow and the liquid sheet flow. Investigation of varying physical properties of liquid is performed in order to demonstrate the effects on the sheet production. It was found that the primary sheet thickness is not sensitive to the variation of liquid viscosity and density. On the other hand, the variation of surface tension greatly affects the thickness and the width of a primary sheet, such as expected in flows where surface tension is the dominating force. Findings demonstrate that by lowering the surface tension of a liquid, i.e. changing liquid from water to alcohol for example, would produce thinner and wider sheets. Simulations were produced with OpenFOAM, relying on finite volume based multiphase solver “compressibleInterFoam”, capable of simulating free surfaces. Mixture formulation of a multiphase system consists of an incompressible liquid phase along with a compressible ideal gaseous phase. Such model was also used in axisymmetric GDVN micro-jet simulations performed in our previous work. Due to the need for 3D simulations and huge computational resources needed, an adaptive approach was chosen. This made the simulations of liquid sheets of thicknesses down to 500 nm possible.
1 INTRODUCTION

Controlled multiphase fluid flows are being utilized in a wide range of scientific research and industrial applications. Generally, these types of flows can be of a wide variety of length scales, ranging from the kilometre down to the nanometre size. In a microfluidics system where typical lengths are measured in few tens of micrometres, the dominant driving force tends to be the surface tension. These types of flows are called surface tension driven flows. Such flows have long been utilized experimentally, to produce droplets of varying sizes, streams of varying diameters etc. The advances in numerical modelling and computational capabilities allow the exploration of these types of flows through simulations. One such application is the use of a gas dynamic virtual nozzle GDVN [1,2] which utilizes flow of a highly compressible gas through a nozzle throat to focus a stream of liquid into a micrometre size jet that eventually breaks up into droplets. Capability of simulating such systems was previously demonstrated [3]. In this paper a somewhat modified GDVN is employed that does not produce an axisymmetric jet, but rather a single stream of perpendicular liquid sheets [4,5]. The work presented here gives a computational insight into behaviour of such liquid sheet systems.

The structure of the paper is organized as follows: Section 2 illustrates the 3D model of the designed nozzle. Section 3 presents the governing equations, while section 4 describes the numerical methods used. The results of this study are shown in section 5. The paper concludes with the final remarks in section 6.

2 LIQUID SHEET NOZZLE

The liquid sheet nozzle design is loosely based on a nozzle design from Koralek et al paper [4], which in turn was based on gas dynamic virtual nozzle (GDVN). Figure 1 depicts the nozzle.

Figure 1: Graphical representation of the nozzle used in the production of liquid sheet viewed from two different directions: (a) front view, (b) side view.
It consists of a central capillary through which a liquid is delivered into the pressure chamber. Gas is injected through two capillaries which are angled at $\beta = \pm 40^\circ$ with respect to the central capillary. All three capillaries are chosen to be of the same diameter $D_c = 20 \, \mu m$. They converge in the nozzle throat of width $D = 25 \, \mu m$ and height $H = 50 \, \mu m$. The nozzle throat forms a rectangular parallelepiped of dimensions $(D, H, D_c)$.

### 3 GOVERNING EQUATIONS

In the present section a set of equations describing the multiphase fluid flow through the nozzle into a pressure chamber is presented. The physical model corresponds to a highly compressible Newtonian fluid in the laminar flow regime, described by the following set of mass (1), momentum (2) and energy conservation equations (3).

\begin{align}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0 \tag{1} \\
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) &= -\nabla p + \nabla \cdot (\mu \nabla \mathbf{u}) + \nabla \cdot (\mu \nabla \mathbf{u}^T) - \frac{2}{3} \nabla (\mathbf{\nabla} \cdot \mathbf{u}) + \mathbf{f}_v \tag{2} \\
\frac{\partial \rho c_T}{\partial t} + \nabla \cdot (\rho c_T \mathbf{u}) &= \frac{\partial \rho U^2}{\partial t} + \nabla \cdot (\rho U^2 \mathbf{u}) + \nabla \cdot (p \mathbf{u}) = \nabla \cdot (k \nabla T) \tag{3}
\end{align}

Velocity, density, pressure, temperature, dynamic viscosity, specific heat, velocity magnitude and thermal conductivity are given by $\mathbf{u}, \rho, p, T, \mu, c, U$ and $k$. In dealings with a multiphase flow an ever present interface needs to be properly solved for. This is handled by an algebraic volume of fluid method, represented by the following two equations:

\begin{align}
\frac{\partial \alpha}{\partial t} + \nabla \cdot (\alpha \mathbf{u}) + \nabla \cdot [(\alpha (1-\alpha) \mathbf{u}_c)] &= 0 \tag{4} \\
| \mathbf{u}_c | &= \min [C_a | \mathbf{u} \cdot \mathbf{n} |, | \mathbf{u} \cdot \mathbf{n} |] \tag{5}
\end{align}

$\alpha$ stands for a volumetric fraction of a liquid accompanied by the interfacial compression velocity $\mathbf{u}_c$, free compression parameter $C_a$ and normal vector to the interface $\mathbf{n}$. Continuum surface force model [6] implements a surface tension force as a body force in the momentum equation by evaluating the curvature of the interface as:

\begin{align}
\mathbf{f}_s &= \sigma \mathbf{\nabla} \alpha \tag{6} \\
\kappa &= -\nabla \cdot \left( \frac{\mathbf{\nabla} \alpha}{| \mathbf{\nabla} \alpha |} \right) \tag{7}
\end{align}

where $\sigma$ is surface tension and $\kappa$ is the mean curvature of the interphase boundary.
4 NUMERICAL METHOD

The simulations in the present work are performed by an open source code OpenFOAM [7] - version 1806, which uses finite volume method alongside with the algebraic volume of fluid method. The nature of the nozzle flow requires the gas flow to be considered as compressible while the liquid flow is of constant density. The proper description of the interphase boundary dictates the choice of “compressibleInterFoam” solver. Non-axisymmetric nozzle design calls for a three dimensional model. A quarter symmetry of the liquid sheets is assumed, which reduces the number of cells by a factor of 4 in comparison to the full 3D simulation. Dynamic meshing capability is utilized to further reduce the calculation time. The refinement criterion is the position of the interface. This results in a basic mesh with 150,000 cells at the beginning of the simulation and 380,000 cells for a fully developed sheet. The interface cell resolution is set to 0.25 µm. Simulations were performed with PISO solver with a maximum Courant number set to 0.95. The simulations were run in parallel on 36 cores on HPC where each simulation took approximately one day to complete. They were run past the time when the sheet stabilized, which occurs at roughly 20 µs real time. Figure 2 depicts a cross-section through a sample mesh where the use of adaptive meshing can be observed clearly, along with an overlying developed sheet.

Figure 2: Scheme of a section of a mesh in a fully developed simulation. Darker regions with the mesh refinement can be observed. The minimum mesh resolution is 0.25 µm.

5 RESULTS

A desire, to know which liquid is most suitable to use for the production of microscopic sheets in the defined nozzle layout, led to the following set of simulations. Here three parametric studies were performed, where a wide range of liquid properties and its effects on the sheet shape were considered (see Table 1). The range was set in such a way that the two most commonly used liquids, water and ethanol, would fall under the investigation. Helium was used
as a focusing gas with pressure chamber gas pressure set to 1 bar. Gas and liquid flow rates were kept constant at 4 mg/min and 80 µL/min, respectively. Due to the microscopic size of the sheet the flow is surface tension driven. We have varied the density, viscosity and the surface tension in the simulations. The quality of the sheets could be evaluated using the number of the perpendicular sheet surfaces, their width, thickness, position relative to the nozzle exit, velocity or the stability of their length. The main criteria in the present study represents the minimization of the sheet thickness. The results are presented below.

Figures 3 to 5 show the vertical symmetry axis thickness of the primary sheet along the horizontal symmetry axis (Figure 1). It can be observed that the thickness of the sheet that emerges from the nozzle is initially 20 µm thick, corresponding to the liquid capillary diameter. The sheet is partially focused already inside the nozzle, shown on graphs left to the vertical black line, and additionally outside to a minimum thickness marked with a circle. The primary sheet then transitions to a perpendicular secondary sheet which can be seen in surface tension variation graphs but not in the density and viscosity graphs. Final results along with corresponding physical parameters are shown in Table 1. The secondary sheets are not investigated here. Figure 3 shows the effect of the density variation of the liquid on the sheet thickness. It is observed that the majority of the focusing happens inside the nozzle and the sheet thickness reaches its minimum roughly 6 µm from the nozzle exit. The 20 percent change in density has virtually no effect on the position of the minimum thickness sheet and only a slight decrease in thickness is observed with the decrease in density.

![Figure 3](image-url)

**Figure 3:** Thickness along the central region of the primary sheet for different liquid densities. The black line denotes the nozzle exit, while the circles represent the minimum achieved sheet thickness.

Figure 4 shows roughly 50 percent variation of the dynamic viscosity of the liquid on the sheet thickness. Similarly as in density, the position of minimum is practically unaffected. The thickness variation is observed to be less than in density study, despite using larger variations. This leads to the conclusion that the flow under these conditions is less sensitive to the liquid viscosity than it is to the liquid density.
Figure 4: Thickness along the central region of the primary sheet for different liquid viscosity. The black line denotes the nozzle exit, while the circles represent the minimum achieved sheet thickness.

Lastly, we examine the effect of the surface tension variation, seen in Figure 5. The variations of the position of minimum thickness and thickness itself are quite substantial in this case. Changing the liquid with surface tension corresponding to water with one corresponding to ethanol results in a sheet thickness reduction from six micrometre thickness down to roughly a micrometre thickness. The simulation with even lower surface tension would thus require an even finer mesh resolution than used in the present work, since the sheet would become thinner and it would breakup due to too rough discretization.

Figure 5: Thickness along the central region of the primary sheet for different surface tensions. The black line denotes the nozzle exit, while the circles represent the minimum achieved sheet thickness.
### Table 1: Liquid properties and minimum thickness measurements.

<table>
<thead>
<tr>
<th>Surface tension coefficient $\sigma \times 10^{-3}$ [N/m]</th>
<th>Density $\rho$ [kg/m$^3$]</th>
<th>Dynamic viscosity $\mu \times 10^{-3}$ [kg/ms]</th>
<th>Primary sheet minimum thickness $\pm 0.25$ [$\mu$m]</th>
</tr>
</thead>
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<tr>
<td>30</td>
<td>1000</td>
<td>1</td>
<td>1.08</td>
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<tr>
<td>50</td>
<td>1000</td>
<td>1</td>
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<tr>
<td>72.8</td>
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<td>1</td>
<td>5.98</td>
</tr>
<tr>
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<tr>
<td>72.8</td>
<td>1000</td>
<td>1.5</td>
<td>6.23</td>
</tr>
</tbody>
</table>

### 6 CONCLUSIONS

Results shown here present the effects of liquid properties on the thickness of liquid sheet, produced from the gas focused liquid nozzles. It can be concluded that, though density and viscosity variations do affect the sheet formation, those changes are minimal in comparison to the surface tension impact. This is to be expected since the underlying force that determines the fluid flow under these operating conditions is the surface tension force. Therefore, we conclude that the changes to the surface tension have the largest effect on the sheet formation. Numerical technique used here, especially algebraic volume of fluid, might not be most suitable technique to use for a surface tension driven flow simulations. With such methods one is effectively artificially compressing the interface in order to preserve its sharpness and then calculating the forces exerted on such interface. This might result in deterioration of accuracy and it can be argued that the surface tension driven flow simulations would benefit greatly from geometrical volume of fluid method where precise geometric reconstruction of the interface is performed. This technique is currently not implemented within OpenFOAM. An alternative would be to use the recently developed meshless technique in connection with the phase field formulation [8] to simulate microfluidic liquid sheets. Nevertheless, the results follow a clear trend with varying liquid properties.

### ACKNOWLEDGEMENT

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REFERENCES


SIMULATION OF MACROSEGREGATION IN LOW-FREQUENCY ELECTROMAGNETIC CASTING BY A MESHLESS METHOD

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Key words: low-frequency electromagnetic casting, macrosegregation, solidification model.

Abstract. The novel use of a meshless numerical approach for simulation of macrosegregation in the low-frequency electromagnetic casting is presented along with the analysis of the simulation results. The casting model includes a coupled set of mass, momentum, energy, and species conservation equations. Lorentz force is computed with the induction equation and used in the solidification model. The coupled physical model is solved in cylindrical coordinate system and can be used to model aluminium alloy billet production. Explicit scheme is used for the temporal discretization, while the meshless diffuse approximate method is used for the spatial discretization. The method is localized with subdomains containing 14 local nodes. The Gaussian weight is used in the weighted least squares minimization. Furthermore, the Gaussian is shifted upstream, when an upwind effect is required in order to increase the convection stability. Direct chill casting under the influence of electromagnetic field (EMF) is simulated for various electric amplitudes and currents. The material properties of Al-5.25wt%Cu are used. The casting parameters and material properties are constant in all presented simulations, while EMF is turned off in some cases in order to study its effect on solidification. The results show that EMF has a large effect on the melt-flow and solidification. Oscillatory, instead of a steady-state, solution is obtained in case of certain geometries in EMF casting. The effect of EMF is hard to predict without the use of numerical simulations, due to strong coupled effects of casting geometry, casting parameters, and EMF parameters. This shows the need for numerical modelling of this strongly coupled problem for its better understanding.

1 INTRODUCTION

Macrosegregation is the chemical inhomogeneity of the composition on the macro-scale level. It is an unavoidable consequence of solidification and one of the major casting defects. It reduces the product quality and is impossible to remove with post-process treatments. The industrial experiments are very expensive and often not possible to perform. That is why the numerical models for prediction of macrosegregation are employed. They can successfully be used to optimize the casting parameters and increase the finished product value. Macrosegregation is caused by various physical phenomena: convection-driven flow,
shrinkage-driven flow, transport of floating grains, deformation-driven flow, and forced flow. The forced flow includes the effect of mechanical, ultrasonic, electromagnetic, etc. stirring and has a very important role in solidification for the low-frequency electromagnetic casting (LFEC).

Complete models for simulation of direct chill casting (DCC), which include mass, momentum, heat, and species transport have been in development for quite a long time. The improvements in the prediction of macrosegregation include: floating grains effect [1], effect of solidification shrinkage [2], multi-component alloys [3], operator splitting scheme [4], and a three-phase model, which includes the effects of intragranular and extragranular liquid [5]. On the other hand, the models for simulation of LFEC have not yet included the prediction of macrosegregation [6]. This is thereby the first investigation of the low-frequency EMF effect on macrosegregation in DCC.

Meshless methods are praised for their flexibility in simplicity of positioning and generation of the computational nodes. Only positions of the computational nodes are required without any other geometrical information. The formulation of the meshless approach is very similar for 2D and 3D, which is a significant benefit in comparison with other numerical methods. Description of the diffuse element method (DEM) is one of the first significant publication on the meshless methods [7]. The diffuse approximation method (DAM), which is employed in the model described in this paper, originates from DEM. The method has successfully been used to solve various thermo-fluid and multi-physics problems [8,9,10].

2 MODEL DESCRIPTION

The volume averaging formulation is used for modelling of the solid-liquid interaction. The conservation equations for mass, energy, momentum, and species are used to model the solidification of aluminium-alloy billets in axisymmetry. The electro-magnetic-induction equation is coupled with the melt-flow. It is used to calculate the magnetic vector potential and the Lorentz force. The Lorentz force is time-averaged and included in the momentum conservation equation, which intensifies the melt-flow. The effect of Joule heating is neglected in the energy conservation due to its insignificant contribution. The semi-continuous casting process is modelled with the Eulerian approach. This implies that the global computational domain is fixed in space. The inflow of the liquid melt is assumed at the top boundary and the outflow of the solid metal is assumed at the bottom. It is assumed that the whole mushy area is a rigid porous media, which is modelled with the Darcy law. Kozeny-Carman relation is used for the permeability definition. The incompressible mass conservation is ensured by the pressure correction, which is performed with the fractional step method. The conservation equations and the induction equation are posed in the cylindrical coordinate system. A linearized eutectic binary-phase diagram is used to predict the solute redistribution in the solid and the liquid phase. The micro model uses the lever rule to determine the temperature and the liquid fraction field from the transport equations.

The solid phase is assumed to be a rigid porous medium, which is traveling with a constant casting speed. The momentum conservation equation is thereby solved only for the liquid phase, which is assumed to be a Newtonian fluid:
\[
\frac{\partial}{\partial t}(\rho g_i \langle v_i \rangle') + \nabla \cdot \left( \rho \nabla \langle p_i \rangle' - g_i^2 \frac{\mu_i}{K} \left( \langle v_i \rangle' - v_{\text{cast}} \right) \right) + g_i \mu_i \nabla \left[ \nabla \left( g_i \langle v_i \rangle' \right) + \left( \nabla \langle g_i \langle v_i \rangle' \rangle \right) \right] + g_i b_{EM} + \rho g_i g \left[ 1 + \beta^T (T_{ref} - T) + \beta^C (C_{ref} - \langle C_i \rangle') \right],
\]

where \( t \), \( \rho \), \( \mu_i \), \( T^C \), \( K \), \( g_i \), \( \langle v_i \rangle' \), \( \langle p_i \rangle' \), \( T_{ref} \), \( T \), \( C_{ref} \), and \( b_{EM} \) are time, density, liquid viscosity, thermal expansion coefficient, species expansion coefficient, permeability, gravity acceleration vector, volume fraction of liquid, intrinsic liquid velocity, casting velocity, intrinsic liquid pressure, reference temperature, temperature, reference concentration, liquid intrinsic concentration, and time-averaged Lorentz force, respectively.

The simple Chorin’s pressure-correction scheme is used to ensure the mass conservation.

Local thermal equilibrium is assumed in the heat transport equation:

\[
\frac{\partial}{\partial t} \left( h_m \right) + \nabla \cdot \left( g_i \langle h_i \rangle' v_{\text{cast}} \right) + \nabla \cdot \left( g_i \langle h_i \rangle' \langle v_i \rangle' \right) = \nabla \cdot \left( \frac{\lambda_m}{\rho} \nabla T \right)
\]

where \( \lambda_m \), \( h_m \), \( \langle h_i \rangle' \), and \( \langle h_i \rangle' \) are thermal conductivity, volume-averaged enthalpy, intrinsic enthalpy of the solid phase, and intrinsic enthalpy of the liquid phase, respectively.

Diffusivity is neglected in both phases in the species transport equation:

\[
\frac{\partial}{\partial t} \left( C_m \right) + \nabla \cdot \left( g_i \langle C_i \rangle' v_{\text{cast}} \right) + \nabla \cdot \left( g_i \langle C_i \rangle' \langle v_i \rangle' \right) = 0
\]

where \( C_m \), \( \langle C_i \rangle' \), and \( \langle C_i \rangle' \) are volume-averaged concentration, intrinsic concentration of the solid phase, and intrinsic concentration of the liquid phase, respectively.

The electromagnetic field is calculated with the induction equation:

\[
\nabla^2 A = \mu_0 \sigma \frac{\partial \mathbf{A}}{\partial t} - \mu_0 \sigma \mathbf{v} \times (\nabla \times \mathbf{A}) - \mu_0 \mathbf{J}_{\text{ext}}
\]

where \( \mathbf{A} \), \( \mathbf{J}_{\text{ext}} \), \( \mathbf{v} \), \( \mu_0 \), and \( \sigma \) are magnetic vector potential, external electric current density, volume-averaged velocity, magnetic permeability of free space, and electrical conductivity, respectively. The current density is the source term, which is calculated from the coil specifications. Harmonic time dependence of magnetic vector potential and current density is imposed. Time-averaged Lorentz force is then calculated as the cross product of the steady parts of current density \( \mathbf{J}_o \) and magnetic field \( \mathbf{B}_o \):

\[ b_{EM}^{EM} = -\frac{1}{2} \text{Re} \left( \mathbf{J}_o \times \mathbf{B}_o \right) \]

3 NUMERICAL METHOD

The partial differential equations are solved with the meshless-diffuse-approximate method. The DAM uses the weighted least squares to determine a locally smooth approximation (\( \hat{f} \))
from a discrete set of data:

\[ f(x) = p(x, x_0) = \sum_{j=1}^{J} p_j(x, x_0) \alpha_j \]  

where \( \alpha \) is the vector of coefficients and \( p(x, x_0) \) is the vector of \( J \) trial functions. The second-order polynomials are used as trial functions. The Gaussian is used as the weight function in the minimization expression:

\[ \theta(x, x_0) = \exp\left(-c \frac{\|x - x_0\|^2}{h^2}\right), \]  

where \( c \) and \( h \) are free-parameter and scaling factor, which are equal to 5 and to the Euclidian distance between \( x_0 \) and the farthest position from \( x_0 \) in the discrete set of data.

The method is localized by defining the smooth approximation for each computational node separately. This is performed by associating each node with an unique local neighbourhood, which is used for minimization. 14 nodes are included in the local subdomains for DCC and LFEC simulations. The stability of the advective term is attained with a shift of the Gaussian weight and evaluation location in the upwind direction. This approach is called adaptive upwind weight function and it is confirmed that is a very successful stabilization procedure [11]. Explicit Euler scheme is used for temporal discretization.

4 SIMULATIONS

Simulations are performed for low-frequency electromagnetic casting process of Al-5.25wt%Cu alloy. Material properties are calculated with the JMatPro software. The secondary dendrite arm spacing is estimated from the literature [12]. The casting temperature and velocity are set to 680 °C and 120 mm/min, respectively. The initial cooling water temperature and discharge are set to 25 °C and 6 m³/h, respectively. The coil is wrapped around the billet and positioned 0.05 m from the billet surface at \( z = 0 \) m. The coil has 40 turns, while the total cross-section area of the windings is \( 9 \times 10^{-4} \) m². The electric current magnitude and frequency are varied in the computational cases and are presented in Table 1.

<table>
<thead>
<tr>
<th>Case</th>
<th>( I ) [A]</th>
<th>( f ) [Hz]</th>
</tr>
</thead>
<tbody>
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<td>LFEC0</td>
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<td>10</td>
</tr>
<tr>
<td>LFEC1</td>
<td>50</td>
<td>10</td>
</tr>
<tr>
<td>LFEC2</td>
<td>150</td>
<td>10</td>
</tr>
<tr>
<td>LFEC3</td>
<td>100</td>
<td>5</td>
</tr>
<tr>
<td>LFEC4</td>
<td>100</td>
<td>20</td>
</tr>
</tbody>
</table>

The casting geometry resembles the realistic industrial geometry and is described by the boundary parametrization points, which are displayed in Figure 1. The length of the billet is limited to 0.9 m, which is enough to reach the steady-state conditions at the outflow.

Symmetry boundary conditions are used at the west boundary. Velocity is set to zero at the
east boundary, while the adiabatic conditions are assumed for the species transport. Robin type of boundary condition is used for heat transfer in all three regions of the east boundary. Heat transfer coefficient is determined differently for each of the three regions; the hot-top is thermally insulated, HTC in the mould-chill depends on the liquid fraction, and HTC in the direct-chill is calculated with the Weckman-Niessen relation [13]. Dirichlet boundary conditions are assumed at the top boundary, where the initial species value and casting temperature are prescribed. A developed Poiseuille flow is assumed for the liquid velocity. Velocity at the bottom boundary is constant and equal to the casting speed. The heat and species conduction at the bottom boundary are both set to zero.

Figure 1: Parametrisation of the domain boundary.

Variable-density adaptive computational node arrangement is used in simulations. The finest node spacing is used in the mushy zone ($r_0=0.32$ mm), while the coarsest is in the solid ($r_0=10.0$ mm). Approximately 85,000 computational nodes are used for computation of mass, momentum, heat, and species transfer. An extended computational domain, which includes approximately 210,000 nodes, is used for computation of the induction equation.

5 RESULTS

In contrary to DCC simulations, the results of LFEC simulations do not always reach a steady-state. An oscillating pattern is observed, where the time interval depends on EMF parameters and the casting geometry. A repeating pattern can roughly be determined by observation of the melt flow structure throughout the simulation. Duration of a single interval is equal to 18.5 s, 9.1 s, and 28.0 s for LFEC0, LFEC2, and LFEC3, respectively. A steady state is achieved for LFEC1 and LFEC4. During a single interval the vortices are broken down in
several smaller ones and reconnected into larger ones (see Figure 2). Although the size, position, and structure of the vortices are not exactly repeated in each interval, it is similar enough to cause a repeating pattern in other fields.

Figure 2: Transient results for the mixture velocity for geometry LFEC0.

Figure 2: Time evolution of the maximum velocity in the billet for all cases.
A decrease and increase of the current amplitude result in a decrease and increase of the maximum velocity, respectively (see Figure 2 and 3). The melt flow in LFEC1 has a reduced amount of vortices. The smaller intensity of the flow results in a steady state without the oscillatory instabilities. The maximum velocity in LFEC2 is almost doubled, while the flow intensity and the frequency of the instabilities are increased. Both simulations with the modified electric frequency result in less pronounced oscillations. The amplitude of the maximum velocity is greatly reduced in the LFEC3 case.

Figure 3: Comparison of the mixture velocity for a single snapshot for all simulation cases.

Figure 4: Comparison of the concentration field for a single snapshot for all simulation cases.
Especially the effect on the concentration field is of great interest. From the contour plot (see Figure 4) it is observed that concentration in the solid along the z-axis is not constant when unsteady conditions are met, which is contrary to what is observed in DCC. Instead, a repeating pattern is formed along the vertical direction.

**Figure 5:** Concentration field for vertical cross sections at the billet center and surface.
Due to fluctuations in the solid species it is hard to quantify macrosegregation, which is usually displayed with horizontal cross section in the solid. But this would not be representative for comparison in the case of unsteady conditions. The comparison of the results for different geometries is therefore made for the vertical cross-sections at the center \((r=0 \text{ m})\) and at the surface \((r=0.12 \text{ m})\) of the billet (see Figure 5). Macrosegregation in the center fluctuates with different frequency and amplitude for each simulated case. Amplitude is largest in LFEC2 and smallest in LFEC1. This corresponds to the maximum velocities observed in the liquid melt. Furthermore, since a steady-state is achieved in LFEC1 and LFEC4, macrosegregation profile along the z-axis is constant in the solidified part of the billet.

6 FINDINGS

Computer simulations of low-frequency electromagnetic casting of Al-5.25wt%Cu alloy are performed with the mathematical model presented in the 2nd and 3rd section of this paper. The effect of EMF parameters in LFEC on melt flow and macrosegregation is evaluated. It is observed that the electric current frequency and intensity have a substantial effect on solidification in LFEC. There is a small effect on temperature distribution and the sump shape, but the effect on the melt flow and macrosegregation is extensive.

By comparing the simulations it can be concluded that an increase in amplitude and frequency of the maximum velocity results in an increase of amplitude and frequency of the macrosegregation evolution. The results show that it is not possible to make any general conclusions about the direct impact of the EMF parameters on macrosegregation formation. The problem is of such complexity that it is seems impossible to predict the melt flow structure and the macrosegregation without numerical simulations or industrial trials.

REFERENCES


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VALIDATION OF A COMPUTATIONAL MODEL FOR A COUPLED LIQUID AND GAS FLOW IN MICRO-NOZZLES

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Key words: Gas Dynamic Virtual Nozzle, Micro-Jet, Jet Shape, Jet Velocity, Coupled Numerical Model.

Abstract. The work presents verification of a numerical model for micro-jet focusing, where a coupled liquid and gas flow occurs in a gas dynamic virtual nozzle (GDVN). Nozzles of this type are used in serial femtosecond crystallography experiments to deliver samples into X-ray beam. The following performance criteria are desirable: the jet to be longer than 100 µm to avoid nozzle shadowing, the diameter as small as possible to minimize the background signal, and the jet velocity as high as possible to avoid sample’s double X-ray exposure. Previous comprehensive numerical investigation has been extended to include numerical analysis of the tip jet velocities. These simulations were then compared with the experimental data. The coupled numerical model of a 3D printed GDVN considers a laminar two-phase, Newtonian, compressible flow, which is solved based on the finite volume method discretization and interface tracking with volume of fluid (VOF). The numerical solution is calculated with OpenFOAM based compressible interFoam solver, which uses algebraic formulation of VOF. In experimental setup for model validation a 3D printed GDVN was inserted in a vacuum chamber with two windows used for illumination and visualization. Once the jet was stabilized
its velocity was estimated based on a distance a droplet traveled between two consecutive illumination pulses with a known time delay. The experimental and computational study was performed for a constant liquid flow rate of 14 μl/min and the gas mass flow rate in the range from 5 mg/min to 25 mg/min. The coupled numerical model reasonably predicts the jet speed and shape as a function of the gas flow.

1 INTRODUCTION

Liquid micro-jets are efficient vectors of mass and momentum, which find applications in countless scientific domains, most recently in serial femtosecond crystallography (SFX) [1]. In SFX they are used as sample carriers for beam interactions, where diffraction patterns of these samples are collected as they interact with femtosecond X-ray pulses from X-ray Free-Electron Lasers (XFELs). These crystal samples are very small with typical dimensions of sub- to few microns and their weak scattering ability requires very high-intensity X-ray beams to produce a sufficient signal for meaningful data collection. The samples are delivered into X-ray beam via a liquid jet, thus some characteristics of the carrier jet are of utmost importance, such as its diameter, length and velocity. The diameter of the jet should be as small as possible to increase the signal of the sample relative to the background from the buffer liquid. In addition, the jet has to be long enough so that the interaction with X-ray beam can be far enough from the nozzle to avoid any shadowing from the nozzle structure in the X-ray diffraction data. The interaction of the jet with the X-ray is normally carried out at a distance of ~100 μm or more. The X-ray beams coming out from XFELs operate with a frequency of 120 Hz (e.g. LCLS) or as high as 4.5 MHz (e.g. European XFEL). In order to avoid a double exposure of the crystal the jet has to be as fast as possible. For biological samples it is also important to know the temperature of the jet.

Liquid jets are produced in many ways starting from Rayleigh sources [2], to more recently, gas dynamic virtual nozzles (GDVNs) [3]–[6]. Rayleigh sources are inefficient for SFX applications because of their limitations in producing fast, micron/sub-micron jets [5]. To overcome these issues, a novel way of producing liquid jets was introduced using a hydrodynamic effect of the co-flowing gas stream [3]. Further improvement was to replace the plate with an orifice with a glass polished converging outer capillary [4]. This increased the harvesting of the focusing moment from the co-flowing gas. An injection molded GDVN [5] was introduced to overcome manufacturing difficulties in glass polished nozzles. More recently 3D printed GDVNs [7] were introduced, enabling advanced micro-nozzle design solutions and manufacturing with high accuracy and reproducibility.

As the jet emanates from nozzle outlet in provided environment various instabilities co-exist on the jet surface. These instabilities determine the jet characteristics, which are either (a) an unstable meniscus with periodic ejection of drops - dripping, (b) a continuous stable liquid thread, which finally breaks into stream of droplets - jetting, (c) spatially unstable jet, which whips with some amplitude - whipping [3], [8]. There are various strongly coupled factors that result in the jet outcome (jetting/dripping/whipping). They include nozzle geometry, liquid and gas operating parameters, gas and liquid material properties.

Numerical simulations have become very successful in studying the jet characteristics. They have been performed for jet emanating in air [9], [10] and vacuum environments [6], [11], [12]. Recently, the jet characteristics have been investigated for injection molded GDVNs using
experimentally validated numerical model for a wide spectrum of liquid and gas flow rates [6], nozzle geometry [11] and type of focusing gas [12].

Present work extends these numerical investigations by using the same numerical model as in [6] for the assessment of the jet speed as a function of gas flow rate for a 3D printed nozzle. A fixed nozzle geometric arrangement is used for numerical study, where the numerical results are compared with the experimentally collected data. The numerical formulation is followed with the short description of governing equations and the basics of the solution procedure. Numerical results are discussed for 5 different cases where the liquid flow rate is kept constant, while the gas flow is changed. Conclusions are drawn in the final section based on the results of the numerical model and its comparison with the related experiment.

2 METHODOLOGY

In this experiment we attempted to collect the jet length, diameter and the velocity of a 3D printed GDVN. The same experimental setup as in [5] was used. However, this time also the jet speed was recorded by using two laser pulses with a known delay. The distance travelled by the first drop detaching from the jet tip was recorded and the speed was measured.

Numerical domain of GDVN used for numerical simulation is shown in Figure 1. The GDVN geometry has a cylindrical symmetry so an axisymmetric modelling approach is applied instead of a full 3D modelling. The numerical model, including the boundary conditions used along with the solution setup are elaborated in [6]. Only basic elements of the numerical model are summarized in the present paper.

![Figure 1](image)

**Figure 1.** Schematic of GDVN used for numerical simulations (not to scale), where \( R_1 = 25 \text{ \(um\) }, R_2 = 70 \text{ \(um\) }, R_3 = 175 \text{ \(um\) } H = 60 \text{ \(um\) } \) and \( D = 60 \text{ \(um\) } \).

A single-domain VOF approach includes a volume fraction variable \( \alpha(p,t) \), bounded between 0 and 1 for gas and liquid, respectively. The interface transport equation along with the mixture formulation of coupled mass, momentum and energy equations are given as follows,
\[ \partial (\rho \alpha) / \partial t + \nabla \cdot (\rho \mathbf{v} \alpha) = 0 \]  

(1)

\[ \partial \rho / \partial t + \nabla \cdot (\rho \mathbf{v}) = 0, \]  

(2)

\[ \partial (\rho \mathbf{v}) / \partial t + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla \cdot \mathbf{f}_s + \mathbf{f}_\sigma \]  

(3)

\[ \partial (\rho e) / \partial t + \nabla \cdot (\rho e \mathbf{v}) = -\nabla \cdot (\rho \mathbf{v}) + \nabla \cdot (\mathbf{f}_s + \nabla \cdot \mathbf{q}) \]  

(4)

where \( \mathbf{v}(p, t) \) is velocity vector and \( \rho \) is density, \( p(p, t) \) denotes pressure, \( \mathbf{f}_s(p, t) \) surface tension forces, \( \mathbf{f}_\sigma \) the viscous stress tensor, defined as \( \mathbf{f}_\sigma = \mu \left( (\nabla \mathbf{v}) + (\nabla \mathbf{v})^T \right) - \lambda \left( \nabla \cdot \mathbf{v} \right) \mathbf{I} \) with viscosity \( \mu \), \( \lambda = (2/3)\mu \) and identity tensor \( \mathbf{I} \), while \( e \) is the specific total energy per unit volume, composed from the specific internal and the kinetic energy per unit volume \( e = c_i T + 0.5 \mathbf{v}^2 \) with \( c_i \) and \( T \) standing for specific heat capacity at constant volume and temperature respectively.

The material properties satisfying equations (1) - (4) are calculated from the phase-weighted averages as,

\[ \partial (\alpha \mathbf{g}) = \alpha \partial \mathbf{g} + (1-\alpha) \partial \mathbf{g}, \]  

(5)

where, \( \partial \) and \( \partial \mathbf{g} \) stand for the liquid and gas material properties, such as density, specific heat, thermal conductivity and viscosity. Ideal gas is considered for density calculation.

The high speeds and micro-dimensionality of the nozzle system allow to neglect the gravitational force. The dominant surface tension force is included as the body force \( \mathbf{f}_s = \sigma \kappa \mathbf{n} \), with \( \sigma \) standing for surface tension, \( \kappa = \nabla \cdot \nabla \alpha \) is the unit normal and the curvature of the interface calculated by using the continuum surface model [13] as, \( \kappa = \nabla \cdot (\nabla / |\nabla|) \).

Numerical simulations are performed with OpenFOAM code [14], which is based on FVM discretization. The liquid-gas interface is captured with VOF method, where the interface diffusion is avoided by using an artificial interface compression counter-gradient approach [15]. PIMPLE algorithm is used for the solution of partial differential equations and an adaptive time stepping approach is used by setting [16] Courant number \( C_O = \left( |\mathbf{v}| \Delta t / \Delta x \right) \) equal to 0.25.

3 RESULTS AND DISCUSSIONS

Numerical simulations were done for a set of 5 different helium gas flow rates (5 mg/min, 10 mg/min, 15 mg/min, 20 mg/min and 25 mg/min), and where the water flow rate was kept constant at 14 µl/min. The jet diameter, length and velocity were analyzed as a function of the gas flow rate. Experimental data was extracted and compared with the numerical simulations in terms of jet length, diameter and velocity in Figure 2, 3 and 4.
It is seen from the jet snapshots in Figure 2, that the jet shape obtained with the numerical simulation reasonably agrees with the experimental one. To analyze the data, the jet shape was averaged over time, once the simulation was stabilized. These time averaged values are presented in Figure 3 - (a, b).

Experimentally measured velocities and velocities obtained from numerical simulations are presented in Figure 4. It is interesting to note a consistent underestimation of the calculated jet velocities as compared to the experimentally measured ones. This difference could potentially be explained with how these velocities were measured. In the experimental setup the velocity of the first detached drop from the jet is monitored as it moves downstream in the nozzle outlet chamber. In the numerical simulations we are extracting the velocity of the tip of the jet. The first detached drop accelerates in high speed gas stream co-flowing with the jet causing the difference in velocity comparison.
4 CONCLUSIONS

The FVM-VOF based numerical model was used to assess the jet focusing for a 3D printed micro GDVN. The measured and calculated jet shapes show reasonable agreement. However, simulated velocities are consistently slower than experimentally measured ones, this difference could possibly be introduced by the velocity measurement. In the experiments we measure the velocity of the first detached drop from the jet, because measuring the velocity closer to the tip of the jet was not possible. Similarly, in numerical simulations it is not easily possible to retrieve velocities of the first detached drop. A more accurate comparisons would require assessing flow characteristics of the jet at same position. In spite of the discrepancies present in measured and calculated velocities, the study overall provides a good way forward for future such investigations. In the numerical simulations there are no such constrains and we can easily retrieve the velocity of the tip of the jet.

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REFERENCES


COUPLED SOIL-STRUCTURE INTERACTION MODELING
AND SIMULATION OF LANDSLIDE PROTECTIVE
STRUCTURES

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Key words: Soil-Structure Interaction, Staggered Coupling, Material Point Method,
Finite Element Method, Landslides

Abstract. Within the past two decades, mass movements hazards involving fast and
large soil deformation have increased significantly in frequency and magnitude due to
their strong relation to climate changes and global warming. These phenomena often
bring along rocks, debris, and heavy materials that can extensively damage and destroy
the landscape and infrastructures, causing devastating economic loss, and often, human
casualties. The risk of future disasters continues to escalate with the increase of real estate
development in suburban areas, including mountainous regions. Further assessment and
prediction on such disasters and their countermeasures are, therefore, in high economic
demands. One of the most intuitive ways is to install protective structures in mountain
slopes and valleys that can hold the materials brought by the moving landslides. While the
current state of the art of landslide prediction using numerical methods has been mainly
dominated by the development of advanced geomechanical models suited for different
types of soil materials, e.g. multi-phase unsaturated soil model, this study focuses more
on the interaction of such phenomena with the installed protective structures. Here, an
implicit formulation of material point method (MPM) is implemented to model the landslides
considering finite strain assumption. Furthermore, a staggered coupling scheme with
traditional Finite Element Method (FEM) is proposed to simulate accurately and robustly
the dynamic force and displacement coupling of soil-structure interaction (SSI). All developments of the method are implemented within the Kratos-Multiphysics framework [1] and available under the BSD license (https://github.com/KratosMultiphysics/Kratos/wiki).

In the future works, more adequate consideration of coupling scheme and material models considering damage and fracture will be investigated before conducting a real-scale landslide simulation.

1 INTRODUCTION

Landslides and other mass movements often carry huge rocks and heavy materials that may, directly or indirectly, cause damage to structures and the landscape. These phenomena are also extremely dangerous and often bring huge losses of lives and properties, resulting in a great economic loss, in particular, in rainy mountainous regions or in major earthquake zones. According to the United Nations Office for Disaster Risk Reduction (UNISDR) and the Centre for Research on the Epidemiology of Disasters (CRED), from 1998 to 2017 [2], landslides and other mass movement hazards have been responsible for 18,779 deaths worldwide, with more than 4.7 million citizens affected, and more than US$ 5.2 billion economic losses. The risk of future disasters is predicted to continue to escalate with the increase of real estate development in suburban areas, including mountainous regions. Even if nothing can be done in a short time to avoid the disasters, protection structures should be designed, or improved, as such that it can minimize the damage induced by the dynamic soil forces.

In this study, the dynamic interaction between landslides and protection structure is selected as a target issue, and it is numerically represented by using a staggered coupling of implicit Material Point Method (MPM) and Finite Element Method (FEM). Introduced by [3, 4] as the extension of Particle-In-Cell (PIC) method [5], the MPM has gained a remarkably increasing popularity due to its capability in simulating solid mechanics problems, which involve historically dependent materials and large deformations. As one of the fully Lagrangian particle methods which combines the strengths of Eulerian and Lagrangian methods, MPM has been utilized in various civil engineering applications, mostly in the analysis of moving discontinuities and large deformation systems such as the free-surface environmental flows with breaking, splash, and fragmentation; those which are difficult to simulate by using traditional FEM due to its mesh distortion issues.

Although MPM has been proven to work robustly for problems involving large deformation materials, the accuracy of the integration done in the particle quadrature is significantly lower than the Gaussian quadrature, which is used in the traditional FEM. It, therefore, produces less accurate and efficient solutions when being used to simulate problems with small deformation in comparison to the ordinary FEM. It is always desirable to combine the FEM with MPM to take respective advantages of these two methods, in particular for soil-structure interactions (SSI) problems.
The objective of this study is to develop an accurate implicit MPM formulation to simulate three-dimensional landslides and SSI considering a robust contact and coupling strategy. Although there were numerous research done to tackle large deformation soil and SSI problems by using MPM, almost all of them are formulated in an explicit way which is easy to implement and computationally less costly. There are, however, still limited research done for the implicit MPM formulation. By using the implicit approach, imposition of nonconforming boundary conditions can be done easily, such as by utilizing the penalty approach. Moreover, the formulation can be smoothly coupled with structural analysis studies by using purely MPM or coupled with other available methods suitable for structural analysis, such as FEM. To achieve the aforementioned motivation, the Kratos-Multiphysics proposed by [1], which is an open-source software available under the BSD license, has been used and continuously developed to treat multi-physics coupling phenomena. This framework allows us to establish a seamless coupling strategy between MPM and FEM, and possibly with other Lagrangian methods in the near future.

2 GOVERNING EQUATIONS

2.1 Strong Form

Consider a body $B$, which occupies an initial domain $\Omega$ at time $t = 0$ of a three-dimensional Euclidean space $E$, with a regular boundary $\partial \Omega$ in its reference configuration. A deformation of $B$ is defined by a one-to-one mapping as:

$$\varphi : \Omega \rightarrow E.$$  

This maps each material point at initial configuration $X \in \Omega_0$ in the body $B$ into a spatial coordinate in deformed configuration $x \in \Omega_t$ as:

$$x = \varphi (X) = x(X, t),$$  

which also represents the location of the same material point in the deformed configuration of $B$. The region of $E$ occupied by $B$ in its new configuration can be denoted similarly by:

$$\Omega_t = \varphi (\Omega_0).$$  

The governing equations, i.e. the mass and the momentum conservation equations, can be written as:

$$\frac{d\rho}{dt} + \rho \nabla \cdot \mathbf{v} = 0 \quad \text{in } \varphi(\Omega),$$  

$$\rho \mathbf{a} = \nabla \cdot \mathbf{\sigma} + \rho \mathbf{b} \quad \text{in } \varphi(\Omega),$$  

where $\mathbf{b}$ is the volume acceleration and $\mathbf{\sigma}$ is the symmetric Cauchy stress tensor. The kinematic variables $\mathbf{a}$ and $\mathbf{v}$, which are the second and the first material derivatives of displacement $\mathbf{u}$, are the acceleration and velocity, respectively. The balance equations
above are to be solved numerically in a three-dimensional field $\Omega \subseteq \mathbb{R}$, within the time range $t \in [0, T]$, considering the following Dirichlet and Neumann boundary conditions:

$$\begin{align*}
    u &= \bar{u} \quad \text{on } \varphi(\partial \Omega_D), \\
    \sigma \cdot n &= \bar{t} \quad \text{on } \varphi(\partial \Omega_N),
\end{align*}$$

(6)

(7)

where $n$ is the outward surface unit normal vector, while $\bar{u}$ and $\bar{t}$ are the corresponding Dirichlet and Neumann boundary displacement and traction, respectively.

## 2.2 Weak Form and Linearization in Spatial Form

In order to solve the momentum balance equation, which was previously written in its strong or derivative form, the weak or integral form of equation (5) should be derived by employing the principle of virtual work [6]. To do that, equation (5) is, first, multiplied by an arbitrary test function $w$, such that $w = \{w \in V | w = 0 \text{ on } \varphi(\partial \Omega_D)\}$, where $V$ is the space of virtual displacements. By using the divergence theorem the weak form of momentum balance can be obtained and written as:

$$R(u, w) \equiv \int_{\varphi(\Omega)} \sigma(\varepsilon(u)) : \nabla^w dw - \int_{\varphi(\Omega)} \rho (b - \ddot{u}) \cdot w dv - \int_{\varphi(\partial \Omega_N)} \bar{t} \cdot w da = 0 \quad \forall w \in V.$$  

(8)

Equation (8) is valid for any kind of strain definitions, including the infinitesimal one. Since, in the current work, strong material and geometric nonlinearities are involved, a linearization of the weak form is, therefore, necessary, and thus, the Newton-Raphson method, which is based on Taylor’s theorem, is used to approximate the solution iteratively. The algorithms of the solving strategy implemented in MPM fashion are explained in detail by [7, 8, 9] considering an implicit time integration scheme of the Newmark-beta method.

## 3 STAGGERED SOIL-STRUCTURE INTERACTION COUPLING

In the current study, a staggered two-way strongly coupled SSI scheme is implemented [10] considering a dynamic relaxation scheme. The SSI interface is implemented to first transfer the soil impact force acting on the structure $F_{s \rightarrow st}$ to the structural solver. The force transferred will further cause deformation on the structure, and this deformation $u_{st \rightarrow s}$ will be then sent back to the soil solver as a response to the given force. This process of transferring and receiving information, namely force and displacement, is then continued in an iterative loop until certain convergence criteria are satisfied, or until the maximum number of iterations is reached (see figure 1 for the illustrative description). Here, the convergence criteria must preserve the continuity of displacement and velocity (or the Dirichlet conditions) as well as the equilibrium of forces or tractions (the Neumann condition) at the boundary $\Gamma$ between the structure and the soil domain. Here, a
penalty-based method is utilized and proposed to impose inhomogeneous Dirichlet condition in the MPM and to approximate contact force at the SSI interface. Note that the discretization of the soil and the structural interface maybe nonconforming, as two different numerical methods are employed, i.e. the MPM and FEM, to discretize the soil and structural domain independently. Therefore, a mapping procedure between the two staggered systems [11] is needed to translate all the scalar or vector quantities required in the coupling.

![Figure 1](image_url): Two-way strongly coupled SSI: Schematic description.

4 NUMERICAL EXAMPLE

In order to test the performance of our staggered coupling of MPM with FEM a similar model to the one created by [9] is constructed by using the proposed SSI interface. The initial geometry for the staggered MPM-FEM coupling can be seen in figure 2. In this validation, the material parameters specified in table 1 is considered. Here, two tests with mesh size $h = 0.005$ and $0.0025$ m are performed to check the mesh-convergence effect in comparison with the result obtained by [9].

The staggered coupling simulations are performed considering a strongly coupled formulation, where a series of iteration is performed to reach a certain convergence of Dirichlet and Neumann conditions at the soil-structure interface. For the MPM simulations, structured triangular meshes are used to generate particles, as such that the initial arrangement is the same with the monolithic SSI simulation done by [9], with MP/cell = 3, while, unstructured triangular background grids are used to perform the MPM computa-
Table 1: Granular flow simulations with an obstacle: Material data.

<table>
<thead>
<tr>
<th>Material type</th>
<th>Density [kg/m³]</th>
<th>Young’s modulus [kPa]</th>
<th>Poisson’s ratio</th>
<th>Friction angle [°]</th>
<th>Cohesion [kPa]</th>
<th>Dilatancy angle [°]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soil</td>
<td>2650</td>
<td>840</td>
<td>0.3</td>
<td>19.8</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Structure</td>
<td>1100</td>
<td>1000</td>
<td>0.0</td>
<td>Neo-Hookean hyperelastic material</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure 2: Granular flow simulations with an obstacle: Initial geometry for staggered MPM-FEM coupling.

Moreover, as the approximated contact forces are often over-estimated at the first coupling iteration, a relaxation method based on the multi-vector update quasi-Newton (MVQN) approach [12] is assumed in this case to ensure and accelerate the convergence of the SSI iteration. Last but not least, for the strong coupling iteration settings, the maximum coupling iteration is set to be 20, and both of the absolute and relative tolerances are set to be $10^{-5}$.

In figure 3 and 4, it can be observed that the simulation results show a very good qualitative agreement with the monolithic MPM-MPM SSI simulations done by [9] with respect to the conducted mesh convergence study. Here, the displacement of the staggered simulations, in particular for $h = 0.0025$ m, shows a higher peak than the one obtained by [9], even though at the end of the simulation the displacement shows a lower displacement. Moreover, the staggered SSI displacements also vibrate with higher amplitude and longer period. These differences in the obtained results are mostly caused by the different contact conditions.
conditions assumed between the two coupling approaches. Unfortunately the current results are not yet validated with any experiments, and thus, further verification and validation test are planned to be performed in the near future.

![Figure 3: Granular flow simulations with an obstacle: Comparisons of deformed configuration at t = 0.5 s between the monolithic MPM-MPM [9] and the proposed staggered MPM-FEM SSI tests.](image)

5 CONCLUSIONS

A staggered coupling scheme to simulate soil-structure interaction problems is presented in the current study by using a coupled implicit material point and finite element method. The staggered coupling technique allows us to utilize the best of each numerical method: the MPM for large and non-linear soil deformation, and the FEM for an accurate evaluation of structural dynamics. Implicit MPM can then be connected to the FEM to adequately simulate fast landslides hazards interacting with complex civil structures with protective purposes. Nevertheless, some future works are necessary to improve the accuracy and quality of the numerical results, such as by improving the numerical stability or reducing the computational cost of the simulations. This will allow to use our approach to predict real-scale landslide hazards involving complex multi-phase flows of particles with different sizes.
**Figure 4:** Granular flow simulations with an obstacle: Comparison of structural displacement at point "A" upon impact between the monolithic [9] and the proposed staggered SSI coupling.

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**REFERENCES**


COUPLING OF STRUCTURAL SOLVER AND VOLUME-CONSERVING SOLVER FOR FORM-FINDING OF MEMBRANE STRUCTURES SUBJECTED TO PONDING

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Key words: Volume-conserving solver, ponding, partitioned FSI, hydrostatic load

Abstract. The current study deals with coupling of a volume conserving solver and a structural solver to calculate the static deformation of flexible structures under the load of a given volume of water. The volume-conserving solver contains a horizontal plane representing the free surface of the fluid, which is moved in the non-linear iterations to conserve the volume. The Partitioned approach is chosen to have code modularity and reusability with many structural codes.

1 INTRODUCTION

Membrane structures have a wide variety of applications spanning across different engineering disciplines, from the construction of light weight structures in civil engineering to the deployment of parachutes during reentry in aerospace industry. Among the various types of light weight structures, tensioned membrane structures may be the most ubiquitous. These structures have a unique load carrying ability relative to their self-weight due to their large deflection behavior. This at the same time makes them vulnerable to ponding, which is the formation of indentation filled with liquid. There are many aspects of an analysis on membrane structures, such as large deformation analysis, form finding [1], wrinkling [2] and membrane wind interaction [3] but the analysis involving ponding water on a membrane structure is relatively rare. However, there are studies [4, 5] where the hydrostatic load is applied as a follower load on the structure and is solved in the non-linear iterations of the structural solver, but this implementation involves access to the structural solver which may not be possible in many structural codes. Therefore, the
approach of partitioned coupling has been chosen for the present work. An example of using this approach to study ponding on membrane structures is performed by Bown et al [6]. In their work, the authors couple their in house structural code inTENS with their shallow water solver in a partitioned manner to predict and analyze ponding on the membrane structure. However, this is computationally expensive as they couple two transient solvers to analyze what is in fact a steady state phenomenon. The volume-conserving solver proposed in this work with an incremental increase of volume should simulate the filling up of water in the local depression without incorporating the transient behavior.

One main motivation to simulate the ponding in membrane structures is to study the case where the ponding water is coupled with a wind excitation. A real-life example where this proved to be fatal is the Pukkelpop accident (Kiewit, Belgium 2011), where a strong wind interacting with ponding water led to huge swaying of a tent in the vertical direction and eventually resulting in the collapse of the structure. Computational methods to investigate this phenomenon will involve a fluid-structure interaction (FSI) simulation with a lightweight structure, ponding water and wind loads. The method discussed in this work will be used to determine the deformed shape of the structure under the influence of ponding, which will be the starting point of the FSI simulation discussed above. Moreover, based on the literature search simulation involving coupling of ponding water, a membrane structure and wind has not been studied before, therefore it is interesting from a research point of view. The proposed method involves coupling a structural solver and a volume-conserving solver in partitioned manner, in the same way how the effect of wind and ponding on a membrane structure will be studied. The volume-conserving solver consists of a plane representing the free surface of the water. The solver updates its position based on the deformation of the underlying structure in order to conserve a given volume of water, which in turn applies hydro-static loads on the structure. When the convergence is achieved in the partitioned iterations, the deformed shape of the structure is determined. The following sections discuss the proposed volume-conserving solver and how it is coupled to a structural solver in KRATOS [7], an open-source finite element framework. At the end, an example is presented where the static deformation of a flexible structure is calculated due to the accumulation of an incompressible fluid.

2 CONTINUOUS PROBLEM

Let us assume a flexible structure which can be modeled as shell or membrane elements with a suitable material model. The surface of the structure is denoted by \( \partial \Omega_s \) which contains a certain volume of incompressible fluid. The free surface of the fluid is horizontal (perpendicular to gravity), denoted by \( \partial \Omega_f \). The part of \( \partial \Omega_s \) which is below \( \partial \Omega_f \) is the fluid-structure interface called wetted surface, denoted by \( \partial \Omega_{fs} \), which experiences hydrostatic pressure from the fluid above. In other words, a point \( S \) on \( \partial \Omega_{fs} \) experiences traction, \( t \) in the form of pressure proportional to the height of the free surface above the point. Mathematically, the traction at a point \( S \) with a position vector \( x \) on the structure
can be stated as:

\[ t = \gamma_f [(x - x_f) \cdot n_f] n \quad \forall x \in \partial\Omega_{fs} \tag{1} \]

\[ t = 0 \quad \forall x \in \partial\Omega \setminus \Omega_{fs} \]

where, \( x_f \in \partial\Omega_f \), \( \gamma_f \) is the specific weight of the fluid, \( n \) is the outward unit normal vector at the point S and \( x_f \) is the position vector of any point at the free surface with an unit normal \( n_f \). The expression \((x - x_f) \cdot n_f\) gives the the vertical height of the point S from the free surface. The symbols and terminologies introduced above are clearly shown in figure 1.

Figure 1: Structure loaded by the hydrostatic pressure from the fluid.

3 VOLUME-CONSERVING SOLVER

The fluid enclosed between \( \Omega_f \) and \( \Omega_{fs} \) is incompressible and therefore during the partitioned FSI iterations, the volume of the fluid should always be conserved. This is achieved by an algorithm called volume-conserving solver. It consists of two building blocks: a volume calculation algorithm and the non-linear iterations responsible for updating the free surface to conserve the volume. The equation for calculating the fluid volume using the points on wetted surface can be obtained by using equation 2 and the Gauss divergence theorem. Following some substitutions, we arrive at the expression of volume \( (V) \) of the fluid domain \( (\Omega_f) \) bounded by the wetted surface \( (\partial\Omega_{fs}) \) and the free surface \( (\partial\Omega_f) \), given in equation 3.

\[ \nabla \cdot [(x - x_f) \cdot n_f] n = 1 \quad \forall x \in \Omega_f \tag{2} \]

\[ \int_{\Omega_f} \nabla \cdot [(x - x_f) \cdot n_f] n \ dV = \int_{\partial\Omega_{fs}} [(x - x_f) \cdot n_f] n \ dS \]

\[ \implies V = \int_{\Omega_f} dV = \int_{\partial\Omega_{fs}} [(x - x_f) \cdot n_f] n \ dS \tag{3} \]
The non-linear iterations to conserve the volume consist of a modification to the Newton’s method called leap-frogging Newton, with residual equal to the difference between the current volume, $V$ (calculated using equation 3) and the target volume, $V_t$. The method is discussed in detail in [9], which consists of a Newton step and followed by a pseudo secant step. The main advantage of this method is that it only involves one derivative evaluation, like Newton’s method and yet it can attain cubic convergence. Both methods were tested for volume conservation with a complicated geometry and it was found that the leap-frogging Newton was much more robust and had faster convergence rate than Newton’s method. Hence, it was chosen over the other.

To understand the method, consider a function $f(x) \in C^2[a, b]$ with a root $x^*$ in the interval $[a, b]$. Let $x_n$ be the solution at $n^{th}$ iteration. The Newton’s step to find the intermediate solution $\tilde{x}_n$ is given as,

$$\tilde{x}_n = x_n - \frac{f(x_n)}{f'(x_n)} \tag{4}$$

In the next step, a secant is constructed from the points $(x_n, f(x_n))$ and $(\tilde{x}_n, f(\tilde{x}_n))$, given by equation 5. The point where the secant line intersects the x-axis is taken as the solution at iteration $n + 1$. By substituting equation 4 in equation 5 and performing some algebraic manipulation, one can obtain an expression to find $x_{n+1}$, given in equation 6. The two steps discussed above are clearly shown in figure 2.

$$y - f(x_n) = \frac{f(x_n) - f(\tilde{x}_n)}{(x_n - \tilde{x}_n)} (x - x_n) \tag{5}$$

$$x_{n+1} = x_n - \frac{(f(x_n))^2}{f'(x_n) (f(x_n) - f(\tilde{x}_n))} \tag{6}$$

For the volume-conserving solver, volume $V - V_t$ is the non-linear function $f$ in equation 6. Considering a case where $n_f$ is along the z-direction, the equation for calculating the volume given in equation 3 simplifies to equation 7, where $z$ and $z_f$ are the z-coordinates of a point in $\Omega_{fs}$ and $\Omega_f$, respectively. Clearly, this is a function of $z$, $z_f$ and $n$. However, it can be noted that during the volume-conserving process the wetted surface doesn’t change, hence the volume depends only on $z_f$. The derivative of the function, $f'$ can be obtained by deriving the equation 7 by $z_f$. As given in equation 8, the derivative of the difference between the target and current volume is equal to the area of the free surface, $A_f$. 

$$f(z) = \frac{z - z_f}{A_f} \tag{7}$$

$$A_f = \int_{z_f}^{z} f(z) \, dz \tag{8}$$
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Figure 2: Leap-frogging Newton method to find the root of a non-linear function.

\[ f(z_f) = V - V_t = \int_{\partial \Omega_{f}} (z - z_f) e_z \cdot n \, dS - V_t \quad (7) \]

\[ f'(z_f) = -\int_{\partial \Omega_{f}} e_z \cdot n \, dS = A_f \quad (8) \]

Using equations 6, 7 and 8, we can write an algorithm for the volume conserving solver as given in algorithm 1, where the free surface is a plane with normal \((n_f = e_z)\). A radius, \(r\) is given as input to give a spatial limit to the volume calculation and hydrostatic load application on the structure.

**Algorithm 1** Leap-frogging Newton’s method for volume-conservation.

1: \( n = 0 \)
2: while \( \| \frac{V - V_t}{V_t} \| > \varepsilon \) do
3: \hspace{1em} if \( n < n_{\text{max}} \) then
4: \hspace{2em} Calculate \( f(x_n) = V - V_t \) using equation 7, where \( x_n = z_f \) at \( n^{th} \) iteration.
5: \hspace{2em} Calculate \( f'(x_n) = A_f \) using equation 8.
6: \hspace{2em} Move the plane to an intermediate position along \( e_z \) using equation 4.
7: \hspace{2em} Calculate \( f(\tilde{x}_n) = \tilde{V} - V_t \) using equation 7.
8: \hspace{2em} Calculate \( x_{n+1} \) using equation 6. Move the plane to \( z_f = x_{n+1} \)
9: \hspace{1em} \( n = n + 1 \)
10: \hspace{1em} end if
11: end while
4 IMPLICIT PARTITIONED COUPLING

The deformed shape of the structure under the load of given volume of fluid, $V_t$ is obtained once the structural equilibrium equations and boundary conditions given in equation 1 are satisfied with fluid volume, $V = V_t$. The implicit partitioned approach to find the solution consists of iterations involving sequential calls to the structural solver to calculate the structural deformation and volume-conserving solver to conserve the volume. In each iteration, the structural solver gets the traction at the wetted surface based on the plane’s position (equation 1), which in turn updates the plane’s position based on the structural deformation so that $V = V_t$ (algorithm 1). Convergence accelerators such as Aitken and IQN-ILS [8] are used to achieve faster convergence. In order to explain the algorithm, we need to define some terms mathematically. Let $\mathbf{d}$ and $\mathbf{t}$ be the displacement and traction on the structure, respectively. With this definition the volume-conserving solver ($\mathcal{F}$) and structural solver ($\mathcal{S}$) can be written as:

\begin{align*}
\mathbf{t} &= \mathcal{F}(\mathbf{d}) \\
\mathbf{d} &= \mathcal{S}(\mathbf{t})
\end{align*}

The problem of finding the equilibrium shape of the structure under the hydrostatic load of a fixed volume of fluid can be written as a fixed point problem,

\[ \mathbf{d} = \mathcal{S} \circ \mathcal{F}(\mathbf{d}) \]  

**Algorithm 2** Partitioned FSI iterations to calculate structural deformation under hydrostatic load.

1: $k = 0$
2: $\tilde{\mathbf{d}}^k = \mathcal{S} \circ \mathcal{F}(\mathbf{d}^k)$
3: $\mathbf{r}^0 = \tilde{\mathbf{d}}^0 - \mathbf{d}^0$
4: while $\| \mathbf{r}^k \| > \varepsilon$ do
5: \hspace{1em} if $k < k_{\text{max}}$ then
6: \hspace{2em} $\mathbf{d}^{k+1} = \mathbf{d}^k + \delta \mathbf{d}^k$
7: \hspace{2em} $\tilde{\mathbf{d}}^k = \mathcal{S} \circ \mathcal{F}(\mathbf{d}^k)$
8: \hspace{2em} $\mathbf{r}^{k+1} = \tilde{\mathbf{d}}^k - \mathbf{d}^k$
9: \hspace{2em} $\delta \mathbf{d}^k = \text{Convergence accelerator.\,ComputeUpdate}(\mathbf{r}^{k+1}, \mathbf{d}^k)$
10: \hspace{1em} $k = k + 1$
11: \hspace{1em} end if
12: end while

In the present work, the solution to the problem given in equation 11 is obtained by implicit partitioned coupling, which involves additional coupling iterations between the structural solver $\mathcal{S}$ and volume-conserving solver $\mathcal{F}$. If $k$ represents the iteration number
for the coupling iterations, then the residual of equation 11 at the $k^{th}$ iteration is given by equation 12, where $d^k$ is the displacement at the $k^{th}$ iteration and $\tilde{d}^k = S \circ F(d^k)$.

$$r^k = \tilde{d}^k - d^k$$  \hspace{1cm} (12)

With all these definitions, we can write the implicit partitioned coupling algorithm for the problem as given in algorithm 2.

5 DISCRETIZED PROBLEM

The structural equilibrium equations with the boundary conditions are generally solved using the finite element method. This involves first discretizing the structure into elements that converts the continuous problem into a discrete set of equations. When the equations are non-linear, an iterative algorithm based on Newton-Raphson is used where the linearized equation given in equation 13 is solved in every iteration to get the solution update until convergence.

$$K_T \Delta d = r_s$$  \hspace{1cm} (13)

where, $K_T$ is the tangent stiffness matrix, $r_s$ is the residual vector of the discretized structural equations and $\Delta d$ is the update in the displacements.

In the current work, the structural-solver responsible for performing non-linear iterations is treated as a black-box. It takes the traction in the form of nodal pressures as input and gives the displacements as output. Consequently, this process introduces an error in the elements that are cut by the free surface plane. As shown in figure 3, the nodes of the cut elements that are below the free surface plane receive pressure values proportional to their vertical distance, as given in equation 1. By contrast, the nodes that are above this plane receive zero pressure, which means equation 1 is not satisfied exactly in the cut elements. However, this error should decrease with a finer discretization.

The volume-conserving solver presented in this paper basically involves computation of two quantities, $V - V_t$ and $A_f$. As evident from the equation 7 and 8, this will involve integration of a scalar quantity in the domain $\partial \Omega_{fs}$, which is performed by numerical integration based on Gauss quadrature in the discretized geometry. This is especially challenging at the cut elements as the elements have to be divided around the free surface plane to resolve the discontinuity. The number and type of divisions will depend on the type of elements. Therefore, it was decided to keep the implementation simple and consider only linear triangular elements for all the simulations. Figure 4 shows the different possibilities and how the elements will be divided to perform the integration. The integration is only performed on the wetted surface and therefore, in the numerical integration only the Gauss points in the shaded region are considered. It can be noted in equation 7 that the volume is calculated by integrating the projection of the distance vector along the surface normal of the wetted surface i.e. $(z - z_f) e_z \cdot n$, also shown in figure 4. Therefore, the volume is calculated by first calculating the distance vector, $(z - z_f) e_z$ for the Gauss
points based on their vertical distance from the plane. Then the weighted sum of their
projection with the unit normal vector gives the volume of the enclosed region.

Figure 3: Hydrostatic pressure applied on the discretized structure.

Figure 4: Volume calculation on the discretized structure using Gauss integration.
6 NUMERICAL EXAMPLES

6.1 Volume enclosed between a plane and hemisphere

Before performing numerical simulation of a structural problem, it is important to validate the volume-conserving solver developed in this work. To this end, let us consider a hollow hemisphere of radius $R = 1.0 \text{ m}$. The volume enclosed by a horizontal plane at vertical distance of $0.5 \text{ m} = z_{\text{ref}}$ below the center of hemisphere would be $V = \frac{2\pi}{3} = 0.6545 \text{ m}^3$. The volume-conserving solver was run with a target volume, $V_t = 0.6545 \text{ m}^3$ and $r = 2.0$ and center coinciding with the center of the hemisphere. Three different meshes were considered with element size $0.1 \text{ m}$, $0.05 \text{ m}$ and $0.025 \text{ m}$ and the results ($z_{\text{comp}}$) for the three cases are summarized in table 1. It clearly shows, that the volume-conserving solver was able to calculate the plane’s position accurately, limited by the discretization error in the surface representation.

Table 1: Results of volume-conserving solver with $V_t = 0.6545 \text{ m}^3$.

<table>
<thead>
<tr>
<th>Mesh size (m)</th>
<th>$z_{\text{comp}}$ (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>-0.4984</td>
</tr>
<tr>
<td>0.05</td>
<td>-0.4996</td>
</tr>
<tr>
<td>0.025</td>
<td>-0.4999</td>
</tr>
</tbody>
</table>

6.2 Hydrostatic load on a hemisphere

In this numerical example, we consider a flexible hemisphere of radius $R = 1.0 \text{ m}$, with thickness $t = 0.05 \text{ m}$, fixed at the top edge. The hemisphere is discretized using linear triangular shell elements with the material properties Young’s modulus $E = 10^4 \text{ Pa}$ and Poisson’s ratio $\nu = 0.3$. A fluid of specific weight $\gamma = 200 \text{ N m}^{-3}$ is gradually filled inside the structure until the fluid volume reaches $V = 1.5 \text{ m}^3$. The simulations are performed using implicit partitioned coupling between the structural solver in KRATOS and the implemented volume-conserving solver. Three different meshes with element size $0.1 \text{ m}$, $0.05 \text{ m}$ and $0.025 \text{ m}$ were considered to study the effect of discretization on the result. Inside the coupling iterations, Aitken relaxation is used as a convergence accelerator for all the simulations. As a quantity for comparison, the vertical displacement of point A ($u_z$) shown in figure 5 is determined for all the meshes. Figure 6 shows the variation of the vertical displacement of point A with the volume of fluid. This data is also presented in table 2 for $V = 1.5 \text{ m}^3$, where we can observe that the difference in the vertical displacements between the meshes decreases as the mesh becomes finer. The table also contains the total vertical reaction force at the fixed top edge. If the loading condition is correct, then this value should be equal to the total weight of the fluid ($W = \gamma V$). From table 2, we can observe that it is indeed the case with small errors. One interesting result
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is that this value approaches the weight of the fluid as the mesh is more refined. This behaviour indicates that the deviation in the reaction force is due the error in the volume calculation and hydrostatic load application on nodes (in section 5) which are directly related to the discretization of the structure. As an example of results, a deformed geometry for mesh with element size 0.05 m and \( V_t = 1.5 \, m^3 \) is shown in figure 7a and 7b, where the distance and displacement field are plotted, respectively. The distance value in the color legend is scaled to positive and negative values very close to zero, to show the wetted region of the structure.

![Figure 5: Problem set up for the hydrostatic load on a hemisphere.](image)

![Figure 6: Vertical displacement vs volume of the fluid for three different meshes](image)
Table 2: Comparison of \((u_z)\) and total reaction force \((F_z)\) for different meshes with \(V = 1.5\ m^3\)

<table>
<thead>
<tr>
<th>Mesh size (m)</th>
<th>(u_z) (m)</th>
<th>(F_z) (N)</th>
<th>(W) (N)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>-0.228121</td>
<td>300.163</td>
<td>300</td>
</tr>
<tr>
<td>0.05</td>
<td>-0.229833</td>
<td>300.050</td>
<td>300</td>
</tr>
<tr>
<td>0.025</td>
<td>-0.23017</td>
<td>300.014</td>
<td>300</td>
</tr>
</tbody>
</table>

Figure 7: Distance and displacement results for mesh with element size 0.05 m and \(V_t = 1.5\ m^3\).

7 CONCLUSIONS AND OUTLOOK

The main objective of this work was to develop an algorithm for calculating the static deformation of a structure under the hydrostatic load from a fixed volume of fluid. The partition approach was chosen to have code modularity and reusability with many structural codes. Consequently, a volume conserving-solver was developed which was coupled to a structural solver to achieve the goal. This procedure will be used in the future to find the shape of the membrane due to ponding. Further, the obtained shape will serve as a starting point for performing FSI simulations with membrane, ponding water and wind loads.
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REFERENCES


A PARAMETRIC TRANSFER FUNCTION FOR REAL-TIME SIMULATION OF COUPLED COMPLEX PROBLEMS

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Abstract. Industrial production lines often involve multistage manufacturing processes with coupled boundary conditions. The output of a process is the input of another processing stage. The end product of such production line is complicated to optimize since its simulation includes countless number of parameters and degrees of freedom. Therefore, incorporating all the end product parameters as extra coordinates of the problem is still an intractable approach, despite the recent advances in computation power and model order reduction techniques.

In this work, we explore an alternative approach using a physically based mechanical transfer function method, which expresses all the physics of the problem in a single function. All part external effects, including boundary conditions for example, become an input of such function. The output result of the proposed function is a real-time simulation of the consider product, for any possible input set of parameters.
1 INTRODUCTION

Numerical simulation is gaining its place at a fast pace in the industrial field [6]. The aim of accurate and optimized manufacturing processes is pushing the manufacturer to adopt the numerical simulation as an uncircumventable numerical tool in their design applications. However, multiple industrial production lines involve multistage manufacturing processes with coupled boundary conditions. The output of a process is the input of another one. Such simulations are still intractable with the current simulation techniques, even with the current progress in computing power. In fact, the solution of a second process in a production line may live in an extremely large dimensionality space, since the first process output value at each node can be considered as an extra parameter of the problem.

Model order reduction techniques are an appealing solution in this situation, since the problem’s number of degrees of freedom scales linearly with respect to the problem dimensionality [5, 11, 2]. The model order reduction techniques were successfully used in different multidimensional problems [7, 8, 4]. However, even with the current model reduction techniques of high dimensionality space, the aforementioned problems with coupled boundary conditions are still intractable. In fact, the dimensionality of the problems explode rapidly, and the model order reduction techniques face « saturation » and thus converge slowly or fail. For example, a multistage metal forming process should consider the residual stresses at each point when coming out of stage $i$, as an extra coordinate of the deformation problem faced at stage $i+1$, to cover all the possible deformations after stage $i+1$. Such approach is prohibitive and involves countless dimensions of the problem. Previous works tried to circumvent this problem by considering the relevant coordinates in a subspace with implicit coordinate system [9, 10]. However, the implicit coordinate system is not trivial to construct and may not exist for every situation. Moreover, identifying these coordinates requires a deep knowledge of the process at hand. Other attempts where do to parametrize the output of process $i$ using the input parameters of the same process $i$ [1].

In this work, we aim at circumventing the complexity of the problem and the dimensionality explosion, by creating a transfer function approach for each manufacturing stage. The transfer function approach shall model the physics inside the material, however all external effects like the loads, boundary conditions... will become an input to the transfer functions. Classical works on transfer functions use the Laplace transformation to find the solution of differential problems for relatively simple cases [3]. In this work, we create a transfer function approach based on the discretized problem stiffness and/or mass matrix, that results in real-time simulation of the depicted problem.
2 Transfer function approach for fixed boundary conditions

In this section, for sake of simplicity, we consider the illustrative example of a 1D steady-state heat transfer problem:

\[-k \frac{\partial^2 T}{\partial x^2} = F\] (1)

where \(k\) the thermal conductivity and \(T\) is the temperature field in a domain \(x \in [0; L]\). The discretized form of the problem is obtained such as:

\[kA\mathbf{T} = \mathbf{B}\] (2)

Where \(A\) is the discretized matrix of the Laplacian illustrated in equation (1), \(\mathbf{T}\) the vector of discretized temperature field values and \(\mathbf{B}\) the vector of the discretized second hand side of the equation. Classical model reduction approaches tend to solve the differential equation of the problem using the parameters of the problem as extra coordinates, for instance if \(F\) is a polynomial function of degree 2

\[F = a + bx + cx^2\] (3)

each coefficient of the polynomial terms \(a, b\) and \(c\) becomes an extra coordinate of the problem. Considering the conductivity as extra coordinate, one have to solve a 5D problem, inside chosen intervals for each parameter, such as:

\[T = f(x, a, b, c, k)\] (4)

Now Considering the following boundary conditions:

\[
\begin{cases}
T(0) = 0 \\
T(L) = 0
\end{cases}
\] (5)

One can find \(R\), the reduced matrix form of \(A\). Using \(R\), One can write:

\[\mathbf{T} = \frac{1}{k} \cdot R^{-1} \cdot \mathbf{B}_r\] (6)

where \(\mathbf{B}_r\) is the reduced form of the second hand size of the discretized problem form \(B\). Since all the parameters appears explicitly in equation (6), it can be used in real time to solve the problem for any chosen value of the parameters \(k, a, b\) or \(c\). This approach does not require a parameter intervals predefinition for \(k, a, b\) and \(c\). Thus, the solution can be literally found in real-time for any value of the chosen parameters. Moreover, the physical properties of the problem are now incorporated into \(R^{-1}\), while all the external effects are fixed on the fly.
Figure 1: Figure illustrating a Matlab GUI slider showing the results of equation (1) in real time for any variation of the input parameters

Figure 2: Figure comparing the classical finite difference solution to the illustrated transfer function approach solution
Figure 1 illustrates a Matlab GUI plugin which uses sliders to change the values of the input parameters and illustrates in real time the solution of the problem. Figure 2 compares the solution of the problem illustrated by the given approach, with the finite differences classical solution.

The disadvantage of this approach is the impossibility of inverting the stiffness matrix $A$ without prescribing the boundary conditions. Boundary conditions are external parameters and one may wish to list them as an input to the transfer function. In such case, no reduced matrix $R$ can be computed and the matrix $A$, being singular, can’t be inversed. Thus, a different approach shall be considered.

3 Transfer function approach with Dirichelet boundary conditions as function input

In this section we illustrate a novel approach to solve the problem while considering the Dirichlet boundary conditions as extra coordinates of the problem. We consider the heat transfer problem depicted in equation (1), with the prescribed Dirichelet boundary conditions:

$$\begin{cases} T(0) = T_0 \\ T(L) = T_L \end{cases}$$

(7)

For sake of simplicity, we consider the conductivity $k = 1$ in the following example. The depicted boundary conditions are extra coordinates of the problem and thus shall not be prescribed to the problem before inverting the matrix. The original discretized system is written as:

$$A \cdot \begin{pmatrix} T_0 \\ T_1 \\ \vdots \\ T_L \end{pmatrix} = B + \begin{pmatrix} -f_0 \\ 0 \\ \vdots \\ f_L \end{pmatrix}$$

(8)

where $f_0$ and $f_L$ are the prescribed heat flux on each of the two sides on the domain, $x = 0$ and $x = L$ respectively. $f_0$ and $f_L$ are unknowns « a priori » and can be found as a post-processing of the discrete problem. However, $f_0$ and $f_L$ should satisfy the first and last equation of the linear system:

$$\begin{cases} \sum_{i=1}^{N} A_{1i} T_i = B_1 - f_0 \\ \sum_{i=1}^{N} A_{Ni} T_i = B_N + f_L \end{cases}$$

(9)

$N$ being the number of nodes in the domain. To define the solution of the problem, we define the matrix $M$ as the pseudo-inverse of the matrix $A$. Then we define the preliminary solution of the problem $P$ by:

$$P = M \cdot (B + f)$$

(10)
where:

\[
\mathbf{f} = \begin{pmatrix}
-f_0 \\
0 \\
\vdots \\
f_L
\end{pmatrix}
\] (11)

Starting with a first random guess for \(f_0\) and \(f_L\), and defining the solution of the problem \(T\) as:

\[
T = \mathbf{P} + d_1 \cdot x + d_2
\] (12)

where \(d_1\) and \(d_2\) two constants defining the potential linear transformation of the preliminary solution. We may define now a system of 4 equations with 4 unknowns:

\[
\begin{aligned}
\sum_{i=1}^{N} \mathbf{A}_{ii} T_i &= \mathbf{B}_1 - f_0 \\
\sum_{i=1}^{N} \mathbf{A}_{ii} T_i &= \mathbf{B}_N + f_L \\
\mathbf{P}_1 + d_1 \cdot 0 + d_2 &= T_0 \\
\mathbf{P}_2 + d_1 \cdot L + d_2 &= T_L
\end{aligned}
\] (13)

where the unknowns are \(d_1\), \(d_2\), \(f_0\) and \(f_L\). Since discretized problems are linear in general, the system depicted in equation (13) is solved with only one iteration using Newton’s algorithm. The solution is obtained almost instantly, for any prescribed boundary condition.

Figure 3 illustrates the solution for a system with \(T_0 = 1\) and \(T_L = 10\), with a constant heat generation term \(F = 100\) in all the domain. The solution is compared to the finite difference one, the relative error does not exceed 1.26%. The solution is obtained within 31.7\(ms\) on a portable PC and the system depicted in equation (13) was solved with only one Newton’s algorithm iteration.

To solve the illustrated problem online, in real-time, only the matrices \(\mathbf{A}\) and its pseudo-inverse \(\mathbf{M}\) should be stored on the simulation platform. All the other parameters, being external to the intrinsic properties of the material, can be considered as an input to the illustrated transfer functions method.

4 Conclusion

In this work we proved the possibility of using a transfer function approach to simulate in real time a problem where coupled boundary conditions are present, or when the boundary conditions of a problem are the result of another one’s solution.
Figure 3: An example illustrating the boundary conditions as extra parameters of the problem, using the transfer function approach, and comparing the obtained solution to classical finite differences.

The presented method uses the pseudo-inverse of the discretized stiffness matrix of the problem to derive the solution of the problem. The method starts with the identification of the heat flux prescribed on the Dirichelet boundary conditions, as well as the linear solution contribution with respect to a preliminary one, obtained directly from the pseudo-inverse matrix. The illustrated method offers the possibility to solve in real-time any problem whose inputs are coupled to another one’s output, or when the inputs are unknown « a priori ». The described method has an advantage over classical model reduction formulations, especially when the number of degrees of freedom increases dramatically.

RÉFÉRENCES


Brittle Cylinder Transfer by a Three-finger Grasp

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ABSTRACT

We consider the problem of the brittle cylinder grasping by the n fingers of the robot-manipulator [1]. Each finger contacts the cylinder in a single supporting point with Amontons-Coulomb or for two footholds spinning friction. Using numerical simulations and analytically, possible locations of contact points on the cylinder, for which there is a kinetostatics problem solution when the cylinder is moved by three fingers, are received.

1 A cylinder grasping problem

In this paper, we consider the problem of curved object grasping by the fingers of the robot-manipulator. For example we discussed a three legged humanoid robot with pair of five arms fingers or a monkey-robot with twenty arms and legs fingers. The robot can hold the object by one and grasp by two or three fingers. An object grasping problem is equivalent to the problem of the walking robot with n legs. Consider a grasp with m fingers. Each finger contacts an object in one foothold.

There is an analogy of this problem to the problem of walking robot dynamics on one-side constraint. While the general walking robot motion on a plane was analyzed in detail in Ref. [1] the case of the dynamics on a curved surface is far more complicated. Model dynamics and control problems was considered in [2]. Equilibrium conditions for a solid on a rough plane was considered in [3]. Walking robot parameters optimization for the motion in tubes was considered in [4], [5]. The special case of a robot with eight legs whose up porting points are restricted to the inner surface of a tube was considered in [6], [7]. In the present work, we consider the more general case of a robot with three arbitrary supporting points on a rough cylinder and on a curved surface.

Let the point O is an origin fixed in absolute space. Suppose that robot arms fingers accomplish the desired motion with respect to the body of the robot. Using general dynamics theorems to describe the cylinder motion, we obtain six different equations for the cylinder dynamics from the momentum and angular momentum theorems [8], [9]. Among them there are three equations of the body translation with point A and another three describe body rotation about point A. For prescribed motion be realized then reaction in m footholds should satisfy following kinetostatic equations [10], [11]:

\[ \sum_{i=1}^{m} \tilde{R}_i = -\tilde{\Phi}, \quad \sum_{i=1}^{m} \tilde{r}_i \times \tilde{R}_i = -\tilde{M}, \]

where \( \tilde{R}_i \) is reaction component, \( \tilde{r}_i \) corresponds to the i-th finger supporting point vector, \( \tilde{\Phi} \) is the sum of the external active forces plus time derivative of desired momentum, and \( \tilde{M} \) is the sum of external active forces momentum and time derivative of desired angular momentum with respect to the point O. In two vector equations in (1), the former corresponds to the momentum of the object (and is equivalent to three scalar equations when projected onto the basis vectors), while the latter defines the desired change of the angular momentum.
Assuming that $\Phi$ is orthogonal to $\dot{M}$, we obtain [12] that the system $\{\Phi, \dot{M}\}$ can be also used at the point $C$

$$\vec{r}_C \times \Phi = \dot{M}, \quad \vec{r}_C = -\frac{\dot{M} \times \Phi}{\Phi^2}, \quad \Phi = |\Phi|,$$

where $\vec{r}_C$ is the vector $OC$, and $C$ corresponds to the point at which the resultant of the reactions is acting.

Further problem of reactions distribution $\dot{R}_i$ in some fixed point of time is investigated by the proposal that force $\Phi$ is acting at the point $\vec{r}_C$ and force moment there is zero. Motion equations (1) for finding reactions of fingers prescribed motion can be transformed [13]:

$$\sum_{i=1}^{m} \dot{R}_i = \Phi, \quad \sum_{i=1}^{m} \vec{r}_C \times \dot{R}_i = \vec{r}_C \times \Phi. \quad (2)$$

For example point $C$ can be the grasping object center of mass.

Assuming that the robot footholds are on the surface of a rough cylinder of radius $\rho$ with a friction coefficient $k$, we introduce the coordinate system $Oxyz$ such that the axis $Ox$ is directed along the cylinder axis (so that the projection of $\Phi$ on the axis $Ox$ is negative – see Fig. 1.), the axis $Oz$ is parallel to the vector $\Phi$, and the angle between the cylinder axis and the vector $\Phi$ is $\alpha$.

![Figure 1: Cylinder.](image)

The problem of finding the reaction forces (2) is similar to the foothold reactions distribution problem for walking robot, when the footholds are on the external surface of a rough inclined cylinder where the axis has an angle $\alpha$ with respect to the vector $\Phi$. It has been considered in the problem of searching of the reactions components along the cylinder axis when $\alpha = 0$.

In the coordinates $Oxyz$ we define $\dot{R}_i = (\ddot{R}_i^x, \ddot{R}_i^y, \ddot{R}_i^z)$, $\vec{r}_C = (\bar{x}_C, \bar{y}_C, \bar{z}_C)$, and $\ddot{R}_i = (-\dot{\Phi} \sin \alpha, 0, -\dot{\Phi} \cos \alpha)$, $i = 1, \cdots, m$. In case of a one-sided surface, and the grasp inside the cylinder, we have additional restrictions on normal reactions $\dddot{N}_i$ [14]:

$$\dddot{N}_i = \dddot{R}_i \cdot \vec{e}_\nu^{i} \geq 0, \quad (3)$$

where $\vec{e}_\nu^{i}$ is an external normal to $i$-th supporting point on the cylinder, while the tangential components are given by $\dddot{F}_i = \dddot{R}_i - \dddot{N}_i \vec{e}_\nu^{i}$.

For brittle cylinder we have to take into account the following inequalities:

$$|\dddot{N}_i| \leq a.$$

When $|\dddot{N}_i| \geq a$, the cylinder is braking.

For the reactions to be in the friction cones (2), we have following inequalities:

$$|\dddot{F}_i| \leq k \dddot{N}_i, \quad (4)$$

i.e. the tangential reactions $\dddot{F}_i$ are restricted by Coulomb limiting friction value. When $\dddot{F}_i$ exceeds this limiting value, the robot legs and arms begin to slide along a surface.
The reaction distribution problem then reduces to the solution of equations (2), and inequalities (3), (4), for reactions limited to the friction cones. The restricted motion can only be realized if the solution of Eqs. (2)-(4) does exist.

The same inequalities are for walking robot on the cylinder [11]. If the grasp is out the cylinder this inequalities (3) have opposite sign.

For example if \( m \) is even. And one of each par of the supporting points is on and another is in the thin surface such that we consider them like one geometrical point. Then we need only inequalities (4).

For \( r_i = \tilde{r}_i/\rho = (x_i, y_i, z_i) \), in the cylinder coordinate:

\[
\begin{align*}
\tilde{r}_i &= (x_i, -\sin \varphi_i, \cos \varphi_i), \\
e_i^x &= (0, -\sin \varphi_i, \cos \varphi_i), \\
N_i &= \tilde{N}_i/\tilde{\Phi} = (0, -N_i \sin \varphi_i, N_i \cos \varphi_i),
\end{align*}
\]

where \( \varphi_i \) is the angles between axis \( Oz \) and cylinder normal \( e_i^x \). We define \( e_x \) as the unitary vector in the \( Ox \) axis, while \( e_i^x = (0, \cos \varphi_i, \sin \varphi_i) \) as the tangential to the cylinder. Then the tangential reaction: \( F_i = (F_i^x, F_i^{yz} \cos \varphi_i, F_i^{y\varphi} \sin \varphi_i) \), where \( F_i^x = F_i \cdot e_x, \ F_i^{y\varphi} = F_i \cdot e_i^x, \ R_i = \tilde{R}_i/\tilde{\Phi} = (R_i^x, R_i^y, R_i^z) \), \( r_C = \tilde{r}_C/\rho = (x_C, y_C, z_C) \).

Projecting onto \( Oxyz \) the first and the second vector equations (2) we obtain

\[
\begin{align*}
\sum_{i=1}^{m} F_i^x &= \sin \alpha, \\
\sum_{i=1}^{m} (N_i \sin \varphi_i - F_i^{y\varphi} \cos \varphi_i) &= 0, \\
\sum_{i=1}^{m} (N_i \cos \varphi_i + F_i^{y\varphi} \sin \varphi_i) &= \cos \alpha, \\
\sum_{i=1}^{m} -y_C \cos \alpha, \\
\sum_{i=1}^{m} (x_i N_i \sin \varphi_i + x_i F_i^{y\varphi} \sin \varphi_i - F_i^{y\varphi} \cos \varphi_i) &= x_C \cos \alpha - z_C \sin \alpha, \\
\sum_{i=1}^{m} (x_i N_i \sin \varphi_i - x_i F_i^{y\varphi} \cos \varphi_i - F_i^{y\varphi} \sin \varphi_i) &= y_C \sin \alpha.
\end{align*}
\]

Let \( p = R_1^x - R_2^x \). We further define the coordinate differences, and the supporting points difference of angles of axis \( Oz \) are \( \Delta x = x_2 - x_1, \ \Delta y = y_2 - y_1, \ \Delta z = z_2 - z_1, \ \Delta \varphi = \varphi_2 - \varphi_1 \), and \( s_{21} = \sin \varphi_2 - \sin \varphi_1, \ c_{21} = \cos \varphi_2 - \cos \varphi_1 \). We then project system (2) onto the axes \( Oxyz \).

For arbitrary surface we find that the second equation of (2) (corresponding to the moment) has the skew-symmetric matrix with respect to the component \( R_i^x \) [11]. These are 2 independent equation, while the third equation corresponds to the restriction of the point \( C \) to the plane containing the two footholds. As a result, the system (2) yields 5 independent equation and a restriction.

In this parer, the general equilibrium conditions for an apparatus and its grasp with support on the surface of a smooth or rough cylinder and on two planes are discussed. Concepts of an isolated equilibrium position and an equilibrium position forming a connected set are introduced. These concepts reflect the possibility of a shift of the center of gravity along the cylinder axis without a disturbance of static stability. In [8] was no constraints on the maximum feasible magnitude of the reactions.

### 2 A Two-finger Grasp

During the robot motion one, two and three supporting points phases are changed. For example, australian lizards - yellow-bellied three-toed skinks (saiphos equalis). First, we consider the one-supporting phase of the grasp. Let \( m = 1 \), then the motion existing condition is reaction is equal to force \( \Phi \) and supporting point and the point \( C \) are on the line along \( \Phi \), while the angle between \( \Phi \) and normal do not exceed the friction angle.

If the grasp inside the surface then point \( C \) is under the surface. In opposite case the grasp is under the surface. Then point \( C \) is inside the surface. Or if one finger out the cylinder, the
center mass of an object is up the finger. And the angle between the weight and the normal not exceed friction angle.

If \( m \) is even. And one of each par of the supporting points is on and another is in the thin surface such that we consider them like one geometrical point. Then it does not matter where the point \( C \) is on the line.

Let \( n = 2 \), and \( x_1 \neq x_2 \). Then 

\[
F^x_1 = \frac{\sin \alpha + p}{2}, \quad F^x_2 = \frac{\sin \alpha - p}{2},
\]

\[
N_1 = \frac{-p \sin^2 \frac{\Delta x}{2} + (x_2 - x_C) \cos \varphi_1 \cos \alpha}{\Delta x} + N_1^\alpha,
\]

\[
N_2 = \frac{-p \sin^2 \frac{\Delta \varphi}{2} + (x_2 - x_1) \cos \varphi_2 \cos \alpha}{\Delta x} + N_2^\alpha,
\]

\[
F^{yz}_1 = \frac{-p \sin \Delta \varphi + 2(x_2 - x_C) \sin \varphi_1 \cos \alpha}{2\Delta x} + F_1^{(yz)\alpha},
\]

\[
F^{yz}_2 = \frac{p \sin \Delta \varphi + 2(x_C - x_1) \sin \varphi_2 \cos \alpha}{2\Delta x} + F_2^{(yz)\alpha},
\]

\[
\tan \alpha = \frac{\Delta x (\sin \varphi_2 + y_C) + (x_2 - x_C) s_{21}}{y_C c_{21} + z_C s_{21} - \sin \Delta \varphi},
\]

where \( N_i^\alpha \) and \( F_i^{yz} \) are the functions of \( x_i, \varphi_i, y_C \) and \( z_C \).

The conditions (4) can be displayed in the form

\[
E p^2 + B_1 p + C_1 \leq 0, \quad E p^2 + B_2 p + C_2 \leq 0,
\]

(7)

where

\[
E = (\Delta x)^2 + \sin^2 \Delta \varphi - 4 k^2 \sin^4 \left( \frac{\Delta \varphi}{2} \right),
\]

\( B_i, C_i \) are the functions of \( x_i, \varphi_i, x_C, y_C \) and \( z_C \).

The boundaries between different regimes can be determined analytically. For example, in the case of \( E < 0 \), the solution exists, and can be obtained analytically [11], as shown in Fig. 2, on the left. Note that in this case it’s limited to the range \( \Delta x \leq 2k\rho \). In contract to this behavior, for \( E \geq 0 \) there is no such restriction and an additional step is required to address the question of the existence of the solution. At the point \((0, 0)\) we find \( E = 0 \), which means that two footholds are orthogonal to the cylinder axis. Here, two possible solution are either identical, or limited to a single diameter. In the latter case, point \( C \) and the reaction have to be in one plane, parallel to force \( \Phi \), and the problem has a solution.

Figure 2: The analytical and the numerical parameter diagrams.
For the desired legs or fingers configurations and given point $C$, the problem can be solved numerically. In Fig. 2, on the right, we present the numerical solution for the example when $x_2 = -x_1 = \rho = k = 1$. Note that in this case $E > 0$.

![Figure 2](image2.png)

**Figure 2:** For $\alpha = \pi/4$; $x_2 = -x_1$, $\varphi_2 = -\varphi_1$.

Specifically, the condition (7) was analyzed in two cases, when $E = 0$ and $E > 0$, and when the solution of the problem does exist, the solutions were shown in the plot.

For $E > 0$, we need to consider two conditions. First is the restriction on the determinants $D \geq 0$, while the second is the requirement of a non-empty intersection of the set of point of the intervals between the roots of quadratic equations. From this plot we see that, if two points are on one diameter, then the solution of the reaction distribution problem exists. The two lines in the plot, correspond to $\varphi_1 = \varphi_2 + \pi$ or $\varphi_1 = \varphi_2 - \pi$. The rhombus form represents the requirement on the determinants $D_i \geq 0$, while additional conditions further restrict the range [13].

In Fig. 3 we present the results for $E > 0$ and $E \leq 0$, when $x_2 = -x_1$, $\varphi_2 = -\varphi_1$ and shows the case of $\alpha = \pi/4$. The figures for $\alpha = 0$ and increased to $\pi/2$ are shown in [?]. Note that when $\alpha = \pi/2$, the solutions exists only for diametrical footholds.

For two-finger robot when $E$ is negative, the solution exists, and obtained analytically [14]. Using numerical simulations we explain the reaction distribution problem existing and build this problem solution existing fields for given footholds and point $C$ position [15]. For example, for two-foothold phase, we consider symmetric, about point $C$, along and orthogonal cylinder axis, robot configurations [16]. For first of these configurations examined cases with nonnegative $E$ coefficient, for distances between point $C$ and footholds [17]. Reactions distribution problem solution existing fields constructed on the two angles plane, correspond to footholds projections on the cylinder base and three dimensional fields which supplement this plane by point $C$ $z$-coordinate altitude [18]. When $x$ equals to 1, 1 for $\alpha$ equals $\pi/3$ in three-dimensional fields observed bundles of separate points, Fig. 4. That means that the point $C$ altitude position more harsh change while changing the angles.

![Figure 3](image3.png)

**Figure 3:** For $\alpha = \pi/4$; $x_2 = -x_1$, $\varphi_2 = -\varphi_1$.

![Figure 4](image4.png)

**Figure 4:** Admissible area for $\alpha = \pi/3$; $\Delta x = 1, 1$. 

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3 A Three-finger Grasp

There is an analogy of supporting on a cylinder and on one or two planes. The same is about holding a cylinder. Let speak about static stability of walking apparatus with support on two unilateral planes. For example a smooth planes in homogeneous gravity field.

We consider the problem of support of an apparatus on two smooth planes in homogeneous gravity field separately for parallel and intersecting planes.

The static-stability conditions for a three-legged walking apparatus with supporting points at the interior surface of a smooth horizontal cylinder and on two smooth planes was studied in [8]. For the cylinder, consequences of equilibrium conditions are considered in the assumption that reaction at the supporting points are directed along the radius of the cylinder. Let speak about a problem of apparatus support on initial surfaces of two smooth parallel planes. Clearly, a necessary condition for equilibrium of the apparatus in support on such parallel planes is a condition of their horizontal.

Problem of static stability of walking robot with support on two smooth unilateral planes in homogeneous gravity field was observed by us in [8]. We consider the problem of support of a robot on two smooth planes in homogeneous gravity field separately for parallel and intersecting planes.

![Figure 5: Two planes.](image)

Assume that supporting points of the apparatus (in all, there are \( n \) points of this kind) with the numbers \( i = 1, \ldots, k \) and \( j = k + 1, \ldots, n \) are located on upper and lower planes, respectively, Fig. 5. Now with a center of gravity of apparatus \( C \) we link the right-handed Cartesian coordinate system \( Cxyz \) such that the axis \( Cz \) is directed upward and the plane \( Cxy \) is horizontal. Equilibrium equations in projections on the axes \( Cxy \) take the form

\[
\sum_{i=1}^{k} x_i N_i + \sum_{j=k+1}^{n} x_j N_j = 0, \quad \sum_{i=1}^{k} y_i N_i + \sum_{j=k+1}^{n} y_j N_j = 0, \quad \sum_{i=1}^{k} N_i + \sum_{j=k+1}^{n} N_j = P,
\]

were \( P \) – is the weight.

Let us introduce the notation:

\[
N^l = \sum_{i=1}^{k} N_i, \quad N^u = \sum_{j=k+1}^{n} N_j.
\]

Consider solutions of equilibrium equations, for which \( N^l \neq 0 \) and \( N^u \neq 0 \). Then, there exist the vector

\[
R^l = \frac{1}{N^l} \sum_{i=1}^{k} r_i N_i, \quad R^u = \frac{1}{N^u} \sum_{j=k+1}^{n} r_i N_j.
\]
Statement 1. That center of reactions and center of gravity of apparatus belong to the same vertical plane is a necessary condition for a nonzero solution of the equilibrium equations.

We consider the problem of robot support on initial surfaces of two smooth parallel planes. Clearly, a necessary condition for equilibrium of the robot in support on such parallel planes is a condition of their horizontal. The rough planes can be not horizontal. We need the less two fingered grasp to hold two parallel planes.

Statement 2. Suppose that \( N_l^i > 0 \) and \( N_u^i > 0 \). The equilibrium conditions have the solution \( N_i > 0, i = 1, \ldots, n \), if and only if there exists a vertical plane (involving the center of gravity) that intersects simultaneously convex hulls of upper and lower supporting polygons; therewith, for \( R_u^i > R_l^i \) it must be \( R_l^i \geq 0 \) and for \( R_u^i = R_l^i \) it must be \( R_l^i = 0 \), were \( R_u^i, R_l^i \) the projections \( R^l \) and \( R^i \) on the plane \( Oxy \).

Problem of conditions for static stability in support on two non coincident intersecting smooth planes was observed by us in [8].

The motion of the walking robot between two horizontal supporting planes has additional possibilities for the distribution of reactions in comparison with the motion on one supporting plane for the cases where a projection of the center of mass of the robot is beyond the supporting polygon. The proposed method of distributions of reactions allows one to estimate the limitations of these possibilities and to use them profitably.

Oscillations of the walking apparatus around the axis of the smooth support cylinder was observed by us in [9].

Let consider equilibrium of a robot that has support with no more than three legs, in cylinder. Or a grasp fingers, which are out of the cylinder. The case: \( m = 3 \). For convenience, we enumerate the supporting points in increasing order of angles \( \varphi_i, i = 1, \ldots, m \). We ignore the configurations, for which there exist coinciding supporting points, along with solutions, for which at least one equality \( N_i = 0 \) holds.

When we speak about \( n = m = 3 \), like in [8], we use \( \varphi_i \) as the angle (2\( \pi \) in magnitude) between the negative direction of the axis \( Oz \) and vector \(-e'_\varphi \).

First, let us study a solution for system (2), assuming that a cylinder provides a bilateral constraint. We present the criterion of a robot equilibrium without constraints on supporting points locations and a geometric criterion of equilibrium for a robot with supporting points below the plane \( Oxy \), assuming that the cylinder is a unilateral constraint. For a grasp, out the cylinder, the same. For a grasp, out of the cylinder, supporting points has to be under the plane.

![Figure 6: Admissible area for m = 3.](image)

For horizontal smooth cylinder, let us consider a subsystem that consists of the second, fourth and fifth equations of system (5) as well as a subsystem that involves the third, second and fifth ones. In the subsequent discussion, we call the first subsystem a homogeneous subsystem and
the second one a inhomogeneous subsystem.

Denote by $\Delta_h$ and $\Delta_{ih}$ the determinants of homogeneous and inhomogeneous subsystems, respectively. Expression for the determinants, as well as the general solution of system (5) for $m = 3$, are given in [7].

**Statement 1.** A necessary condition for the static stability of a walking robot on a smooth cylindrical surface is the center of gravity belongs to the vertical longitudinal plane of the cylinder symmetry.

For the grasp it is about the center of mass of the transferred cylinder.

**Corollary 1.** Statement 1 becomes a sufficient equilibrium condition if all supporting points are located on one vertical plane that is normal to the axis of the cylinder and contains the center of gravity, but for the given configuration the conditions of the first two items of Statement 1 [8], are not fulfilled.

**Corollary 2.** Assume that all supporting points are located on one vertical plane that is normal to the axis of the cylinder and contains the center of gravity of the apparatus. Then, a necessary and sufficient condition for static stability of the considered configuration is the availability of one or two supporting points that provide equilibrium if we suppose that reactions at the other supporting points are equal to zero.

Let us introduce the new system of coordinates $Ox'y'z'$, rotated by the angle of $\varphi^*$ about the axis $Oy$ with respect to the system $Oxyz$.

**Statement 2.** If there exists a plane $Ox'y'$ such that orthogonal projections of the supporting points on this plane are located only in two alternate quadrants (except the boundaries) then a corresponding configuration is not an equilibrium position.

**Statement 3.** If there exists a plane $Ox'y'$ such that all supporting points are located on one side of this plane and orthogonal projections of the supporting points on this plane are located only on one side of the straight line $Ox'$, except for the boundary, then a corresponding configuration is not an equilibrium.

**Statement 4.** Assume that all supporting points are located below the plane $Oxy$. Then, static stability of the apparatus is disturbed if vertical projections of all supporting points on the plane $Oxy$ belong to one of the quadrants including its boundaries formed by the axes of the coordinates, with the deleted point $O$.

**Statement 5.** Assume that all supporting points are located below the plane $Oxy$. In this case, if one can select a straight line $l$ parallel to the axis $Ox$ such that with respect to the projection of the straight line $l$ to the plane $Oxy$ and the axis $Oy$, the vertical projections of all supporting points are located only in two alternate quadrants, then the corresponding configuration is not an equilibrium (Fig. 7).

![Figure 7: Selection of the line l.](image-url)
Statement 6. Assume that \( x_1 \neq x_2; \varphi_1 \neq \varphi_2 + \pi k, k \in \mathbb{Z}; \varphi_i \neq \pi l, l \in \mathbb{Z}; x_i \neq 0, i = 1, 2, 3. \) Then, the equality \( \Delta_h = 0 \) is equivalent to the ratio

\[
\frac{x_3^{-1} - x_2^{-1}}{x_2^{-1} - x_1^{-1}} = \cot \varphi_3 - \cot \varphi_2 \quad \cot \varphi_2 - \cot \varphi_3.
\] (9)

Statement 7. Assume that \( x_1 \neq x_2; \varphi_1 \neq \varphi_2 + \pi k, k \in \mathbb{Z}; \)

\[
\varphi_i \neq \pi/2l_1, \quad l_1 \in \mathbb{Z}; \quad x_i \neq 0, \quad i = 1, 2, 3.
\] (10)

Then, if

\[
\varphi_1 \neq \varphi_3 + \pi l, \quad \varphi_2 \neq \varphi_3 + \pi j, \quad l, j \in \mathbb{Z},
\] (11)

the determinants \( \Delta_h \) and \( \Delta_{ih} \) cannot simultaneously be equal to zero. In the case where relations (11) do not hold, the equalities \( \Delta_h = 0 \) and \( \Delta_{ih} = 0 \) are equivalent.

Assume that \( m = 3 \) and generalized coordinates satisfy constraints (10), (11). System (5) has a unique solution if and only if \( \Delta_h = 0. \)

Corollary 3. Let \( m = 3. \) Then, with the fulfillment of constraints (10), (11), a necessary and sufficient condition that a configuration provides an equilibrium, assuming that the cylinder realized an unilateral constraint, is the equation (9) with the constraints (3).

Consider the question of the connectedness of a set of equilibriums. For example for a smooth cylinder. Examples of isolated equilibriums are presented in [7].

Statement 8. An equilibrium, for which none of the supporting points belong to the vertical plane of the smooth cylinder symmetry, is isolated.

Statement 9. Classification of equilibrium positions. In the case where \( m = 3, \) a shift center of gravity of the walking apparatus along the axis of the smooth cylinder, given fixed supporting points, is possible only for the configurations presented below as well as for those symmetric to them with respect to the plane \( Oxz \) and \( Oyz. \)

(1) Configurations for which all supporting points belong to the plane \( Oxy. \)

(a) \( \varphi_1 = \varphi_2 = \varphi_3 - \pi = 0. \) Two supporting points are located below the plane \( Oxy \) and one supporting point is located above this plane.

(a1) \( x_1 < x_2 \leq x_3; \ x_2 \geq 0. \)

(a2) \( x_1 < x_3 < x_2. \)

(b) \( \varphi_1 = \varphi_2 = \pi, \varphi_3 = 0. \) Two supporting points are located above the plane \( Oxy \) and one supporting point is below this plane.

(b1) \( x_1 < x_2 \leq x_3; \ x_3 \leq 0. \)

(b2) \( x_1 < x_3 < x_2. \)

(c) \( \varphi_1 = \varphi_2 = \varphi_3 = 0. \) The center of mass of the robot (or for a grasp, of a cylinder) must belong to a segment with ends at the projections of supporting points onto the axis of the smooth cylinder.

(1) Configurations for which one of supporting points belongs to the plane \( Oxy \) and two other point have the same coordinates (Fig. 6 on the right).

(a) \( \varphi_1 = 0, \ x_2 = x_3. \) The first supporting point is located below the plane \( Oxy. \)

(a1) \( \varphi_2 \in (3\pi/2, 2\pi), \varphi_3 \in [0, \pi/2]. \) A projection of the center of gravity of the apparatus must belong to an interval with ends at supporting point projections to the axis of the cylinder.
(a2) $\varphi_2 \in [\pi, 3\pi/2]$, $\varphi_3 \in [0, \pi/2]$, $\varphi_2 + \varphi_3 \neq \pi k$, $k \in \mathbb{Z}$. If $\varphi_2 - \varphi_3 < \pi$, then the inequality $x_1 \leq 0$ must hold, and if $\varphi_2 - \varphi_3 \geq \pi$, the projection of the center of gravity of the apparatus must belong to an interval with ends at projections of supporting point onto the axis of the cylinder.

(a3) $\varphi_2 \in (\pi, 3\pi/2)$, $\varphi_3 \in [\pi/2, \pi/2]$; $x_1 < 0$.

(b) $\varphi_1 = \pi$, $x_2 = x_3$. The first supporting point is located above the plane $Oxy$.

(b1) $\varphi_2 \in (3\pi/2, 2\pi)$, $\varphi_3 \in [0, \pi/2]$; $x_2 > 0$.

(b2) $\varphi_2 \in [\pi, 3\pi/2)$, $\varphi_3 \in [0, \pi/2]$, $\varphi_2 + \varphi_3 \neq \pi k$, $k \in \mathbb{Z}$, $\varphi_2 - \varphi_3 > \pi$; $x_2 > 0$.

Other variants of configurations, i.e., not included in this classification, may be isolated equilibrium positions only, for a smooth cylinder.

Now, we consider configurations with three supporting points located strictly below the plane $Oxy$. For these points, a geometric criterion of equilibrium of the walking apparatus is also obtained.

Statement 10. Assume that three supporting points are located below the plane $Oxy$. Let $\Delta_h = 0$ and $\Delta_{ih} \neq 0$.

(1) For $\varphi_1 = 0$, $x_2 = x_3$, $sgn x_2 = -sgn x_3$, a necessary and sufficient condition for equilibrium is that the projection of the center of gravity belong to an segment between projections of the first and second (and, along with it, also the third) supporting points to the axis of the smooth cylinder. The set of equilibrium is a connected set.

(2) Assume that $\varphi_1 \neq 0$ and $x_2 \neq x_3$. A configuration is an equilibrium if conditions of Statements 2 – 5 from [8] not fulfilled. Otherwise, a configuration is not an equilibrium. Equilibriums are isolated.

Statement 11. Assume that the apparatus has $n$ points in the support and $n \geq 3$. Then, if there exists a triple of supporting points, for which the conditions of Statement 10 are fulfilled, the considered configuration is an equilibrium.

Robot can hold the horizontal cylinder by three fingers. Let one of the points is in vertical plane containing cylinder axis and another are in the plane orthogonal to the axis. Without friction, the cylinder center of mass has to be in the vertical plane that contain the cylinder axis. The supporting points are on the external surface of the lower semi-cylinder and the center mass of the cylinder is in the footholds triangle, Fig. 6. If one of supporting points is in the lower semi-cylinder and another are on the upper, the point $C$ has to be out of the footholds triangle.

So the robot can transfer the cylinder by one, two or three fingers.

4 Conclusion

A solution of the problem of reaction distribution with respect to supporting points on the cylinder, both for walking robot and its grasp, demonstrates a great variety of cases that must be analyzed individually. Therewith, it turns out that there exist isolated equilibriums, even if support polygon does not degenerate. For example, for a smooth cylinder or surface. Such a specify principally differentiates the problem of reaction distribution on a cylinder or a surface from the problem of reaction distribution on a horizontal plane, two or some planes. For a set of equilibriums to be connected in the case of three supporting points, this provides a means for comfortable quasi stationary motion, it is necessary to select supporting points in a special way, so that one of them be located in the lower or upper element of the smooth cylinder. For rough cylinder this solution exists. If between the surface of the cylinder and legs of walking robot or it fingers, viscous friction arises, then this condition is essential, therewith, given dry friction, it is of lesser importance for algorithm of motion control.
The motion of the walking robot between two horizontal supporting planes has additional possibilities for the distributions of reactions in comparison with the motion on one supporting plane for the cases where a projection of the center of mass of the robot, or part of planes, is beyond the supporting polygon. The proposed method of distribution of reaction allows one to estimate the limitations of these possibilities and to use them profitably.

During the robot motion, one, two and three supporting point phases are changed. And for example the humanoid robot with five arm fingers can hold the object by one and grasp by two or three-fingers. The reaction distribution problem have a solution in following cases. Let we give some examples.

1. One-supporting point phase. So the motion existing condition is reaction is equal to force $\Phi$ and supporting point and the point $C$ are on the line along $\Phi$. And the angle between $\Phi$ and the normal not exceed friction angle.

1.1 If the grasp inside the surface then point $C$ is under the surface. In opposite case the grasp is under the surface. Then point $C$ is inside the surface.

1.2 If $m$ is even. And one of each par of the supporting points is on and another is in the thin surface such that we consider them like one geometrical point. Then it does not matter where the point $C$ is on the line.

2. Two-supporting point phases. In case when the grasp is inside the cylinder. The point $C$ and the reactions have to be in the plane parallel to force $\Phi$.

2.1 If supporting points are on one diameter.

2.2 When coefficient $E < 0$. And in some fields with connected set of points, when $E \geq 0$. Robot can hold the cylinder by two fingers on one diameter.

3. Robot can hold the horizontal cylinder by three fingers. Let one of the points is in vertical plane containing cylinder axis and another are in the plane orthogonal to the axis. Without friction, the cylinder center of mass has to be in the vertical plane that contain the cylinder axis. The supporting points are on the external surface of the lower semi-cylinder and the center mass of the cylinder is in the footholds triangle. If the first supporting point is in the lower semi-cylinder and two another are on the upper, the center of mass has to be out of the footholds triangle.

So the robot can transfer the cylinder by one, two or three fingers.

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**REFERENCES**


COMBINED DRY FRICTION MODELS IN THE CASE OF RANDOM DISTRIBUTION OF THE NORMAL CONTACT STRESSES INSIDE CONTACT PATCHES

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Key words: Combined Dry Friction, Random Distribution of the Normal Contact Stresses.

Abstract. We propose a further development of the theory of multi-component dry friction [5-10] by offering a dry friction model with random distribution of contact stresses across the contact spot. Special attention is devoted to investigation of the dry friction effects that arise in the traditional systems that consist of solid disks and spheres sliding or rolling on a horizontal plane. Applications of the proposed model for description of the interaction between a pneumatic aviation tire and the surface of a landing strip are outlined.

1 INTRODUCTION

The theory of poly-component dry friction has proved its efficiency in the investigation of the dynamics of solids for a variety of types of kinematic interaction between them. The theory allowed a relevant description of the overall effects that the poly-component friction can produce and also helped create physically consistent phenomenological models of friction.

Tackling real engineer problems within the framework of the theory (such as rolling of aviation pneumatic tires) revealed that the model must be further improved by taking into account the environmental and physical realities which in its turn seriously affect the value of the coefficients involved. In particular, the anisotropy of the dry friction coefficient should be taken into consideration [9, 18].

Another factor that influences the coefficients of the model is the non-homogeneity of the spot across which the bodies interact which leads to a certain randomness in the distribution of the contact stresses within the spot. This phenomenon of “randomness” shows itself not only in real-life problems [2-4, 16,17] but also in model experiments [11] aimed at verification of the theory we offer. First attempts to account for this “randomness” are due to
Burlakov and Treschev [1] where they suggested a simplified contact stress model (e.g. a rigid circle is assumed to touch the plane in a three randomly emerging supporting points). Below we present a model in which the normal contact stresses contain some randomly distributed components. Such an approach seems to be relevant for the study of an amount of classical problems such as sliding and spinning of a massive disk (cylinder) and rolling accompanied with slipping and spinning of a heavy sphere over a rough surface. In spite of its seeming simplicity this approach serves a good and convenient basis for further more sophisticated analysis.

2 PROBABILISTIC MODEL OF SLIDING FRICTION

2.1 Basic assumptions

Consider a system that consists of two rigid bodies that interact frictionally. A complicated (combined) kinematics within the contact area is assumed meaning that any combination of sliding, spinning and rolling may occur (Fig. 1). The contact spot is assumed to be of circular (or nearly circular) shape. It was shown in the previous studies [5-14] that the spot’s shape seriously influences the net force that the bodies experience and especially the occurrence of the essentially non-zero dry friction component $F_\perp$, which is orthogonal to the velocity of the relative sliding. Nevertheless, if the spot is almost a circle this component exerts but a negligible effect on the $F_\parallel$ component, which opposes the relative sliding velocity.

The dry friction models describing the interaction within a contact spot are constructed under the assumption that the Coulomb law in generalized differential form holds for a small surface element $dS$ in the interior of the contact spot. According to the law the differentials of the resultant vector $d\mathbf{F}$ and the moment of friction $dM_C$ with respect to the contact spot center are determined by the formulae:

![Figure 1: Kinematics inside the contact spot](image)
Here $f$ is the coefficient of friction, $r = (x, y)$ is the position vector of an elemental area in the interior of the contact spot with respect to its center Fig. 1, $\omega$ is the angular velocity of rotation about the center and $\sigma(x, y)$ is the distribution of the normal contact stresses.

Formulas (1) clearly manifest the following important feature: the distribution of velocities and normal contact stresses within the spot uniquely determine the corresponding distribution of forces.

Since the contact spot possesses radial symmetry, it seems reasonable to assume that the distribution of normal contact stresses $\sigma_0$ at rest also has this property.

In the next section we propose a simple analytic representation for the contact stresses distributions $\sigma_0$ assuming its radial symmetry

$$\sigma_0(x, y) \equiv \sigma_0(\sqrt{x^2 + y^2})$$

After the body is set in motion, there occur tangent stresses which “deform” the originally symmetric distribution of stresses by sort of “shifting” the whole picture in the direction of the instantaneous sliding velocity $v$ or in the direction of rolling.

This “shift of symmetry” can be modelled by introducing a factor linear in coordinates $x$ and $y$ in the following way [5,6,8,10]:

$$\sigma(x, y) = \sigma_0(x, y)(1 + k_x x/R + k_y y/R)$$

2.2 Integral dry friction models and its analytical approximations

Integrating the differentials (1) over the contact spot yields the resultant vector $F$ of the friction force and torque $M_c$:

$$dF = -f\sigma\frac{V}{|V|}dS, \quad dM_c = -f\sigma\frac{r \times V}{|V|}dS, \quad (1)$$

$$V = (v - \omega y, \omega x), \quad r = (x, y), \quad \sigma = \sigma(x, y)$$

$$F = -f\int_G \sigma(x, y)\frac{V}{|V|}dxdy, \quad M_c = -f\int_G \sigma(x, y)\frac{r \times V}{|V|}dxdy, \quad (4)$$

$G = \{(x, y): x^2 + y^2 \leq R^2\}$, $F = (F_\parallel, F_\perp)$

After normalization of the variables $x$ and $y$ by using the characteristic size equal to the radius of the contact area $R: x = \hat{x}R, y = \hat{y}R$ and introduction of the dimensionless distribution function $\hat{\sigma}(\hat{x}, \hat{y}) = \hat{\sigma}(\hat{x}, \hat{y})N/R^2$ the components (4) can be rewritten as [17]:
Here the symbol ^ is omitted for brevity.

In applications, in the case of radial symmetry of the contact area, spinning distorts the originally symmetric distribution of stresses to a considerably lesser extent than so do rolling and sliding. Therefore, it seems reasonable to assume \( k_x \ll k_y \) in (3) and thereby neglect the corresponding terms in (5).

The exact integral models (4-5) give a good description of the dry friction effects in the case of combined kinematics. However, it is inconvenient to use them straightforwardly as it implies dealing with multiple integrals in the right-hand sides of the equations of motion. Approximated analytical models [4-13, 17] can help to avoid this inconvenience:

\[
F_{\parallel} = \frac{F_0 v}{\sqrt{u^2 + au^2}}, \quad F_{\perp} = \frac{\mu k_x u}{\sqrt{u^2 + bv^2}}, \quad M_C = \frac{M_0 u}{\sqrt{u^2 + mv^2}}, \quad u \equiv \omega R
\]  

(6)

The coefficients in (6) can be found as follows [5-6, 8]:

\[
F_0 = F_{\parallel}(0,v) = 2\pi f R^2 \int_0^1 r \sigma_0(r) dr, \quad \frac{1}{\sqrt{a}} = \frac{u}{F_0} \frac{\partial F_{\parallel}(u,0)}{\partial v} = \pi f R^2 \int_0^1 \sigma_0(r) dr,
\]

\[
\frac{1}{\sqrt{b}} = \frac{v}{k_x} \frac{\partial F_{\perp}(0,v)}{\partial v} = \pi f R^3 \int_0^1 r^3 \sigma_0(r) dr
\]

(7)

\[
M_0 = M_C(u,0) = 2\pi f R^3 \int_0^1 r^2 \sigma_0(r) dr, \quad \frac{1}{\sqrt{m}} = \frac{v}{M_0} \frac{\partial M_{\parallel}(0,v)}{\partial u} = \pi f R^3 \int_0^1 r^3 \sigma_0(r) dr
\]

In what follows we inject a certain randomness into the expression of the distribution \( \sigma_0 \) and show how this affects the parameters of the model (7).

2.3 Probabilistic model of friction

Assuming the distribution of the normal stresses to contain a certain random ingredient we however suppose that when the body is at rest the graph of \( \sigma_0 \) has the form qualitatively depicted in Fig. 2. Such a distribution was obtained numerically when studying the rolling motion of an aviation pneumatic tire with radial construction [5-8, 18]. As a first approximation we use a combination of the Hertz and Galin distributions of the form:

\[
\sigma_0(r) = \left( \frac{1}{\sqrt{R^2 - r^2}} - \frac{\sqrt{R^2 - r^2}}{\varepsilon^2 - R^2} \right) \frac{3P_0 (R^2 - \varepsilon^2)}{2\pi R (4R^2 - \varepsilon^2)}.
\]

(8)

Here \( P_0 \) is the force of normal pressure or simply the body’s weight and \( \pm \varepsilon \) are the
coordinates of the points at which the distribution in Fig. 2 has minima. The variable $\xi$ is assumed to be a stochastic function of time.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure2.png}
\caption{Typical distribution of the normal contact stresses for radial aviation pneumatic tire}
\end{figure}

To obtain explicit expressions of the force and moment one has to insert the formula (8) for $\sigma_n(r)$ into (5). The integrals that ensue can be calculated analytically but the final formulas are still too bulky.

From the point of view of engineer applications it seems to be effective to use the approximate model (7) whose coefficients in terms of dimensional variables now read

\begin{equation}
F_0 = f P_0, \quad M_0 = \frac{3 f \pi R \left(5 R^2 - 4 \xi^2\right)}{16 \left(4 R^2 - 3 \xi^2\right)}, \quad \mu = \frac{M_0}{2}, \quad b = \frac{m}{4}
\end{equation}

\begin{equation}
a = \left(\frac{8 R \left(4 R^2 - 3 \xi^2\right)}{3 \pi \left(3 R^2 - 2 \xi^2\right)}\right)^2, \quad m = \left(\frac{15 \pi \left(5 R^2 - 4 \xi^2\right)}{16 R \left(6 R^2 - 5 \xi^2\right)}\right)^2
\end{equation}

The graphs of the exact (5) and approximate (6) component $F_\parallel$ and the moment $M_C$ as functions of $k = v/u$ are shown in (Fig. 3). The graph of the normal component resembles (at least qualitatively) the graph of $M_C$.

3 CONCLUSIONS

We offered a model of combined dry friction that accounts for randomness in the distribution of the normal stresses within the contact spot.

For a typical distribution of stresses for a pneumatic aviation tire with radial construction [5-8, 18] the model’s coefficients are calculated.

The graphs plotted show a good agreement between the friction force and moment components derived from the exact integral representation (5) and their analytical approximations (6).
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REFERENCES


GENERAL CASE OF MOVEMENT OF SOLID SYSTEM WITH TWO MASSIVE ECCENTRICS ON A ROUGH PLANE

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Key words: Coupled Dynamics, Solid System, Internal Movers, Dry Friction.

Abstract. The mechanism consisting of the tripod with two rotating eccentrics as internal movers is investigated. The tripod moves with dry friction on horizontal plane. Rotating massive eccentrics enable the tripod to slide and spin. In mathematical model general equations of motion are considered for sliding and spinning of the tripod.

1 INTRODUCTION

In two previous papers [1-2], a solid system with two massive eccentrics, standing on a rough surface as a tripod, was considered in two special cases: purely translational motion without rotation and purely rotational motion with one fixed support point. In this paper a general case is considered where the system can move in a plane without restriction on the type of motion.

The main result of this work is that the equations of motion for the general case of motion of a tripod with two eccentrics are obtained.

The main feature of this study is that there is an experimental stand that allows you to study the behaviour of the mechanical system in full-scale tests.

The significance of the work is that the direction of research – movement due to internal movers and systems with three points of contact with surface – is quite interesting for many researchers [3-9].

2 MECHANISM

The solid system with two massive eccentrics on a rough plane is presented on the Fig. 1. It is the mechanism that consists of mechanical and electronical parts. Mechanical parts and motors are taken from Makeblock. Microcontroller and motor driver are Arduino compatible.

3 MATHEMATICAL MODEL

For consideration of our system it is convenient to divide the system into three components interacted with each other – a tripod and two pendulums. View from above is presented on the Fig. 2. The tripod has three points of contact with horizontal surface in points $A, B, C$. Pendulum $OP$ has cylindrical hinge in point $O$ and rotates around $\xi$-axis (Fig. 2, 3). Pendulum $SQ$ has cylindrical hinge in point $S$ and rotates around $\eta$-axis (Fig. 2, 4).
Figure 1: CAD model of the mechanism and the assembled mechanism

Figure 2: Tripod with two pendulums. View from above

System of axes $\xi \eta \zeta$ is connected to the tripod and moves with it. System of axes $xyz$ is connected to the surface and does not move. Hence, $\xi \eta \zeta$ is non-inertial, $xyz$ is inertial. Cylindrical hinges $O$ and $S$ are above the surface at the heights $h$ and $H$, respectively. Lengths of pendulums $OP$ and $SQ$ are $l$ and $L$, respectively. Geometrical parameters of the tripod in horizontal plane are described by $a, b, d$.

Figure 3: Pendulum P in cylindrical hinge O. View from $\xi$-axis
The movement in horizontal plane of point $C$ of the tripod is determined by variables $x, y$. Rotation of the tripod is determined by variable $\Psi$. Rotation of pendulums $OP$ and $SQ$ is determined by $\beta$ and $\gamma$, respectively.

Now let us consider the general case of mechanism’s movement on the rough surface when the pendulums rotate and the tripod moves in plane with sliding and spinning and without jumping above the surface.

For the tripod we can write equation of forces in the inertial reference system:

$$F_x + F_y + F_z + N_A + N_B + N_C + Mg + R_O + R_S = M\ddot{R}_C,$$

where $F_A, F_B, F_C$ – friction forces in points $A, B, C$; $N_A, N_B, N_C$ – normal reactions in points $A, B, C$; $Mg$ – gravity force; $R_O$ – reaction in point $O$, where the tripod is connected with the pendulum $OP$ through a cylindrical hinge $O$; $R_S$ – reaction in point $S$, where the tripod is connected with the pendulum $SQ$ through a cylindrical hinge $S$; $C$ – center of inertia of the tripod (for simplicity); $\ddot{R}_C$ – acceleration of point $C$.

In projections on axes $\xi \eta \zeta$ equation (1) looks like:

$$F_{A\xi} + F_{B\xi} + F_{C\xi} - R_{O\xi} - R_{S\xi} = MW_{C\xi},$$
$$F_{A\eta} + F_{B\eta} + F_{C\eta} - R_{O\eta} - R_{S\eta} = MW_{C\eta},$$
$$N_A + N_B + N_C - R_{O\zeta} - R_{S\zeta} - Mg = 0.$$

Now let us write for an angular momentum of the tripod relative to its center of inertia:

$$\frac{d\vec{R}_{C_{tripod}}}{dt} = \vec{CA} \times (\vec{N}_A + \vec{F}_A) + \vec{CB} \times (\vec{N}_B + \vec{F}_B) + \vec{CO} \times \vec{R}_O + \vec{CS} \times \vec{R}_S + \vec{\mu}_O + \vec{\mu}_S,$$

where $\vec{R}_{C_{tripod}} = J\vec{\omega}_C$ – angular momentum of tripod with respect to the point $C$; $\vec{\mu}_O, \vec{\mu}_S$ – moments of reaction to the electric motors, rotating pendulums in hinges $O, S$.

For the vectors in (3) we have:

$$\vec{CA} = \begin{bmatrix} d & a & 0 \end{bmatrix}^T,$$
$$\vec{CB} = \begin{bmatrix} d & -a & 0 \end{bmatrix}^T,$$
$$\vec{CO} = \begin{bmatrix} d & 0 & \mu \end{bmatrix}^T,$$
$$\vec{CS} = \begin{bmatrix} 0 & 0 & H \end{bmatrix}^T,$$
$$\vec{\mu}_O = \begin{bmatrix} \mu_o & 0 & 0 \end{bmatrix}^T,$$
$$\vec{\mu}_S = \begin{bmatrix} 0 & \mu_s & 0 \end{bmatrix}^T.$$
After calculating vector products in (3) we get:

\[
\begin{bmatrix}
  a(N_A - N_B) + hR_{\delta y} + HR_{\delta z} + \mu_0 \\
  -d(R_{\delta y} - N_A - N_B) - hR_{\delta z} - HR_{\delta y} + \mu_1 \\
  d(F_{\delta y} + F_{\delta z} - R_{\delta y}) + a(F_{\delta z} - F_{\delta y})
\end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ J\Psi \end{bmatrix}. \tag{4}
\]

For the pendulum \( P \) in cylindrical hinge \( O \) we can write equation of forces in the non-inertial reference system:

\[
\frac{d\vec{p}_{rel}^P}{dt} = \vec{R}^{ext.} + \vec{R}^{in.1} + \vec{R}^{in.2},
\]

where \( \vec{p}_{rel}^P \) – momentum of pendulum \( P \) in non-inertial frame; \( \vec{R}^{ext.} \) – the sum of the external forces acting on the pendulum \( P \), \( \vec{R}^{in.1} \), \( \vec{R}^{in.2} \) – forces of inertia.

For the relative momentum of pendulum \( P \) with the mass \( m_P \) and the length \( l \) we have:

\[
\vec{p}_{rel}^P = m_P\vec{v}_P^P = m_P\vec{v}_{rel}^P \times \vec{OF} = m_P \begin{bmatrix} 0 \\ -\beta \cos \beta \\ \beta \sin \beta \end{bmatrix},
\]

where \( \beta \) – angle between the \( OP \) and the vertical \( \zeta \).

For external forces in (5):

\[
\vec{R}^{ext.} = \vec{R}_O + m_P\vec{g} = \begin{bmatrix} R_{\delta y} \\ R_{\delta z} \\ R_{\delta z} - m_Pg \end{bmatrix},
\]

where \( \vec{R}_O \) here for pendulum \( P \) is opposite to the \( \vec{R}_O \) in the equations for tripod.

For inertia force \( \vec{R}^{in.1} \) we have:

\[
\vec{R}^{in.1} = -m_P \left( \frac{\Omega^2}{4} \vec{C} \times \vec{C} \right) \left( \psi \vec{e}_x \times \vec{C} \right) = -m_P \begin{bmatrix} \psi^2 l \sin \beta \\ \psi^2 l \sin \beta + \psi d \\ 0 \end{bmatrix},
\]

and for inertia force \( \vec{R}^{in.2} \):

\[
\vec{R}^{in.2} = -2m_P \psi \vec{e}_x \times \vec{V}_{rel}^P = -m_P \begin{bmatrix} 2\psi \beta l \cos \beta \\ 0 \\ 0 \end{bmatrix}.
\]

So finally for the relative momentum of pendulum \( P \) after calculating derivatives:

\[
m_P \begin{bmatrix} 0 \\ \beta l \cos \beta + \beta^2 l \sin \beta \\ \beta l \sin \beta + \beta^2 l \cos \beta \end{bmatrix} = \begin{bmatrix} R_{\delta y} - m_P \left( \psi^2 d + \psi \sin \beta + 2\psi \beta l \cos \beta \right) \\ R_{\delta z} - m_P \left( \psi^2 l \sin \beta + \psi d \right) \\ R_{\delta z} - m_P \left( \psi^2 l \sin \beta + \psi d \right) \end{bmatrix}.
\]
From here we can express reaction in hinge \( O \):

\[
\begin{bmatrix}
R_{iO} \\
R_{oO} \\
R_{jO}
\end{bmatrix} =
\begin{bmatrix}
\frac{m_p}{2} (W_{C,i} - \psi^2 d + \psi l \sin \beta + 2\psi l \cos \beta) \\
\frac{m_p}{2} (W_{C,o} - \beta l \cos \beta + \beta l \sin \beta + \psi^2 l \sin \beta + \psi d) \\
\frac{m_p}{2} (\beta l \sin \beta + \beta^2 l \cos \beta + g)
\end{bmatrix}.
\tag{6}
\]

For the pendulum \( Q \) in cylindrical hinge \( S \) we can write equation of forces in the non-inertial reference system:

\[
\frac{d\vec{p}^\text{rel}_Q}{dt} = \vec{R}^\text{rel}_Q + \vec{R}^\text{in} \in Q + \vec{R}^\text{in} \in 2 \in Q,
\tag{7}
\]

where \( \vec{p}^\text{rel}_Q \) – momentum of pendulum \( Q \) in non-inertial frame; \( \vec{R}^\text{rel} \in Q \) – the sum of the external forces acting on the pendulum \( Q \), \( \vec{R}^\text{in} \in Q \), \( \vec{R}^\text{in} \in 2 \in Q \) – forces of inertia.

For the relative momentum of pendulum \( Q \) with the mass \( m_Q \) and the length \( L \) we have:

\[
\vec{p}^\text{rel}_Q = m_Q \vec{\omega}^\text{rel} = m_Q \vec{\omega}_S \times \vec{SO} = m_Q \begin{bmatrix}
L \gamma \cos \gamma \\
L \gamma \sin \gamma
\end{bmatrix},
\]

where \( \gamma \) – angle between the \( SQ \) and the vertical \( \zeta \).

For external forces in (7):

\[
\vec{R}^\text{rel} \in Q = \vec{R}_S + m_Q \vec{g} = \begin{bmatrix}
\vec{R}_{c,i} \\
\vec{R}_{c,o} \\
\vec{R}_{j,o} - m_Q \vec{g}
\end{bmatrix},
\]

where \( \vec{R}_S \) here for pendulum \( Q \) is opposite to the \( \vec{R}_S \) in the equations for tripod.

For inertia force \( \vec{R}^\text{in} \in Q \) we have:

\[
\vec{R}^\text{in} \in Q = -m_Q \left( \vec{\omega}_C + \psi \vec{\epsilon}_C \times \vec{CQ} + \psi \vec{\epsilon}_C \times \left( \psi \vec{\epsilon}_C \times \vec{CQ} \right) \right) = -m_Q \begin{bmatrix}
W_{C,i} - \psi^2 L \sin \gamma \\
W_{C,o} + \psi L \sin \gamma \\
0
\end{bmatrix},
\]

and for inertia force \( \vec{R}^\text{in} \in 2 \in Q \):

\[
\vec{R}^\text{in} \in 2 \in Q = -2m_Q \psi \vec{\epsilon}_C \times \vec{\omega}^\text{rel} = -m_Q \begin{bmatrix}
0 \\
2\psi \gamma l \cos \gamma \\
0
\end{bmatrix}.
\]

So finally for the relative momentum of pendulum \( Q \) after calculating derivatives:

\[
m_Q \begin{bmatrix}
\gamma L \cos \gamma - \psi^2 L \sin \gamma \\
0 \\
\gamma L \sin \gamma + \psi^2 L \cos \gamma
\end{bmatrix} =
\begin{bmatrix}
\vec{R}_{c,i} - m_Q \left( W_{C,i} - \psi^2 L \sin \gamma \right) \\
\vec{R}_{c,o} - m_Q \left( W_{C,o} + \psi L \sin \gamma + 2\psi \gamma L \cos \gamma \right) \\
\vec{R}_{j,o} - m_Q g
\end{bmatrix}.
\]
From here we can express reaction in hinge $S$:

$$
\begin{bmatrix}
R_{S_x} \\
R_{S_y} \\
R_{S_z}
\end{bmatrix} =

\begin{bmatrix}
m_q \left( \gamma L \cos \gamma - \gamma^2 L \sin \gamma + W_{C_x} - \psi^2 L \sin \gamma \right) \\
-m_q \left( W_{C_y} + \psi L \sin \gamma + 2 \psi \gamma L \cos \gamma \right) \\
m_q \left( \gamma L \sin \gamma + \gamma^2 L \cos \gamma + g \right)
\end{bmatrix}.
$$

Let's return to the equation (4). From the first and the second line in (4) we have the system for normal reactions in points $A, B$:

$$
\begin{align*}
N_b - N_a &= \frac{1}{d} \left( hR_{Oy} + HR_{Sq} + \mu_O \right) \\
N_b + N_a &= R_{OC} + \frac{1}{d} \left( \mu_S - hR_{OC} - HR_{SS} \right)
\end{align*}
$$

Solving this system we obtain:

$$
\begin{align*}
N_a &= \frac{1}{2} \left( R_{OC} + \frac{1}{d} \left( \mu_S - hR_{OC} - HR_{SS} \right) \right) - \frac{1}{d} \left( hR_{Oy} + HR_{Sq} + \mu_O \right), \\
N_b &= \frac{1}{2} \left( \frac{1}{d} \left( hR_{Oy} + HR_{Sq} + \mu_O \right) + R_{OC} + \frac{1}{d} \left( \mu_S - hR_{OC} - HR_{SS} \right) \right).
\end{align*}
$$

These normal reactions we can substitute in the third line of (2) where:

$$
N_c = Mg + R_{OC} + R_{SS} - N_a - N_b. \tag{10}
$$

Let us write equation for angular momentum of the pendulum $P$ in non-inertial reference frame $O\xi\eta\zeta$:

$$
\frac{dK_{Orel}^{pend,P}}{dt} = \bar{M}_{O}^{ext,P} + \bar{M}_{O}^{in1,P} + \bar{M}_{O}^{in2,P}, \tag{11}
$$

where $\bar{K}_{Orel}^{pend,P} = -m_P l^2 \beta \bar{e}_z$ – relative angular momentum of the pendulum; $\bar{M}_{O}^{ext,P}$ – moment of external forces; $\bar{M}_{O}^{in1,P}, \bar{M}_{O}^{in2,P}$ – moments of inertia forces. All these moments are taken with respect to the point $O$.

For the derivative in left we have:

$$
\frac{dK_{Orel}^{pend,P}}{dt} = -m_P l^2 \beta \bar{e}_z.
$$

For $\bar{M}_{O}^{ext,P}$ we have:

$$
\bar{M}_{O}^{ext,P} = \bar{OP} \times m_P \bar{g} + \bar{P}_O = (m_P g l \sin \beta - \mu_O) \bar{e}_z,
$$

where $\bar{P}_O$ – moment of the electric motor rotating pendulum $P$ – here it is opposite to the $\bar{P}_O$ in equation for tripod (3).

For $\bar{M}_{O}^{in1,P}$ we have:
\[
\begin{align*}
\vec{M}_{O}^{inl. P} &= \overrightarrow{OP} \times \vec{R}^{inl. P} = m_{l}J \begin{bmatrix}
-\cos \beta \left(W_{c_{g}} + \psi l \sin \beta + \psi d \right) \\
\cos \beta \left(W_{c_{g}} - \psi d + \psi l \sin \beta \right) \\
-\sin \beta \left(W_{c_{g}} - \psi d + \psi l \sin \phi \right)
\end{bmatrix},
\end{align*}
\]

For \(\vec{M}_{O}^{ina2. P}\) we have:
\[
\begin{align*}
\vec{M}_{O}^{ina2. P} &= \overrightarrow{OP} \times \vec{R}^{ina2. P} = m_{l}J^{2} \begin{bmatrix}
0 \\
2\psi \beta \cos^{2} \beta \\
-2\psi \beta \sin \beta \cos \beta
\end{bmatrix}.
\end{align*}
\]

Substituting these expressions into equation (11), we obtain:
\[
\begin{bmatrix}
-m_{l}J^{2}\dot{\beta} \\
0 \\
0
\end{bmatrix} = \begin{bmatrix}
m_{g}gl \sin \beta - m_{o} - m_{l} \cos \beta \left(W_{c_{g}} + \psi l \sin \beta + \psi d \right) \\
m_{l} \cos \beta \left(W_{c_{g}} - \psi d + \psi l \sin \beta + 2\psi \beta \cos \beta \right) \\
m_{l} \sin \beta \left(W_{c_{g}} - \psi d + \psi l \sin \beta + 2\psi \beta \cos \beta \right)
\end{bmatrix}.
\]

Let us write equation for angular momentum of the pendulum \(Q\) in non-inertial reference frame \(S\xi\eta\zeta\):
\[
\frac{d\vec{K}_{Srel}^{pend, Q}}{dt} = \vec{M}_{S}^{ext, Q} + \vec{M}_{S}^{in1, Q} + \vec{M}_{S}^{in2, Q},
\]
where \(\vec{K}_{Srel}^{pend, Q} = -m_{g}L^{2}\ddot{\gamma} \bar{\eta}\) – relative angular momentum of the pendulum; \(\vec{M}_{S}^{ext, Q}\) – moment of external forces; \(\vec{M}_{S}^{in1, Q}, \vec{M}_{S}^{in2, Q}\) – moments of inertia forces. All these moments are taken with respect to the point \(S\).

For the derivative in left we have:
\[
\frac{d\vec{K}_{Srel}^{pend, Q}}{dt} = -m_{g}L^{2}\ddot{\gamma} \bar{\eta},
\]

For \(\vec{M}_{S}^{ext, Q}\) we have:
\[
\vec{M}_{S}^{ext, Q} = \overrightarrow{SQ} \times m_{g}L \bar{\gamma} + \bar{p}_{S} = \left(m_{g}gL \sin \gamma - \mu_{S}\right) \bar{\eta},
\]
where \(\mu_{S}\) – moment of the electric motor rotating pendulum \(Q\) – here it is opposite to the \(\mu_{S}\) in equation for the tripod (3).

For \(\vec{M}_{S}^{in1, Q}\) we have:
\[
\vec{M}_{S}^{in1, Q} = \overrightarrow{SQ} \times \vec{R}^{in1, Q} = m_{g}L \begin{bmatrix}
-\cos \gamma \left(W_{c_{g}} + \psi L \sin \gamma \right) \\
\cos \gamma \left(W_{c_{g}} - \psi^{2} L \sin \gamma \right) \\
-\sin \gamma \left(W_{c_{g}} + \psi L \sin \gamma \right)
\end{bmatrix}.
\]

For \(\vec{M}_{S}^{in2, Q}\) we have:
\[ \Omega^* = \overrightarrow{SQ} \times \Omega^* = m_y L^2 \begin{bmatrix} -2\dot{\gamma} \cos^2 \gamma & 0 \\ 0 & -2\dot{\gamma} \sin \gamma \cos \gamma \end{bmatrix}. \]

Substituting these expressions into equation (13), we obtain:

\[ \begin{bmatrix} 0 \\ -m_y L^2 \ddot{\gamma} \\ 0 \end{bmatrix} = \begin{bmatrix} -m_y L \cos \gamma \left(W_{Cq} + \dot{\psi} L \sin \gamma + 2L \dot{\psi} \dot{\gamma} \cos \gamma \right) \\ m_y g L \sin \gamma - \mu_s + m_y L \cos \gamma \left(W_{Cq} - \dot{\psi}^2 L \sin \gamma \right) \\ m_y L \sin \gamma \left(W_{Cq} + \dot{\psi} L \sin \gamma + 2L \dot{\psi} \dot{\gamma} \cos \gamma \right) \end{bmatrix}. \tag{14} \]

The dynamics of the electric motors can be described by the equations:

\[
\begin{align*}
\tau_0 \frac{d\mu_0}{dt} + \mu_0 &= b_0(U_o - b_0) \beta \\
\tau_s \frac{d\mu_s}{dt} + \mu_s &= b_s(U_o - b_s) \ddot{\gamma}
\end{align*}
\tag{15}
\]

where \(\mu_0, \mu_s\) – torque of electric motors in hinges \(O, S\); \(\tau_0, b_{01}, b_{02}, \tau_s, b_{s1}, b_{s2}\), – electric motors constants; \(U_o, U_s\) – voltage applied to the motors; and also:

\[\tau_0, b_{01}, b_{02}, \tau_s, b_{s1}, b_{s2}, U_o, U_s, \beta, \ddot{\gamma} > 0.\]

4 CONCLUSIONS

- General equations of motion are obtained for the mechanism consisting of the tripod and two pendulums as internal movers.
- General case of motion of the tripod is considered on a rough horizontal plane – the tripod moves not only translationally and not only rotationally but with sliding and spinning at the same time.

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REFERENCES


MODEL OF THE TETHERED SPACE SYSTEM IN VICINITY OF ELLIPSOIDAL ASTEROID AND ITS APPROXIMATIONS

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Abstract. While planning missions in vicinity of an asteroid/comet body one has to take into account several dynamical problems to overcome and among them are: (a) irregular distribution of the body internal masses; (b) too weak gravity acceleration near the body surface. In case of (a) one offers to apply approximate models of gravity. As an example we consider the case of a triaxial ellipsoid. For the problem (b) we apply docking procedures with help of anchor and a connecting tether.

For computing the force field of gravity being generated by the ellipsoid of three axes one has to calculate several values of elliptic integrals at each instant of the simulation process. For this we apply original algorithm interpreting elliptic integrals as a state variables in additional to dynamics system of ODEs. To resolve the problem (b) we use so-called hybrid automata to build up the tethered interconnection between a spacecraft and the asteroid.

Ellipsoidal asteroid performs free rotary motions about its mass center thus performing the Euler case of the rigid body rotary motion. The spacecraft moves under the force of
gravity from the asteroid and under the tether tension, in case of the constraint being imposed. So we have so-called restricted dynamical model because the asteroid does not “feel” any force from the spacecraft.

In addition to the hybrid automata dynamical model including impacts on constraint we also consider approximations of this model being really regularizations of the impact process. All these models are analysed and compared numerically.

1 INTRODUCTION

Pendulum system under consideration may be regarded as a delivery facility to transport payloads to/from the spacecraft from/to the asteroid surface, some kind of space elevator. This idea is close to that one, belonging to Tsiolkovsky and known as a space elevator located nearby the Earth. Engineering development of this construction concerns the pioneer work [1], see also [2]. Close idea of the Moon elevator probably arises due to works of F. Zahnder [3]. This latter idea was rediscovered in [4, 5, 6].

Specific property of the problem under analysis consists of typically irregular shape and mass distribution of asteroids. Another property relates to asteroid’s motion as the Euler top, which is not a permanent rotation in general situations.

Studying of pendulums concerning the dynamical problems of orbital mechanics goes back to probably pioneer work [7]. Existence and conditions of stability for orbital pendulums in different formulations were investigated in [8, 9, 10], and also in papers [11, 12, 13, 14, 15, 16, 17, 18]. Investigation of space tethered systems is tightly interconnected with activity of Beletsky and his pupils and colleagues: [19, 20, 21, 22, 23, 24]. Dynamics of tethered systems attached to an asteroid is studied intensively in [25, 26, 27, 28, 29]). Orbital motion of compound satellites was studied in [30, 31]. The model useful for simulation the contact between particular spacecraft of the tethered system and the asteroid surface see in [32].

2 PROBLEM FORMULATION

When planning missions in vicinity of minor celestial body of the Solar system one has to take into account at least two serious difficulties to overcome: (a) internal masses distribution inside asteroid/comet is as a rule irregular; (b) gravity of such a body is too weak such that it makes practically impossible the traditional “landing” of the spacecraft onto the celestial object surface. For solving two problems mentioned we apply proper methodics. In case of (a) one offers to apply approximate models of gravity. As an example we consider gravity of the asteroid having a shape of triaxial ellipsoid. To overcome problems in case of (b) one can apply docking procedures with help of anchor and cable connection.

One encounters frequently celestial bodies of ellipsoidal shape or close to it in Solar system. For computing the force field of gravity being generated by such a body one
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has to calculate elliptic integrals on each step of the integration process for the dynamical model under construction. As it turned out one can use special additional system of ODEs for this problem efficient solution. For solving the problem (b) one uses so-called hybrid automata to build up the dynamical model of a spacecraft. There are exactly two states of this automata: free flight of the spacecraft: cable is slack; flight along the constraint: cable is tensed.

Ellipsoidal asteroid performs free rotary motions about its mass center. The spacecraft moves under the force of gravity from the asteroid and under the tension, in case of the constraint being imposed. Dynamical model under analysis can be classified as a restricted one. Indeed, spacecraft does not influence the motion of the asteroid.

Besides the hybrid automata dynamical model, which includes impacts on constraint, approximations of this model are also under consideration. These approximations are reduced to replacement of “exact” model of impact by its different schemes of regularization. Some of these models are analysed and compared numerically.

Thus first of all consider a tethered system (TS), consisting of a weightless tether of length $\ell$, an asteroid $A$, and a particle $Q$ of mass $m$, see Figure 1. Suppose the tether connects a point $P$ fixed on the asteroid surface $\Sigma$ and a particle $Q$.

Figure 1: Mechanical system.

Let $OX_\alpha X_\beta X_\gamma$ be an absolute frame of reference (ARF). Assume that its origin coincides with the asteroid center of mass. Also let $Ox_1x_2x_3$ be the mobile reference system (MRF), connected with the asteroid. Its axes are assumed to be directed along its principal central axes of inertia. Unit vectors of the ARF base with respect to MRF can be represented in the following way

$$\alpha = (\alpha_1, \alpha_2, \alpha_3)^T, \quad \beta = (\beta_1, \beta_2, \beta_3)^T, \quad \gamma = (\gamma_1, \gamma_2, \gamma_3)^T.$$  \hspace{1cm} (1)
Using components of these vectors one can compose an orthogonal matrix

$$\mathbf{S} = \begin{pmatrix} \alpha_1 & \alpha_2 & \alpha_3 \\ \beta_1 & \beta_2 & \beta_3 \\ \gamma_1 & \gamma_2 & \gamma_3 \end{pmatrix},$$  

allowing to implement transfers from MRF to ARF and back: if a vector $\vec{OQ}$ is described as

$$\mathbf{X} = (X_{\alpha}, X_{\beta}, X_{\gamma})^T, \quad \mathbf{x} = (x_1, x_2, x_3)^T$$

in ARF and MRF respectively, then

$$\mathbf{X} = \mathbf{S}\mathbf{x}.$$  

The angular velocity

$$\mathbf{\omega} = (\omega_1, \omega_2, \omega_3)^T$$

given by its projections onto the axes of the MRF satisfies a matrix equation

$$\dot{\mathbf{S}} = \mathbf{S} \cdot \mathbf{\hat{\omega}}, \quad \mathbf{\hat{\omega}} = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix},$$

that can be treated as a matrix form of the Poisson equations describing variations of the body orientation. The same equations in the vector form read

$$\dot{\mathbf{\alpha}} = \mathbf{\alpha} \times \mathbf{\omega}, \quad \dot{\mathbf{\beta}} = \mathbf{\beta} \times \mathbf{\omega}, \quad \dot{\mathbf{\gamma}} = \mathbf{\gamma} \times \mathbf{\omega}.$$  

If in the ARF velocity and acceleration of the particle $Q$ are represented as

$$\mathbf{V} = \begin{pmatrix} \dot{X}_{\alpha} \\ \dot{X}_{\beta} \\ \dot{X}_{\gamma} \end{pmatrix}^T \quad \text{and} \quad \mathbf{A} = \begin{pmatrix} \ddot{X}_{\alpha} \\ \ddot{X}_{\beta} \\ \ddot{X}_{\gamma} \end{pmatrix}^T$$

respectively, then, as is known from kinematics, in the MRF velocity and acceleration are given as

$$\mathbf{V} = \mathbf{S}^T \cdot \mathbf{V} = \mathbf{\omega} \times \mathbf{x} + \dot{\mathbf{x}},$$

$$\mathbf{A} = \mathbf{S}^T \cdot \mathbf{A} = \mathbf{\omega} \times (\mathbf{\omega} \times \mathbf{x}) + \dot{\mathbf{\omega}} \times \mathbf{x} + 2\mathbf{\omega} \times \dot{\mathbf{x}} + \ddot{\mathbf{x}}.$$  

respectively.

Since the point of fixation $P$ given by the vector $\overrightarrow{OP}$ with

$$\mathbf{P} = (P_{\alpha}, P_{\beta}, P_{\gamma})^T, \quad \mathbf{p} = (p_1, p_2, p_3)^T$$

is fixed in asteroid, then its velocity and acceleration are

$$\mathbf{V}_P = \mathbf{S} (\mathbf{\omega} \times \mathbf{p}), \quad \mathbf{A}_P = \mathbf{S} (\mathbf{\omega} \times (\mathbf{\omega} \times \mathbf{p}) + \dot{\mathbf{\omega}} \times \mathbf{p})$$

respectively in the ARF. They also read

$$\mathbf{v}_P = \mathbf{\omega} \times \mathbf{p}, \quad \mathbf{a}_P = \mathbf{\omega} \times (\mathbf{\omega} \times \mathbf{p}) + \dot{\mathbf{\omega}} \times \mathbf{p}$$

respectively in the MRF.
3 DYNAMICS

Let the pendulum be hanged at the point $P$ of the asteroid surface with a massless inextensible tether of the length $\ell$: $|PQ| \leq \ell$. The mass $m$ of the pendulum is supposed being concentrated at its endpoint $Q$. The asteroid is assumed performing rotation about its mass center as the Euler top. One also assumes that the pendulum motion does not affect the asteroid rotation. The tether length we in general assume as known predefined function of time. Then equations of the particle $Q$ motion w. r. t. MRF read

$$ma = f_\ast + \lambda_\ast \frac{\partial \varphi}{\partial x},$$

(12)

where $f_\ast$ and $\lambda_\ast$ are the active force and the Lagrange multiplier respectively. The latter one is determined from the equation of the exerted constraint:

$$\varphi(x, p, \ell) = \frac{1}{2} \left[ (x - p, x - p) - \ell^2 \right] \equiv 0 \quad (13)$$

and two its time derivatives

$$(x, x - p) - \ell \dot{\ell} \equiv 0, \; (\dot{x}, x - p) - (\ddot{x}, \ddot{x}) - \ddot{\ell} \ell - \ddot{\ell}^2 = 0. \quad (14)$$

Since the point $P$ is assumed to be fixed in the MRF the equalities $\dot{p} = 0, \ddot{p} = 0$ are fulfilled.

Denoting $f_\ast = mf, \lambda_\ast = m\lambda$ and using identity (9) we find out from (12) that

$$(\omega \times (\omega \times x) \dot{+} \omega \times x + 2\omega \times \dot{x} + \ddot{x}) = f + \lambda \frac{\partial \varphi}{\partial x} \quad (15)$$

or in the equivalent form:

$$\ddot{x} = ((\omega \times x) \times \omega + x \times \dot{\omega} + 2x \times \omega) + f + \lambda \frac{\partial \varphi}{\partial x}. \quad (16)$$

Substituting of acceleration $\ddot{x}$ from (16) into second identity (14) we have

$$((\omega \times x) \times \omega + x \times \dot{\omega} + 2\dot{x} \times \omega + f + \lambda(x - p), x - p) - (\dot{x}, \ddot{x}) - \ddot{\ell} \ell - \ddot{\ell}^2 = 0,$$

and one obtains the Lagrange multiplier

$$\lambda = \left[ (\omega \times (\omega \times x) + \dot{\omega} \times x + 2\omega \times \dot{x} - f, x - p) + (\ddot{x}, x) + \dddot{\ell} + \dddot{\ell}^2 \right] / \ell^2. \quad (17)$$

We assume that active forces are potential, and potential energy has the form $U_\ast = mU(x)$. Then

$$f = -\frac{\partial U}{\partial x}. \quad (18)$$
Explicit expression of force (18) will be used below in equations (16). However it is impossible to write down an exact expression for potential energy for an arbitrary celestial body, because of the absence of exact data about its mass distribution. Nevertheless if the point \( Q \) is located far enough from the asteroid then we can assume that

\[
U = -GM \left[ \frac{1}{r} + \frac{I_1 + I_2 + I_3}{2r^3} - \frac{3(Ix, x)}{r^3} + \ldots \right]
\]  

(19)

where \( r = (x, x)^{1/2} \), and \( I = \text{diag} (I_1, I_2, I_3) \) is asteroid’s central tensor of inertia, divided by its mass and represented in asteroid’s principal central axes of inertia. In the further course we assume that selection of physical dimensions is such that \( GM = 1 \).

Remark 1 Approximate expression (19) for the potential is derived, as usual, from the exact one:

\[
U(x) = -\frac{1}{m} \int \int \int_A \rho u(x, y) dy
\]  

(20)

via a standard expansion of the integrand multiplier

\[
u(x, y) = (x - y, x - y)^{-1/2}
\]  

(21)

with respect to the parameter \( \varepsilon = (-2(x, y) + (y, y)) / (x, x) \). However, the potential can be also expanded with respect to \( \varepsilon_* = -2(x, y) / ((x, x) + (y, y)) \). This parameter has no singularity at the origin. This representation has been applied in [33] for gravitating rings and in [34] for tetrahedral bodies

\[
u(x, y) = \frac{1}{((x, x) + (y, y))^{1/2}} \left( \frac{1}{1 + \varepsilon_*^{1/2}} = u_0 + u_1 + \cdots = \right)
\]  

(22)

\[
= \frac{1}{((x, x) + (y, y))^{1/2}} \left( 1 - \frac{1}{2} \varepsilon_* + \frac{3}{8} \varepsilon_*^2 - \frac{5}{16} \varepsilon_*^3 + \cdots \right).
\]

In contrast to the standard expansion, integration of terms \( u_n \), which are not homogeneous function of the vector \( y = (y_1, y_2, y_3)^T \) components usually is non-trivial. Properties of this approximation for the potential, in particular, its behaviour in vicinity of the asteroid surface were not deeply investigated.

Equations (17), (19) are suitable to describe motion of a massive particle in Euler case of asteroid’s rotation as well as in particular cases of precessions and permanent rotations. In the latter case

\[
\omega = \dot{\psi} e_\psi,
\]  

(23)

where \( \dot{\psi} = \text{const} \) is the magnitude of angular velocity which is invariable in the body coordinate system, \( e_\psi \) is the unit vector which is directed along axis of rotation.
Regular precessions exist in the case of the body $\mathcal{A}$ dynamical symmetry. If $\mathbf{f}_1$, $\mathbf{f}_2$, $\mathbf{f}_3$ are unit vectors directed along its principal central axes of inertia, and $\mathbf{f}_3$ is directed along the axis of symmetry, then

$$\mathbf{\omega} = \dot{\psi} \mathbf{e}_\psi + \dot{\phi} \mathbf{e}_\phi.$$  \hspace{1cm} (24)

Here and below the constant quantities $\dot{\psi}$ and $\dot{\phi}$ denote magnitudes of angular velocities of precession and proper rotation respectively; $\theta$ is a constant angle of nutation;

$$\mathbf{e}_\psi = \cos \theta \mathbf{f}_3 + \sin \theta (\cos (\dot{\phi}t) \mathbf{f}_1 + \sin (\dot{\phi}t) \mathbf{f}_2)$$

is a unit vector of the axis of precession, fixed in the absolute space; $\mathbf{e}_\phi = \mathbf{f}_3$.

Remark 2 If the value $\lambda$, determined by (17) is negative on the motions under consideration, then the constraint is tensed, and it can be implemented using the tether. Otherwise for the constraint implementation one needs a weightless rod. If the value $\lambda$ can change its sign then releasing the constraint as well as its tension are possible.

It is natural to expect that the tether model is applicable if its length is large enough and its free endpoint $Q$ is located in the region where a centrifugal force dominates over the force of gravity. At the same time, it is natural that the rod model ought be applied near the body surface, where force of gravity dominates.

### 4 MODEL OF A SPACECRAFT TETHERED WITH ASTEROID

The tether, implementing a unilateral constraint and connecting an asteroid surface and a massive particle, can be in a stretched or slackened state. We build up a computer model of the mechanical system consisting of a free rigid body and a massive particle, connected by a massless inextensible tether. The problem is considered within a restricted formulation: a particle, the spacecraft, does not affect dynamics of a rigid body, asteroid. At the same time, the particle moves under gravitational attraction of the asteroid and simultaneously under reaction of the tether. The unilateral constraint allows impacts satisfying, for example, the Newton model.

Description of the typical mission in vicinity of the asteroid including slack mode of the tether connecting the asteroid surface and the spacecraft, its decreasing oscillations with impacts, final landing on the constraint and the limit pendulum-like motions of the tethered system we undertook in [29].

Let us apply the model described above. Let the asteroid be a homogeneous triaxial ellipsoid with semi-axes $a_1 > a_2 > a_3$, described by

$$\frac{x_1^2}{a_1^2} + \frac{x_2^2}{a_2^2} + \frac{x_3^2}{a_3^2} = 1$$

in the MRF. Assume that ellipsoid’s center of mass is fixed, and the ellipsoid itself rotates uniformly about its axis of inertia, corresponding to the maximal moment of inertia. Without loss of generality this is the axis $Ox_3$ of the ARF, coincident to the axis $Ox_3$. 

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of the MRF. In case of Euler such solution is possible. Suppose the point of tether’s attachment \( P \) is located on the ellipsoid surface at the point of intersection with the axis of inertia, corresponding to the minimal moment of inertia. Without loss of generality this is the axis \( Ox_1 \) of the MRF.

Model of the tether as a unilateral constraint was implemented as a hybrid automata with a properly defined automata state variable. This variable takes two possible values: (a) “constraint is in a slackened state”; i. e. the spacecraft freely flies in field of the asteroid gravity; (b) “constraint is in a stretched state”, i. e. the spacecraft moves as a spherical pendulum also in field of asteroid gravity.

In [29] we also demonstrated so-called “landing-on-the-constraint” process with repetitive impacts and final change motion to constrained mode of spherical pendulum. Really hybrid automata is one of possible implementations for unilateral constraint which in turn is sufficiently rough model for the tethered system of two bodies. The cable is assumed weightless and inextensible in the simplest case and without any resistance to bending. Thus when the distance between endpoints is less than the cable length then the tension force is equal to zero. The force interaction takes place only if the unilateral constraint arises with impacts or impactless. Evidently the case of the impact is the most general one. Here we use the simplest case of Newtonian impact model.

Approximations are known [35] for systems with impacts having potential energy of large value. Elastic and viscous components are included in frame of Newtonian impact model. We performed comparison of pure impact model with linear elastic and viscous models during the process of “landing on constraint” as an example. The first model performs multiple impacts and soon starts its limit pendulum-like motions. The second, linear, model performs its decreasing oscillations in much more slow pace.

At the same time if we consider the non-linear model of repulsing force instead of linear model then this force supposed to act inside the thin, of thickness \( \varepsilon \ll 1 \), layer. This layer simulates the boundary compliance for the constraint under analysis. The force can have the following expression

\[
F_{\text{elast}} = \begin{cases} 
  c \cdot \tan \left( \frac{\pi \Delta \ell}{2 \varepsilon} \right) & \text{for } \Delta \ell \geq 0 \\
  0 & \text{for } \Delta \ell < 0
\end{cases}
\]

where \( c \) is the stiffness coefficient, \( \Delta \ell \) is the deviation from the constraint virtual boundary such that for \( \Delta \ell < 0 \) the constraint/contact are absent and for \( \Delta \ell \geq 0 \) the constraint is simulated by the elastic resistance force being increased fast up to infinity.

Numeric results are shown in Figure 2 where two variables \( \Delta \ell \) for two models under verification, one with impacts and nonlinear with compliance, are compared in the process of landing on the constraint. One can see easily that non-linear model represented above gives an approximation of much more better quality while the landing process.

Let us consider in more detail the motivation of the last model use. The complicated dynamical picture can arise in case of the account for the interconnecting tether mass.
Let for definiteness and simplicity we have the tether lumped model as a chain sufficiently long and consisting of the discrete elements which are particles of sufficiently small masses being interconnected by weighless and inextensible cable segments. In such the model if each the segment is simulated as a hybrid automata then it is easy to see that combining interactions via impacts is transformed to the problem of large computational complexity.

To resolve this problem we can undertake the replacement of inextensible segments by ones of the model described above with sufficiently small compliance. Computational experiments show that inextensible and compliant segments demonstrate dynamical close-ness. As a result we can conclude that application of lumped model with compliance can be useful for efficient approximation of the tethered system dynamics with massive interconnected cables. For this we also have to remark that real cables are sooner compliant than inextensible.

5 CONCLUSION

As a result we can make some numerical observations:

–Lumped model with inextensible elements with impacts approximates source problem
having massive tethers;
–Lumped model with compliance approximates model of the hybrid automata with impacts;
–The latter model can be used for approximating dynamical problems with tethers having non-zero masses.

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REFERENCES


NUMERIC-ANALYTICAL METHODS OF THE COEFFICIENTS DEFINITION OF THE ROLLING FRICTION MODEL OF THE PNEUMATIC AVIATION TIRE

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Key words: Combined Dry Friction, Numeric-Analytical Methods, Pneumatic Aviation Tire.

Abstract. A new approximate models of the tire rolling accounting for coupled longitudinal and lateral sliding as well as the spinning and the deformed state resulting in elastic forces were proposed in previous works [1-7]. The main goal of this investigation consists in the development of the numeric-analytical methods of these models coefficients definition.

1 INTRODUCTION

The intensive oscillations of main landing gears were observed at initial stages of landings of some modern aircrafts. Some of the registered cases of oscillations resulted the destruction of torque links and the alarm conditions with hard damaging of aircraft's frame. Among the main features of this phenomena are the following:

- the high-intensive coupled longitudinal, lateral, and spinning oscillations of "shimmy" type observed directly after touchdown (i.e. at the stage of non-steady rolling with longitudinal sliding) as well as directly after the end of the unstably rolling stage;

- the high-amplitude oscillations are coupled with significant wheels’ sliding that is proved by the tracks of wheels at runaways’ surfaces.

The last specificity leads to the main conclusion: the classical shimmy models cannot be applied to the theoretical description of the investigated phenomenon. Indeed, the hypothesis of sliding and spinning absence is the background of these models. Thus, a qualitatively new model with no non-holonomic constraint and accounting the dry friction forces is needed. This kind of models was proposed by the Russian academicians D.M.Klimov and V.Ph.Zhuravlev in 2009 on the groundwork of the multi-component dry friction theory. Their dry friction theory was efficiently used to model the shimmy of the rigid wheel without tire, i.e. with vanishing deformations and significant sliding during the unstable rolling. It is to be
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noted that their solution of the rolling stability problems was obtained for the Hertzian contact pressure distribution that is allowed only for small strains and deformations of tires, i.e. the approximation of the pressured thick-walled shell by an elastic solid. Nevertheless, the pressure distributions obtained from the numerical simulation on the groundwork of 3D finite element models as well as on the known approximate analytical solutions for the nonlinear problem of the soft shell theory differ significantly from the Hertzian distribution if even the quasi-statics is investigated. The real contact pressure distribution or its approximation has to be taken into account to compute the friction parameters, primarily for the friction torque due to its significant effect on the stability of rolling [5, 6, 7, 12]. Such a distribution can be obtained on the background of the finite element simulation in dynamics or in quasi-statics. On the other hand the three-dimensional finite element modeling of such strongly nonlinear systems is very resource consuming. Thus, the numerical simulation of the dynamics of systems like aircraft landing gears become practicable only at the stage of final calculations if the transient contact interaction of a pneumatic wheel and a road is modeled in details; it remains almost meaningless at the stage of the preliminary engineering design. Roughly speaking, it is strictly required to know what effect will be studied before the detailed quantitative dynamics analysis is performed.

Such a qualitative analysis must result in the knowledge about main specificities of the system and requires approximate models up to the simplest ones allowing analytical estimates construction. For instance, the study of the stability of the wheel rolling can use different three-dimensional models as well as the shell models or even the simplest approximations of the contact pressure to compute the dry friction forces and torque, etc. This approach was realized by the authors in the previous works [3, 4, 6, 7, 8, 9]. These results were obtained with the aid of theory of multi-component dry friction which makes it possible to correctly and qualitatively describe the effects of dry friction in the case of combined kinematics. The narrow field of theoretical mechanics that began in the early 2000's with a few publications has formed in integral scientific direction, now, and has effectively used not only in works of authors [3-10] but in different publications of researchers from different scientific groups [1, 2, 11].

Unfortunately, the application of the theory of combined dry friction was limited by the need to calculate the coefficients of the models based on the calculation of the distribution of normal tangential stresses within the contact patch. The technique of experimental investigations of these coefficients and its validation on the base of numerical experiment is presented below. The verification procedure consists in two main stages: at the beginning the models coefficients are calculated on the basis of analytical formulae [3,4,6,8] with aid of numerical simulation of the stress distribution inside contact areas, then these coefficients are defined from the numerical dependence for dry friction torque and force components.

2 NUMERICAL EVALUATION OF THE COEFFICIENTS OF THE COUPLED DRY FRICTION MODEL ON THE BACKGROUND OF THE FINITE ELEMENT SIMULATION OF TIRE-ROAD CONTACT INTERACTION

The normal reaction $N$ for an arbitrary pneumatic tire could be defined as follows:
Here $\sigma_v(r, \varphi)$ denotes the contact pressure distribution over the contact spot.

Let us consider the static deformed state corresponding to the maximum vertical deformation equal to 29 mm. The corresponding distribution of the dimensionless contact pressure $\sigma_v(r, \phi)$ referred to the boost pressure $P^* = 200$ kPa is shown on the Figure 1:

![Figure 1. Spatial distribution of the static contact pressure in a typical tire](image)

Now let us consider the distribution of the contact pressure for the rolling tire corresponding to the same boost pressure as well as to the same maximum vertical deformation before rolling initiation. The spatial distribution of the dimensionless pressure $\sigma_v(r, \phi)$ is shown below on the Figure 2:
For the diameter section of the contact spot we have the contact pressure distribution that is shown on the Figure 3.

Let us define hence the rolling correction factor $k_x$. In general, the pressure could be approximated as follows [3, 4, 6, 8]:

$$\sigma_v(r, \varphi) \approx \sigma_0(r, \varphi) \left(1 + k_x \frac{x}{R} \frac{\theta_v}{\Theta_v}\right)$$

where $R$ is the contact spot radius and $k_x$ is interpreted as a shift of the gravity center of the contact pressure distribution due to the rolling. As a result, we obtain

$$\begin{align*}
S_x &= \frac{2\pi R}{\int_0^R \int_0^{2\pi} \sigma_v(r, \varphi) r^2 \cos \varphi dr d\varphi} \\
k_x &= \frac{S_x}{R}, \quad s = \pi \int_0^R \sigma_v(r, \varphi) r^3 dr
\end{align*}$$

(1.2)

As the contact spot could be considered as a circle, the numerical evaluation of the formulae (1.2), (1.3) and (1.4) could be based on the trapezoid formula referred to the polar
frame. As a result, we obtain \( N = 2.41 \times 10^5 \) N, \( M_0 = 1.07 \times 10^4 \) N m, \( m = 0.025 \) m, \( a = 0.052 \) m\(^2\), \( s = \frac{k_s}{s} = 0.13 \).

**Figure 3.** Distribution of the dimensionless static contact pressure over the diameter section of the contact spot, finite element simulation

The approximate formulae for the longitudinal dry friction force as well as for the dry friction torque could be written as follows [3, 6, 8]:

\[
F_\parallel = \frac{F_0 v}{\sqrt{v^2 + au^2}}, \quad F_\perp = \frac{k b u}{\sqrt{u^2 + bv^2}}, \quad M_c = \frac{M_0 u}{\sqrt{u^2 + mv^2}}. \tag{1.3}
\]

Here the following coefficients are introduced:

\[
F_0 = 2\pi f R^2 A^1, \quad M_0 = 2\pi f R^3 A^2. \tag{1.4}
\]

\[
\frac{1}{\sqrt{a}} = \frac{1}{F_0} \pi f R^2 A^0 = \frac{1}{2} \frac{A^0}{A^1}; \quad \frac{1}{\sqrt{m}} = \frac{1}{M_0} \pi f R^3 A^3 = \frac{1}{2} \frac{A^3}{A^2}. \tag{1.5}
\]

\[
b_1 = \frac{\pi f R^3 A^2}{2}; \quad \frac{b_1}{\sqrt{b}} = \frac{\pi f R^3 A^3}{\sqrt{m}} = \frac{M_0}{\sqrt{m}} \Rightarrow \frac{1}{\sqrt{b}} = \frac{2}{\sqrt{m}} = \frac{A^3}{A^2}. \tag{1.6}
\]

\[
A^4 = \int_0^1 \sigma_0(\rho) \rho^4 d\rho, \quad \rho = \frac{r}{R}.
\]
Thus, the formula for $F_{\perp}$ can be rewritten as follows:

$$F_{\perp} = \frac{k_{c}M_{u}u}{2\sqrt{u^{2} + \frac{1}{2}m\nu^{2}}}$$  \hspace{1cm} (1.7)

Let us introduce dimensionless variables, $\psi = \nu / u$ and $\mu = u / \nu$. Thus, the one-dimensional dependencies for both dry friction force and torque could be derived from (1.1):

$$F_{\parallel} = \frac{F_{0}}{\sqrt{1 + a\psi^{2}}}, \hspace{1cm} F_{\perp} = \frac{k_{c}M_{0}}{2\sqrt{1 + \frac{1}{2}m\psi^{2}}}, \hspace{1cm} M_{C} = \frac{M_{0}}{\sqrt{1 + m\psi^{2}}}.$$  \hspace{1cm} (1.8)

The corresponding diagrams are shown on Figures 4, 5, 6 as solid lines for $f = 0.3$.

We could consider these diagrams as test data; thus, the factors $F_{0}, M_{0}, k_{c}, a,$ and $m$ of the model (1.8) could be obtained from these diagrams, therefore the model could be interpreted as a rheological one. Indeed, let us perturb the diagrams by applying the random distribution with amplitude equal to $0.2 \max(F_{\parallel})$ and $0.2 \max(M_{C})$, respectively. In the other words, the 20% measurement error level is assumed. The corresponding “test values” are shown on Figures 4-6 as dotted lines.

![Figure 4. Dependence of the longitudinal friction force on the ratio between the sliding velocity and spinning angular velocity, $\psi$](image-url)
Figure 4. Dependence of the friction torque on the ratio between the spinning angular velocity and sliding velocity, $\psi$

Figure 5. Dependence of the lateral friction force on the ratio between the spinning angular velocity and sliding velocity, $\psi$
The model factors could be obtained by the nonlinear least squares fitting [13]:

\[
\min \sum_{k=1}^{N} \left\| f \left( x_k \right) - y_k \right\|
\]

(1.6)

where \( x_k \) are the values of \( \psi \) and \( \nu \) and \( y_k \) are measured values of the longitudinal force \( F_l \), lateral force \( F_\perp \) and friction couple \( M_\nu \). The dry friction factor could be obtained as

\[
f = \frac{F_0}{N}
\]

(1.6)

The fitting of the test data results in the following coefficients of the investigated model obtained with 95% confidence bounds:

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Theoretical value</th>
<th>Experimental value</th>
<th>Bounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>( f )</td>
<td>0.3</td>
<td>0.301</td>
<td>0.296, 0.305</td>
</tr>
<tr>
<td>( F_0 )</td>
<td>72219</td>
<td>72370</td>
<td>71200, 73530</td>
</tr>
<tr>
<td>( M_0 )</td>
<td>3215</td>
<td>3252</td>
<td>3182, 3322</td>
</tr>
<tr>
<td>( a )</td>
<td>0.690</td>
<td>0.714</td>
<td>0.603, 0.825</td>
</tr>
<tr>
<td>( m )</td>
<td>1.595</td>
<td>1.607</td>
<td>1.348, 1.867</td>
</tr>
<tr>
<td>( k_i )</td>
<td>0.130</td>
<td>0.129</td>
<td>0.128, 0.131</td>
</tr>
</tbody>
</table>

3 CONCLUSIONS

- The model of the dry friction with combined kinematics is considered accounting for the contact pressure distribution obtained from the finite element simulation of the quasi-static deformed state of the pneumatic tire.
- The factor of the rolling friction as well as other coefficients of the model based on analytical approximations are obtained on the background of the numerical simulation of the steady rolling of the tire.
- The dimensionless dependencies of the longitudinal dry friction force, lateral dry friction force, and dry friction torque are obtained.
- The experimental data are simulated by adding of random noise to the theoretical curves, then the model factors are obtained from noised curves by nonlinear least squares procedure.
- The good correlation between the exact model coefficients and the ones obtained from the simulated test curves is shown, therefore the possibility of identification of the model parameters after typical tests is proven.
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REFERENCES

ON THE OPTIMIZATION
OF A CAPSUBOT WITH A SPRING

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Key words: Capsule Robots, Friction Based Locomotion, Optimal Control

Abstract. A capsule robot (capsubot) without external drivers is considered. The device consists of a shell, an actuator, and certain equipment. It can move on a rough surface due to the controlled movement of an internal mass and external friction. The mass is driven by the actuator according to a given program, which ensures the movement of the shell due to the inertia forces. The system includes an elastic spring, connecting the shell with the internal mass. A control is proposed that allows to maximize the average velocity under given technological restrictions.

1 INTRODUCTION

A capsule robot (capsubot) is a type of compact mobile device which can explore fields inaccessible to humans. In recent years, such devices received intensive attraction mostly in connection with medical purposes: a tiny capsbot with camera can be swallowed by patient to diagnose diseases; another application is inspection of pipelines. Some methods of active locomotion were developed. The simplest approach is based on internal control forces and external static friction [1-5]. Comparatively to a legged design, it leads to more save interaction between the capsule and the explored area. Similar idea was used to study floating robots [6,7]. A capsbot without external moving parts contains an internal mass, being put in motion by an actuator. As the internal mass changes its position relative to the capsule, the center of gravity shifts. An appropriate control strategy is needed to provide periodic motion of the capsbot in desired direction. Due to limited resources (size and mass of the robot, power supply, etc.), the optimization problem (in a sense) is of great practical importance. A number of results in this direction are obtained [1,2,8]. Further modifications of the capsbot include elastic springs [9-11]. Numerical studies and experiments show that the addition of springs leads to improved technical characteristics such as the average velocity of the robot and energy consumption. Generally speaking, the use of springs allows to increase the maximum force during acceleration of the internal body, as well as to reduce the energy consumption during its braking. The present paper is devoted to the control of a capsbot with a linear spring. Taking as a basis the results of cited papers, we will look for the parameters of the spring and the control law, providing the maximal average velocity of the robot.
2 PROBLEM STATEMENT

The physical model of the capsubot is shown in Fig. 1. It consists of a capsule shell \( m_1 \), interacting with an internal moving mass \( m_2 \) and with a horizontal support. Let \( y \) be the relative position of the inner body, \( x \) is the position of the shell with respect to an external fixed frame, and \( v = \dot{x} = \frac{dx}{dt} \). The following forces will be taken in account: (i) a control force \( F(t) \) is generated by an actuator, attached to the shell (not shown), and acts on the inner body; (ii) a force \( G(y) \), generated by a linear spring, acts on the inner body (the opposite force is applied to the shell); (iii) friction force \( T(v) \) between the shell and support.

Equations of motion in Newton form are

\[
(m_1 + m_2) \ddot{y}_0 = (m_1 + m_2) \dot{v} + m_2 \ddot{y} = T(v), \quad m_2 (\dot{v} + \dot{y}) = F(t) + G(y)
\]  

(1)

where \( v_0 \) is velocity of the mass center. Define friction force by the Coulomb friction law

\[
T(v) = -T_0 \operatorname{Sign} v, \quad T_0 = k (m_1 + m_2), \quad k = fg, \quad \operatorname{Sign} v = \begin{cases} 
1, & v > 0 \\
-1, & v < 0 \\
[-1,1], & v = 0
\end{cases}
\]

(2)

where \( g \) is acceleration of gravity and \( f \) is the coefficient of friction. If the capsule moves to the right, then \( v > 0 \) and \( T = -T_0 \); similarly, we have \( v < 0 \) and \( T = T_0 \) for sliding to the left. In the stick phase \( v = 0 \), then according to (1)

\[
\alpha \ddot{y} \in [-k,k], \quad \alpha = \frac{m_2}{m_1 + m_2}
\]

(3)

Assume that control function \( F(t) \) is \( \tau \) - periodic, piecewise continuous, and has zero mean value, i.e.

\[
\langle F(t) \rangle = \frac{1}{\tau} \int_{0}^{\tau} F(t) dt = 0
\]

(4)
then \( v(t) \) is continuous, and \( y(t) \) is smooth. We look for such control that functions \( v(t) \) and \( y(t) \) are \( \tau \) - periodic and maximize average velocity of the robot:

\[
\langle v(t) \rangle = \frac{1}{\tau} \int_0^\tau v(t) dt \to \max \quad \text{s.t.} \quad |F(t)| \leq M, \quad y(t) \in [0, L]
\]  

(5)

3 SIMPLEST CASE: NO SPRING

First discuss the case \( G(y) \equiv 0 \) [2]. Then in eqs (1) \( v \) does not depend on \( y \) directly:

\[
m_1 \ddot{y} = -k(m_1 + m_2) - F(t), \quad \alpha m_2 \ddot{y} = km_2 + F(t)
\]  

(6)

In such statement, problem (5) has the optimal periodic solution (period \( \tau \) being fixed) [2]:

\[
F(t) = \begin{cases} 
-M, & t \in [0, \tau_1) \\
M, & t \in [\tau_1, \tau_2), \\
T_0, & t \in [\tau_2, \tau] 
\end{cases}
\]

\[
\tau_1 = \frac{\tau}{4} \left( 1 + \frac{T_0}{M} \right), \quad \tau_2 = \frac{\tau}{2}
\]

(7)

According to (7), the three-step control profile is used here: acceleration of the shell, its deceleration, and rest. The conditions of Pontryagin’s principle are satisfied, since the maximal admissible control is used at each phase of motion. A geometric interpretation of the optimal solution is presented in the phase plane \((y, \dot{y})\) (Fig.2, a). Each of the three steps is depicted by a parabolic arc; these lines form a closed loop.

![Fig.2. Periodic motions of the robot a) no spring: (i) acceleration AB (green); (ii) deceleration BC (red); (iii) rest phase CA (black); b) with spring: acceleration AC, two-step rest phase CCA.](image)

4 ADDING A LINEAR SPRING

Suppose now that function \( G(y) \) in eq. (1) is linear: \( G(y) = -c(y - y_0) \) and modify formula (7) for this case. In the acceleration phase we have \( F(t) = -M \), and the equations of motion are
\[ \ddot{v} + \alpha \dot{v} = -k, \quad \dot{m}_2 (\ddot{v} + \dot{v}) = -M + G(y) \]  

(8)

Therefore,

\[ m_1 \ddot{v} = -k(m_1 + m_2) + M - G(y), \quad \alpha m_1 \ddot{y} = km_2 - M + G(y) \]  

(9)

The second equation here can be considered separately. It admits one-parameter family of solutions, satisfying given length restriction:

\[ y(t) = \frac{L}{2} \left(1 + \cos \omega t\right), \quad \dot{y}(t) = -\frac{\omega L}{2} \sin \omega t \]

(10)

\[ c = \frac{m_1 m_2}{m_1 + m_2} \omega^2, \quad y_0 = \frac{L}{2} + \frac{M - km_2}{c} \]

The presence of the spring allows to increase the acceleration of the shell, as well as eliminate the braking phase. Let \( A \) be such point at which the shell begins to move (Fig.2,b), its position on the curve (10) is defined by a value \( t = t_A \). Substituting expressions (10) into the first formula (8), we obtain after integration:

\[ v(t) = -k \left(t - t_A\right) + \alpha \omega \frac{L}{2} \left(\sin \omega t - \sin \omega t_A\right) \]  

(11)

Now we can determine point \( C \) as first root of equation \( v(t_C) = 0 \). Thus, \( t_C = t_A + 2 \theta / \omega \), where \( \theta \) is first positive root of equation

\[ \theta = \sigma \sin \theta \cos (\varphi_A + \theta), \quad \theta = \frac{\varphi_C - \varphi_A}{2}, \quad \sigma = \frac{cL}{2 km_1}, \quad \varphi = \omega t \]  

(12)

Further, in the rest phase \( v \equiv 0 \), hence

\[ m_2 \ddot{y} = T, \quad m_2 \ddot{y} = F(t) + G(y) \]  

(13)

which is consistent provided

\[ F(t) + G(y(t)) = T \]  

(14)

In view of (5) we should minimize the duration of this part. This is known minimum time control problem: how to get point \( A \) starting from point \( C \) as fast as possible under restriction \( \alpha |\dot{y}| \leq k \). The solution curve is either parabola \( \alpha \dot{y} = k \) or two parabolic arcs \( \alpha \dot{y} = \pm k \) depending on the coordinates of points \( C \) and \( A \). Both arcs belong to the region \( y \in [0, y_A] \). If \( \alpha \dot{y} = k \), then \( T = T_0 \) and to fulfil equality (14) for any \( y \in [0, L] \) it is sufficient that

\[ 2M \geq k(m_1 + 2m_2) + \frac{cL}{2} \]  

(15)
In fact, in this case we can impose condition (14) only on the interval \( y \in [0, y_A] \) (which covers the arc \( CC' \)). Similarly, in the case \( T = -T_0 \) non-slip condition (14) must be satisfied for \( y \in [y_C, y_A] \), i.e.

\[
y_C \geq \frac{L}{2} \left(1 + \frac{1}{\sigma} \right)
\]

which is rather restrictive. To satisfy both conditions (15) and (16), it is necessary that \( M \geq T_0 \).

To evaluate duration of the rest phase, note that equation \( \alpha \ddot{y} = k \) is equivalent to

\[
y = \frac{\alpha}{2k} \dot{y}^2 + \gamma, \quad \gamma = \text{const}
\]

If points \( C \) and \( A \) belong to the same line (17), then the black line in Fig.2,b is single parabolic arc, and duration of the rest phase equals

\[
\tau_0 = \alpha \left( \dot{y}_A - \dot{y}_C \right) / k
\]

Otherwise, the fastest path from \( C \) to \( A \) consist of two arcs: \( \alpha \ddot{y} = k \) and \( \alpha \ddot{y} = -k \). The total duration of such path is

\[
\tau_0 = \frac{\alpha}{k} \left( 2 \sqrt{ \frac{k|\gamma_A - \gamma_C|}{\alpha}} + \dot{y}_A^2 - \dot{y}_A - \dot{y}_C \right)
\]

where the values \( \gamma_A \) and \( \gamma_C \) are defined by (14) for points \( A \) and \( C \), correspondingly. With account of (10) and (12),

\[
\gamma_A - \gamma_C = L \sin(\varphi_A + \theta) (\sin \theta + \vartheta \cos \theta)
\]

The total period \( \tau \) is the sum of \( \tau_0 \) and the duration of the first phase \( \tau_1 = t_C - t_A \).

The path \( S \), taken by the shell in one period, can be calculated by integration of (11):

\[
S = \alpha L \sin(\varphi_A + \theta) (\sin \theta - \vartheta \cos \theta)
\]

Finally,

\[
\langle v(t) \rangle = \frac{S}{\tau_0 + 2\vartheta / \omega}
\]

5 RESULTS AND DISCUSSION

We discuss the feasibility of adding a spring for two cases: \( \chi = M / T_0 < 1 \) and \( \chi \gg 1 \). Take initial point \( A \) (see Fig.2,b) such that
\[c(y_A - y_0) = M + T_0\]  
(22)

In view of (9), the value of \(y_A\) is maximum possible to keep the shell at rest just before the acceleration phase (we set here \(F = M\)). To start the acceleration, we assume \(F = -M\), so at this moment first eq. (9) becomes

\[m_1\dot{v} = 2M > 0\]

Note that the acceleration rate here is maximal regardless the coefficients of elasticity and friction. Therefore, the capsubot can move even for \(\chi < 1\) in contrast to a robot without spring. However, in this case motion in the rest phase will be rather slow. Indeed, in this case inequality (15) is violated. To ensure the rest phase, we should modify formulas (15), (16) by replacing \(k\) with such value \(k' < k\) that they became true, i.e.

\[\beta + (1-\alpha)\sigma \leq \min\{\alpha, 2\chi - \alpha\}, \quad \beta = \frac{k'}{k} < 1\]  
(23)

Note that the value \(k'\) will appear in denominator of (18) instead of \(k\), thus there is a reason to increase \(\beta\). In turn, the parameter \(\sigma\) is proportional to the spring elasticity, it determines the duration of the propulsion phase and the distance travelled. In view of physical restriction (25), it’s impossible to increase both parameters. Hence, an optimal relation between them is to be found. For this purpose, the following algorithm can be implemented.

Suppose that the parameters \(m_1, m_2, k_1, k_2\), and \(\chi < 1\) are given. Explore admissible scope of variables \(\beta\) and \(\sigma\) in accordance with inequality (23). First we choose maximal value \(y_A\) with account of restriction (23). Unfortunately, the solution to (22)

\[\alpha(1-\alpha)\cos\phi_A = 2\chi + \beta - \alpha\]  
(24)

is not admissible, and we are to replace the control force \(M\) in equation (21) with some \(M' < M\). This implies the relation

\[\sigma(1-\alpha)\cos\phi_A = 2\chi' + \beta - \alpha, \quad \chi' = M'/T_0 < \chi\]  
(25)

Then the conditions \(\cos\phi_A \leq 1\) and (23) are equivalent to the system

\[\chi' + \beta \leq \alpha, \quad \chi' + \beta \leq \chi\]  
(26)

Then find the first positive root of equation (12). At last, perform the calculations by formulas (18)-(21).

**Example.** Let \(\alpha = \chi = 0.8, \phi_A = 0\). To satisfy (23), put

\[\sigma = 4 - 5\beta, \quad \beta \in (0, 0.8)\]

then equation (12) has form

\[2\theta = \sigma \sin 2\theta\]  
(27)
The interval $\sigma \in (0, 4)$ correspond to the root of eq.(27) in the range $\theta \in (0, 1.2)$. Numerical calculations by formulas (18) – (21) lead to the dependence $\langle v(t) \rangle (\theta)$, shown in Fig.3. A single maximum is situated at

![Fig.3. Typical dependence of normalized average velocity on the parameter $\theta$ (radians)](image)

The case $\chi \gg 1$ can be considered qualitatively. In view of (10), (21) we assume

$$\sigma = \frac{km_1 \cos \varphi_4}{km_1 + 2M} = O(\chi^{-1}), \quad c = \frac{2km_1 + 4M}{L \cos \varphi_4} = O(\gamma)$$

We are free to choose $\varphi_4 \in (-\pi/2, 0)$, then we determine $\theta$ as first root of eq. (12):

$$\theta = \left( \frac{\pi}{2} - \varphi_4 \right)(1 - \sigma) + O(\chi^{-2})$$

Keeping in mind that the differnce $\gamma_4 - \gamma_C$ is bounded, we obtain

$$\langle v(t) \rangle \approx \frac{\alpha L \sqrt{c}}{4 \sqrt{\alpha m_1}} (\cos \varphi_4 - (\pi/2 - \varphi_4) \sin \varphi_4) \approx 2 \sqrt{\frac{\alpha LM}{m_1}} \frac{\cos \varphi_4 - (\pi/2 - \varphi_4) \sin \varphi_4}{\sqrt{\cos \varphi_4}}$$

As $\chi \to \infty$, the value $c$ is large, and in theory the last fraction in (28) can be arbitrary big. We conclude that the use of springs is advisable both to increase the speed of the mobile device, and to ensure its movement with a low-power motor.

**ACKNOWLEDGEMENTS**

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REFERENCES


A HYBRID METHOD FOR THE SIMULATION OF
AEROACOUSTIC EFFECTS INDUCED BY RIGID BODY
MOTION IN TURBULENT FLOW

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Key words: Aeroacoustics, Fluid-Structure Interaction (FSI), Splitting Approach

Abstract. In the present work an approach for the simulation of aeroacoustic effects induced by the interaction of a turbulent flow with moving structures is presented. The aeroacoustic sound field computation is based on an acoustic/viscous splitting approach. Acoustic radiation is computed based on the linearized Euler equations (LEE) and acoustic sources are derived from the incompressible flow field solution. An arbitrary Lagrangian-Eulerian (ALE) method is applied for coupling the fluid and acoustic fields with the mechanical field. The validity of this approach for acoustic simulations is shown using two classical acoustic test cases, which are extended to moving grids. Finally, the aerodynamic and acoustic effects induced by an oscillating cylinder in a turbulent flow are presented.

1 INTRODUCTION

The turbulent flow around blunt bodies induces aeroacoustic sources. This flow induced noise is one of the major contributors to transportation noise and has therefore a significant impact on our quality of life. The progress made in computational aeroacoustics (CAA) during the last few years has increased the use of simulations for acoustic research. While the majority of this research is focused on stationary geometries, surface deformations or low-frequency structural movements induced by fluid-structure interaction (FSI) are rarely considered. However, understanding the interaction between fluids and solids and its influence on aeroacoustic source mechanisms remains a crucial step towards understanding noise generation of real-world applications, such as wind turbines or aircraft wings.

Numerous hybrid methods exist for sound field computation which are based on the acoustic/viscous splitting approach. These methods are considered to be an efficient
way for computing aeroacoustic sound generated in turbulent flows at low Mach numbers ($Ma \leq 0.3$). The original idea, introduced by Hardin and Pope [1], is based on a decomposition of the flow field into incompressible and perturbed compressible variables. Further formulations were for example proposed by Seo and Moon [2] or Ewert and Schröder [3]. In this work a modification of the original acoustic/viscous splitting approach is used, which was proposed by Kornhaas et al. [4]. Acoustic sources are derived from the incompressible flow field solution and acoustic radiation is computed based on the LEE.

The efficient computation of FSI is still a demanding task. This is due to the coupling of two problems with different foundations, the Lagrangian structural field with the Eulerian fluid field. A widely used approach is the ALE method, introduced by Hirt et al. [5]. The boundary-fitted fluid grid is deformed in every time step depending on the structural displacement. The application of the ALE method to acoustic radiation can be found in Flitz [6]. An approach for modelling fluid-solid-acoustics interactions is presented by Link et al. [7] in the context of human phonation. A strong coupling between the fluid and solid was considered in this work. Schäfer et al. [8] studied the acoustic field induced by a thin and flexible structure in a turbulent wake. The influence of structural deformation on the flow field was not considered in this work. Both works based their aeroacoustic approach on a finite-element discretization of Lighthill’s equation [9]. In contrast, the present work investigates the application of a finite-volume discretization of the acoustic equations derived from an acoustic/viscous splitting approach. Using the same discretization method for the acoustic field and for the incompressible flow field reduces communication costs and allows the influence of background flow on the acoustic field to be accounted for more easily.

The goal of the present work is to investigate an application of the ALE method to hybrid methods in CAA. Therefore, acoustic radiation and source term calculation on moving grids are investigated. Finally, the forced oscillation of a cylinder in a turbulent flow and the induced aeroacoustic effects are presented. This is considered an essential step towards computing aeroacoustic effects induced by a fully coupled FSI.

2 GOVERNING EQUATIONS

The acoustic/viscous splitting approach used is introduced in the following section and the governing equations for fluid mechanics and acoustics are described. Both fields are computed in the in-house finite-volume solver FASTEST [10]. Further emphasis is placed on the field interactions considered: solid-fluid and fluid-acoustics. The acoustic/viscous splitting approach is based on a decomposition of the total flow variables density $\rho$, pressure $p$ and velocity $\vec{v}$ into

$$
\rho = \rho^I + \rho^a,
$$

$$
\vec{v} = \vec{v}^I + \vec{v}^a,
$$

$$
p = p^I + p^a,
$$

where $\rho^I$, $\rho^a$, $\vec{v}^I$, $\vec{v}^a$, $p^I$, $p^a$ are the incompressible and perturbed compressible variables, respectively.
where the incompressible variables are denoted by \((I)\) and the acoustic fluctuations are denoted by \((a)\).

### 2.1 Fluid mechanical setup

The fluid field is determined by the incompressible Navier-Stokes equations in ALE formulation

\[
\nabla \cdot \vec{v}^I = 0 ,
\]

\[
\rho^I \frac{\partial \vec{v}^I}{\partial t} + \rho^I (\vec{v}^I - \vec{v}^g) \cdot \nabla \vec{v}^I + \nabla p^I - \mu^I \Delta \vec{v}^I = 0 ,
\]

where \(\mu^I\) is the dynamic viscosity. The ALE approach includes the velocity of the reference system \(\vec{v}^g\) into the Navier-Stokes equations (2) in order to account for moving boundaries. In the present work structural movements are prescribed. At the interface of solid and fluid kinematic continuity has to be ensured with

\[
\vec{v}^I = \vec{v}^S ,
\]

where \(\vec{v}^S\) is the structural velocity.

### 2.2 Aeroacoustic setup

Inserting the acoustic/viscous splitting approach (1) into the compressible Navier-Stokes equations after simplifications, results in a set of partial differential equations describing the acoustic field [4]

\[
\frac{\partial \rho^a}{\partial t} + (\vec{v}^I - \vec{v}^g) \cdot \nabla \rho^a + \rho^I (\nabla \cdot \vec{v}^a) = 0 ,
\]

\[
\rho^I \frac{\partial \vec{v}^a}{\partial t} + \rho^I (\vec{v}^I - \vec{v}^g) \cdot \nabla \vec{v}^a + \nabla p^a = 0 ,
\]

\[
\frac{\partial p^a}{\partial t} + \rho^I c^2 (\nabla \cdot \vec{v}^a) + (\vec{v}^I - \vec{v}^g) \cdot \nabla p^a = -\frac{\partial p^I}{\partial t} + \vec{v}^g \cdot \nabla p^I ,
\]

where \(c\) is the speed of sound. The left hand side of this set of acoustic equations are the LEE, which describe acoustic wave propagation. An ALE approach is used analogously to the fluid mechanical setup. The equations return to the Eulerian formulation if the system is not moved \((\vec{v}^g = 0)\). The acoustic sources on the right hand side are derived from the incompressible flow field and provide a coupling mechanism between both fields. The ALE approach is also applied here.

### 3 NUMERICAL METHODS FOR ACOUSTICS

The set of acoustic equations (4) can be reduced to a one-dimensional problem at each cell interface. This is achieved by transforming the state of both neighbouring cells into
a local coordinate system \( \{ \vec{e}_\xi, \vec{e}_\eta, \vec{e}_\zeta \} \), which is normal to the cell interface. The matrix form of the set of acoustic equations (4) becomes

\[
\frac{\partial \vec{q}}{\partial t} + A \frac{\partial \vec{q}}{\partial \xi} = \vec{s}
\]

with the variable vector

\[
\vec{q} = \begin{bmatrix} \rho_a v_\xi^a & v_\eta^a & v_\zeta^a & p^a \end{bmatrix}^T,
\]

the coefficient matrix

\[
A = \begin{bmatrix}
v_\xi - v_\xi^g & \rho_I & 0 & 0 & 0 \\
0 & v_\xi - v_\xi^g & 0 & 0 & \frac{1}{\rho_I} \\
0 & 0 & v_\xi - v_\xi^g & 0 & 0 \\
0 & 0 & 0 & v_\xi - v_\xi^g & 0 \\
0 & \rho_I c^2 & 0 & 0 & v_\xi - v_\xi^g
\end{bmatrix}
\]

and the source vector

\[
\vec{s} = \begin{bmatrix} 0 & 0 & 0 & -\frac{\partial p_I}{\partial t} + \vec{v}^g \cdot \nabla p_I \end{bmatrix}^T.
\]

A fractional step method is applied in order to split the matrix form (5) into the homogeneous LEE and an ordinary differential equation describing acoustic source terms. The solution of this first sub-problem is obtained by solving a Riemann problem normal to the cell interface. The resulting waves are then rotated back into the original coordinate system and the neighbouring cell states are updated. A high-resolution scheme is applied for the acoustic fluxes using the first-order Godunov method in combination with the second-order Lax-Wendroff method and a van Leer limiter [11] if not stated otherwise. A forward Euler method is applied to solve the ordinary differential equation. The acoustic source term described in equation (8) is computed from the incompressible flow field using a first-order backward scheme

\[
\frac{\partial p_I^{l,n}}{\partial t} = \frac{p_I^{l,n} - p_I^{l,n-1}}{\Delta t},
\]

where \( \Delta t \) is the time step size and \( n \) indicates the time step.

4 ACOUSTIC ON MOVING GRIDS

The application of an ALE approach to the set of acoustic equations (4) has been assessed by a number of test cases. Two test cases are presented as follows. The first case is a Gaussian pulse and the second a monopole source. Dimensionless variables with respect to the following scales are used: The speed of sound \( c \) and the ambient density \( \rho_I \) are used as the velocity and density scales, respectively. The pressure is nondimensionalized by \( \rho_I c^2 \). The length and time scales are case-dependant. Both test cases have been extended to moving grids.
4.1 Gaussian pulse

In order to verify the ALE approach with respect to acoustic wave propagation, a 2D Gaussian pulse is considered. The length scale is given by $0.05L$, where $L$ is the domain width and time is scaled with $0.05L/c$. The Gaussian pulse is emitted with the initial values

$$p_{t=0}^a = \exp\left(-4\alpha \left(x^2 + y^2\right)\right),$$

$$v_{x,t=0}^a = \beta y \exp\left(-\alpha \left((x - 6.7)^2 + y^2\right)\right),$$

$$v_{y,t=0}^a = -\beta (x - 6.7) \exp\left(-\alpha \left((x - 6.7)^2 + y^2\right)\right),$$

$$\rho_{t=0}^a = \exp\left(-4\alpha \left(x^2 + y^2\right)\right) + 0.1 \exp\left(-\alpha \left((x - 6.7)^2 + y^2\right)\right)$$

with $\alpha = \ln(2)/4$ and $\beta = 0.04$. The analytical solution to this setup can be found in [12]. The computational domain has an extension of $(x, y) \in [-10, 10] \times [-10, 10]$ with $513 \times 513$ grid points and a regular grid spacing at initialization ($t = 0$). After the initialization a time-dependent displacement $\Delta x$ and $\Delta y$ is prescribed at each grid point with

$$\Delta x (t) = \left(L \exp\left(x_0/L + 0.5\right) - 1 \exp(1) - 1 \right) \frac{t}{T},$$

$$\Delta y (t) = \left(L \exp\left(y_0/L + 0.5\right) - 1 \exp(1) - 1 \right) \frac{t}{T},$$

where $(x_0, y_0)$ is the corresponding starting position and $T = 5$ is the final time of evaluation. Figure 1 shows the final grid point distribution and the corresponding acoustic pressure $p^a$.

![Figure 1: Instantaneous acoustic pressure $p^a$ (every 8th grid line shown)](image)
pressure field. The instantaneous acoustic pressure fields along the line $y = 0$ computed by the ALE approach and the Eulerian description ($\vec{v}_g = 0$) are compared in Figure 2. The acoustic pressure distribution computed with an Eulerian formulation results in a shift of the pulse due to the grid movement while the ALE approach agrees well with the exact solution.

The convergency of the acoustic scheme is investigated by varying the grid spacing $h$ while keeping a constant CFL number ($c\Delta t/h$) of 0.2 at initialization. Even though the CFL number changes during the simulation due to the grid movement, it is consistent between the different grid resolutions. Figure 3 presents $L_1$ and $L_2$ pressure errors calculated with the exact solution. The expected behaviour of a first-order Upwind and a second-order Lax-Wendroff scheme is maintained on moving grids. The Van Leer limiter reproduces a second order for this relatively smooth test case. The results show that the ALE approach is well suited for computing acoustic radiation on moving grids.

![Figure 2: Comparison of acoustic pressure $p^a$ along the line at $y = 0$](image1)

![Figure 3: $L_1$, $L_2$ error for Upwind, Van Leer (VL) and Lax-Wendroff (LW)](image2)

### 4.2 Monopole source

In order to assess the acoustic source term calculation on moving grids, a two-dimensional monopole source is considered. The length scale is given by $0.01L$, where $L$ is the domain width and time is scaled with $0.01L/c$. A sinusoidal sequence of the incompressible pressure is prescribed by

\[
p^I (x, y, t) = -A \omega \sin(\omega t) \exp \left( -\ln (2) \frac{x^2 + y^2}{w^2} \right)
\]

(12)
with an amplitude of \( A = 0.01 \), an angular frequency of \( \omega = \pi/5 \) and the pulse half width \( w = 25/8 \). The analytical solution to this setup can be found in [12]. The computational domain has an extension of \((x, y) \in [-50, 50] \times [-50, 50]\) with 513 \times 513 grid points and a regular grid spacing at initialization \((t = 0)\). After the initialization a time-dependent displacement \( \Delta x \) and \( \Delta y \) is prescribed at each grid point with

\[
\begin{align*}
\Delta x (t) &= \left( L \exp \left( \frac{x_0}{L} + 0.5 \right) - 1 \right) \left( \frac{x_0}{L} - \frac{L}{2} \right) \sin (2\pi \omega g t), \\
\Delta y (t) &= \left( L \exp \left( \frac{y_0}{L} + 0.5 \right) - 1 \right) \left( \frac{y_0}{L} - \frac{L}{2} \right) \sin (2\pi \omega g t),
\end{align*}
\]

where \((x_0, y_0)\) is the corresponding starting position and \( \omega g = 2\pi/100 \) is the circular oscillation frequency of the grid. The locations of the control volume centres, where flow field variables are stored, change from one time step to the next due to the grid movement as illustrated in Figure 4 exemplary for one location \( Q \).

![Schematic of the bilinear interpolation method](image)

Figure 4: Schematic of the bilinear interpolation method

As an alternative to the ALE approach described in equation (4), an Eulerian description of the acoustic source term \( (\vec{v}^g = 0) \) is investigated in combination with a bilinear interpolation of the incompressible pressure field from one time step to the next. For Cartesian grids the pressure from the old time step \( p^{I,n-1} \) but at the new location \( Q^n \), which is required in equation (9), can be approximated with

\[
p^{I,n-1} (x, y) = \frac{1}{(x_2 - x_1)(y_2 - y_1)} \begin{bmatrix} x_2 - x \\ x - x_1 \end{bmatrix}^T \begin{bmatrix} p^{I,n-1} (x_1, y_1) & p^{I,n-1} (x_1, y_2) \\ p^{I,n-1} (x_2, y_1) & p^{I,n-1} (x_2, y_2) \end{bmatrix} \begin{bmatrix} y_2 - y \\ y - y_1 \end{bmatrix}
\]

As an example of the results, Figure 5 presents the final acoustic pressure field \((t = 100)\) computed with the ALE description of the acoustic source term. Figure 6 compares the final acoustic pressure fields along a section of the line \( y = 0 \) for both investigated methods. The Eulerian formulation without interpolation induces erroneous acoustic sources due to the grid adaptation. The ALE approach and the bilinear interpolation method reduce
these errors significantly and show a good agreement with the analytical solution. The results show that the ALE approach is well suited for computing acoustic source terms on moving grids.

5 OSCILLATING CYLINDER IN TURBULENT FLOW

The aerodynamic and aeroacoustic effects induced by the flow past a cylinder undergoing forced oscillation at Reynolds number $Re_D = 10000$ and Mach number $Ma = 0.044$ are investigated. This Reynolds number was chosen due to the availability of reference data for aerodynamic quantities [13, 14]. It should be noted that the experiments were conducted in a water channel, while air is used in the present work with the fluid properties given in Table 1.

<table>
<thead>
<tr>
<th>Table 1: Fluid properties</th>
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</thead>
<tbody>
<tr>
<td>Fluid density $\rho^f$</td>
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<tr>
<td>Dynamic viscosity $\mu^f$</td>
</tr>
<tr>
<td>Speed of sound $c$</td>
</tr>
</tbody>
</table>

5.1 Aerodynamic results

The unsteady incompressible flow field is computed via Large Eddy Simulation (LES), using a Smagorinsky subgrid-scale model with the dynamic approach of Germano [15].
Convective and diffusive fluxes are approximated with a second-order central difference scheme. A fully implicit first-order scheme is applied for time discretization. The flow computation is performed on an O-grid with a radial extension of $L_r = 225D$ and a spanwise extension of $L_z = \pi D$. The domain consists of $580 \times 480 \times 32$ grid points in the circumferential, radial, and spanwise directions, respectively. Periodic boundary conditions are applied in the $z$-direction and no slip walls are applied at the cylinder surface. The boundary layer is resolved with a dimensionless wall distance of $y^+ \approx 1$. The time step for the LES is $\Delta t = 2.0 \cdot 10^{-6}$ s, which results in a CFL number below unity. A comparison of the computed aerodynamic coefficients for the flow past a stationary cylinder with experimental data and DNS results is presented in Table 2.

### Table 2: Comparison of aerodynamic coefficients

<table>
<thead>
<tr>
<th></th>
<th>Stationary</th>
<th>Oscillating</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$C_{Dm}$</td>
<td>$C_{L,rms}$</td>
</tr>
<tr>
<td>Exp., Gopalkrishnan [13]</td>
<td>1.186</td>
<td>0.384</td>
</tr>
<tr>
<td>DNS, Dong [14]</td>
<td>1.143</td>
<td>0.448</td>
</tr>
<tr>
<td>LES, Present</td>
<td>1.170</td>
<td>0.439</td>
</tr>
</tbody>
</table>

The Strouhal number $St$, the mean drag coefficient $C_{Dm}$ and the root mean square value of the lift coefficient $C_{L,rms}$ are found to be in good agreement with reference data. In the case of forced oscillation the rigid cylinder is moved with

$$y = Y_0 \sin (2\pi f_0 t) \quad ,$$

where $Y_0 = 0.15D$ is the maximum displacement of the cylinder and $f_0 = 0.165U_0/D$ is the oscillation frequency. The grid adaptation is limited to a radius of $r = 20D$ around the cylinder and is performed with transfinite interpolation [16]. The experiments conducted by Gopalkrishnan [13] showed that this oscillation frequency falls into the range of a quasi-periodic non-lock-in region. The lift force measured in these experiments shows an irregular time response with random fluctuations between the natural Strouhal frequency and the oscillation frequency and the same behaviour is also observed for the present LES results. Table 2 compares the computed aerodynamic coefficients for the flow past an oscillating cylinder with experimental reference data. The phase angle $\Phi_0$, which describes the phase difference between the lift component oscillating with the same frequency as the body motion and the imposed displacement, is at the higher end of the range of measured values. The resulting lift coefficient in phase with the oscillation velocity $C_{L,V_0}$ is therefore at the lower end of the range of measured values. A possible reason for this is that the oscillation frequency lies in a range where a small difference in oscillation frequency results in a large change in aerodynamic coefficients.
5.2 Acoustic results

Applying periodic boundary conditions to the spanwise width used for the incompressible flow field results in an un-physically correlated acoustic field. In order to avoid this, the approach introduced by Oberai et al. [17] is followed. A two-dimensional acoustic field is calculated on the mid-span plane ($z = 0$) with acoustic sources integrated in the spanwise direction:

$$\tilde{s}_{2D}(x, y, t) = \int_{-L_z/2}^{L_z/2} \tilde{s}_{3D}(x, y, z, t) \, dz .$$  \hfill (16)

The three-dimensionally radiated acoustic pressure in the far field $p_{3D}^a$ is approximated from the two-dimensional acoustic pressure $p_{2D}^a$ in the frequency domain with

$$p_{3D}^a(x, y, 0, \omega) \approx p_{2D}^a(x, y, \omega) \frac{1 + i}{2} \frac{\omega}{\omega_{cr}} ,$$  \hfill (17)

where $r$ is the distance from the source to the observer. The acoustic time step is set to $\Delta t^a = \Delta t/150$, which results in an acoustic CFL number of 0.41. The acoustic pressure field is evaluated in the mid-span plane at a distance $r = 50D$ from the cylinder centre and at 90° to the flow direction. Overall 40 cycles of the natural shedding frequency are analysed after a quasi-periodic stage of the flow is established. The acoustic power spectral density $PSD$ is calculated by segmenting the obtained time signal into seven blocks with an overlap of 50% and averaging the results. Figure 7 presents the $PSD$ for a stationary and an oscillating cylinder. The main peak in $PSD$ occurs for both cases at the natural vortex shedding frequency. In the case of forced oscillation a second peak is observed at oscillation frequency. This coincides with the lift coefficient, which also has components at both the natural Strouhal and oscillation frequency.

![Figure 7: Power spectral density of acoustic pressure at $r = 50D$](image-url)
6 CONCLUSIONS

A hybrid method for the numerical simulation of aeroacoustic phenomena associated with rigid body motion has been investigated. The outlined method is based on an acoustic/viscous splitting approach in combination with an ALE approach. The validity of the equations describing acoustic radiation and acoustic source terms on moving grids has been shown using two classical acoustic test cases. The results show a very good agreement with the analytic solutions. The approach has been used to study aeroacoustic effects induced by a cylinder undergoing forced oscillation.

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REFERENCES


ELASTOPLASTIC ANALYSIS OF MISES METAL
BY RETURN-MAPPING ALGORITHM
FOR EXTENDED SUBLOADING SURFACE MODEL

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Key words: Finite Element Method, Return-mapping, Subloading Surface Model, Consistent Tangent Modulus Tensor, Metal

Abstract. The extended subloading surface model is capable of representing not only monotonic but also cyclic loading behaviors accurately. The various return-mapping methods have been adopted to for the elastoplastic deformation analysis in FEM incorporating the subloading surface model. However, the past algorithms based on the expansion of the subloading surface is inapplicable to the cyclic loading behaviors. Then, the rigorous complete integration algorithm for Mises metal is adopted in this study. Additionally, it is implemented into the FEM software ABAQUS through the user-subroutine UMAT. The numerical calculations are performed for the forward and inverse loading processes by use of the proposed and the past implicit algorithms. A more accurate elastoplastic deformation analyses can be conducted by the proposed algorithm. Thus, it may be stated that the accurate numerical solution can be attained by adopting the proposed return-mapping algorithm for the general loading process.

1 INTRODUCTION

The subloading surface model does not incorporate the yield surface enclosing a purely-elastic domain. Instead, it is based on the natural postulate that the plastic strain rate develops as the stress approaches the yield surface [1, 2]. Therein, the subloading surface is incorporated, which passes through always the current stress point and keeps the similarity to the yield surface (the normal-yield surface). Therefore, the smooth transition from the elastic to the plastic state leading to the description of the continuous tangential modulus represents always in the subloading surface model. Moreover, the subloading surface model is capable of describing not only monotonic but also cyclic loading behaviors accurately.

The implicit stress integration algorithm based on the return-mapping for the subloading surface model in Mises metal has been studied in various approaches [3-7]. These loading criteria are based on the premise that the plastic strain rate is occurred by the expansion of the
subloading surface. Thus, these are limited to the description of monotonic loading behaviors and are unsuitable to the cyclic loading behaviors. In fact, the plastic strain rate is induced even when the subloading surface contracts in the elastic trial step if it once contracts but expands thereafter.

The return-mapping algorithm for the extended subloading surface model is formulated by incorporating the rigorous loading criterion in this study. It is capable of describing elastoplastic deformation in the general loading process involving not only monotonic but also cyclic loading for the Mises metals. Moreover, it has been implemented in the FEM software ABAQUS through the user-subroutine UMAT. Numerical analyses were performed not only for the forward loading but also the inverse loading in the multi-axial loading. In addition, the numerical calculations were performed by use of the past loading criterion in order to verify the necessity of the incorporation of the rigorous loading criterion.

2 EXTENDED SUBLOADING SURFACE MODEL

The constitutive equations in the extended subloading surface model [8] are addressed. The infinitesimal strain theory is adopted and the infinitesimal strain $\varepsilon$ is additively decomposed into the elastic strain $\varepsilon^e$ and the plastic strain $\varepsilon^p$. The Cauchy stress $\sigma$ is given by as following equation using Hooke’s law with the elastic modulus tensor $E$.

$$\varepsilon = \varepsilon^e + \varepsilon^p$$  \hspace{1cm} (1)

$$\sigma = E : \varepsilon^e = E : (\varepsilon - \varepsilon^p)$$  \hspace{1cm} (2)

The normal-yield surface for Mises metal is adopted. The subloading surface, which is similar to the normal-yield surface and passes though the current stress point, is given (Figure 1).

$$f(\sigma) = F(H)$$  \hspace{1cm} (3)

$$f(\sigma) = RF(H), \quad f(\sigma) = \sqrt{\frac{3}{2}} \|\sigma\|$$  \hspace{1cm} (4)

The following relations hold in the variables for the normal-yield surface and subloading surface.

Figure 1: Normal-yield, subloading, and elastic-core surfaces.
\[ \dot{\sigma} = \sigma - \alpha, \quad \tau = \sigma - \tilde{\alpha}, \quad \dot{\tau} = \tau - \alpha, \quad \ddot{\tau} = \tau - c = R(\sigma - \alpha) = \sigma - R\dot{\tau} \]

(5)

Where \( \alpha \) is the kinematic hardening variable, \( c \) is the elastic-core, and \( \tilde{\alpha} \) is the center of the subloading surface and the conjugate point to the kinematic hardening variable in the normal-yield surface. \( R (0 \leq R \leq 1) \) is the normal-yield ratio denoting the ratio of the size of the subloading surface to that of the normal-yield surface. The subloading surface coincides with the normal-yield surface when \( R=1 \). By contrast, the subloading surface become a point when \( R=0 \). The following equation is the evolution rule for the normal-yield ratio. \( R_\infty (0 \leq R_\infty < 1) \) is the material constant expressing the normal-yield ratio in the limit of the purely-elastic domain.

\[ R = U(R)||\dot{\tau}^p|| \text{ for } \dot{\tau}^p \neq 0 \]

(6)

\[ U(R) = u \cot \left( \pi \frac{R - R_\infty}{1 - R_\infty} \right) \]

(7)

\[ R = \frac{2}{\pi} \cos^{-1} \left\{ \cos \left( \frac{R_\infty - R}{1 - R_\infty} \right) \exp \left( -u \frac{||\dot{\tau}^p||}{1 - R_\infty} \right) \right\} + R_\infty \]

(8)

Where \( (*) \) denotes the material time derivative and \( \{ \} \) is Macauley's bracket.

The elastic-core surface, which passes through the elastic-core and is similar to the normal-yield surface with respect to the kinematic hardening variable is introduced. \( R_\infty (0 < R_\infty < 1) \) is the ratio of the size of the elastic-core surface to that of the normal-yield surface. The elastic-core limit surface is introduced to regulate the elastic-core to move only inside of it because it is inapplicable that the elastic-core coincides normal-yield surface.

\[ f(\dot{\tau}) = g_\infty F(H) \]

(9)

\[ f(\dot{\tau}) = \chi F(H) \]

(10)

Where \( \chi (<1) \) is a material constant expressing the limit of the elastic-core surface.

The plastic strain rate is given by the associated flow rule and the normalized outward-normal vector of the subloading surface \( \vec{n} \).

\[ \dot{\varepsilon}^p = \dot{\lambda} \vec{n}, \quad \vec{n} = \frac{\partial f(\sigma)}{\partial \sigma} \left| \frac{\partial f(\sigma)}{\partial \sigma} \right| \]

(11)

Where \( \dot{\lambda} (\geq 0) \) is the plastic multiplier. The evolution of the elastic-core, isotropic and kinematic hardening is given by the non-linear hardening rule.

\[ \dot{\tilde{\alpha}} = s \lambda C_\alpha \left( \vec{n} - \frac{g_\infty}{\chi} \vec{a} \right) \]

(12)

\[ F(H) = F_0 \left\{ 1 + h_1 \left[ 1 - \exp(-h_2 H) \right] \right\}, \quad \dot{H} = \frac{2}{3} ||\dot{\varepsilon}^p|| \]

(13)

\[ \dot{a} = a \lambda = a \left( \vec{n} - \frac{\sqrt{3}}{r_a F(H) a} \right) \lambda \]

(14)

\( F_0 \) is the initial value for isotropic hardening function, and \( C_\alpha, h_1, h_2, a_\alpha \) and \( r_\alpha \) are the material constants.
3 RETURN-MAPPING ALGORITHM

3.1 Rigorous loading criterion

The complete implicit stress integration algorithm based on the return-mapping is adopted, in which the strain increment $\Delta \varepsilon_{n+1}$ inputs the elastic deformation in the elastic trial step [9]. The elastic trial stress $\sigma_{\text{trial}}^{n+1}$ is calculated by the elastic equation using the elastic strain $\varepsilon_{n}$ in step n and the strain increment, where, the subscript denotes the number of steps.

$$\sigma_{\text{trial}}^{n+1} = E : (\varepsilon_{n} + \Delta \varepsilon_{n+1})$$  \hspace{1cm} (15)

The following loading criterion has been adopted for the subloading surface model in the past [3-6].

$$\begin{cases} f \left( \sigma_{n+1}^{\text{trial}} - \bar{\sigma}_{n} \right) - R_{s} F \left( H_{s} \right) \leq 0 \text{ or } f \left( \sigma_{n+1}^{\text{trial}} - \bar{\sigma}_{n} \right) - R_{s} F \left( H_{s} \right) \leq 0 : \Delta \sigma_{n+1}^{p} = 0, \ σ_{n+1}^{\text{trial}} = \sigma_{n+1}^{\text{trial}} \\
\text{Otherwise} \quad : \Delta \varepsilon_{n+1}^{p} \neq 0, \ σ_{n+1}^{\text{trial}} \neq \sigma_{n+1}^{\text{trial}} \end{cases}$$  \hspace{1cm} (16)

The past loading criterion is based on the premise that the elastic trial stress goes out for the plastic loading process from the subloading surface and the purely-elastic domain in the step n. In fact, however, the plastic strain rate is induced even when the subloading surface contracts in the elastic trial step if it once contracts but expands thereafter. In order to explain this fact concisely, the example of inverse monotonic loading process is shown in Figure 2. The elastic trial stress is directed toward the interior of the current subloading surface, and the subloading surface in elastic trial step once contracts. However, it re-expands larger than purely-elastic domain. Therefore, this elastic trial step is the plastic loading process which the elastic trial stress goes out from the subloading surface and the purely-elastic domain. It is necessary to occur the plastic strain rate even when subloading surface contracts in the elastic trial step if it once contracts but expands thereafter. However, the past loading criterion can’t consider this fact and is inapplicable to describe of cyclic loading behaviors.

The numerical errors using the past loading criterion can be prevented by setting the input increment to be sufficiently small. However, the advantage of highly accurate and efficient calculation in return-mapping is not performed. Then, the rigorous loading criterion is adopted in this study. In the rigorous loading criterion, it formulated based on the fact in Figure 3.

(1) When the elastic trial stress increment $\Delta \sigma_{n+1}^{\text{trial}} = \sigma_{n+1}^{\text{trial}} - \sigma_{n}$ goes out from the subloading surface and the purely-elastic domain in the step n, the plastic strain rate is induced.

![Figure 2](image-url): Inverse loading process: the subloading surface in elastic trial step re-expand after once contraction.
When the elastic trial stress increment \( \Delta \sigma_{\text{trial}} \) goes in for an inverse loading process the subloading surface in the step \( n \) (\( \hat{n} : \Delta \sigma_{\text{trial}} > 0 \)). The plastic strain rate is induced even when the subloading surface contracts in the elastic trial step if it once contracts but expands thereafter. In this case elastic trial stress increment and outward-normal vector of the subloading surface in the elastic trial step (\( \hat{n} : \Delta \sigma_{\text{trial}} > 0 \)) forms an acute angle (\( \theta \leq 90^\circ \)). However, the plastic strain rate is not induced when the elastic trial stress (\( \hat{n} : \Delta \sigma_{\text{trial}} > 0 \)) is inside the purely-elastic domain (\( f(\hat{\sigma}_{\text{trial}} - \hat{a}_n^* ) = R_F(H_e) < 0 \)).

Thus, the following loading equations are introduced as the rigorous loading criterion.

\begin{align}
(1) \quad \hat{n}_{\text{trial}} : \Delta \sigma_{\text{trial}} \geq 0 & \quad \text{(Forward loading)} \\
& \begin{cases} 
(i) & f(\hat{\sigma}_{\text{trial}} - \hat{a}_n^* ) - R_F(H_e) \leq 0 : \Delta \varepsilon_{\text{trial}}^p = 0, \quad \sigma_{\text{trial}} = \sigma_{\text{trial}} \nn 
(ii) & f(\hat{\sigma}_{\text{trial}} - \hat{a}_n^* ) - R_F(H_e) > 0 : \Delta \varepsilon_{\text{trial}}^p \neq 0 
\end{cases} \\
(2) \quad \text{Otherwise} (\hat{n} : \Delta \sigma_{\text{trial}} < 0) & \quad \text{(Inverse loading)} \\
& \begin{cases} 
(i) & \hat{n}_{\text{trial}} : \Delta \sigma_{\text{trial}} \leq 0 : \Delta \varepsilon_{\text{trial}}^p = 0, \quad \sigma_{\text{trial}} = \sigma_{\text{trial}} \\
(ii) & \text{Otherwise} (\hat{n} : \Delta \sigma_{\text{trial}} > 0) \\
& \begin{cases} 
(a) & f(\hat{\sigma}_{\text{trial}} - \hat{a}_n^* ) - R_F(H_e) \leq 0 : \\
& \Delta \varepsilon_{\text{trial}}^p = 0, \quad \sigma_{\text{trial}} = \sigma_{\text{trial}} \\
(b) & f(\hat{\sigma}_{\text{trial}} - \hat{a}_n^* ) - R_F(H_e) > 0 : \\
& \Delta \varepsilon_{\text{trial}}^p \neq 0 
\end{cases} 
\end{cases}
\end{align}

Where, the variables for the loading criterion are expressed by

\begin{align}
\Delta \sigma_{\text{trial}} &= \hat{\sigma}_{\text{trial}} - \sigma_n \\
\hat{a}_{\text{trial}} &= c_n - R \hat{\varepsilon}_n, \quad \hat{a}_{\text{trial}} = c_n - R \hat{\varepsilon}_n \\
\sigma_n &= \sigma - \hat{a}_n = \sigma + R \hat{\varepsilon}_n, \quad \sigma_{\text{trial}} = \sigma_{\text{trial}} - \hat{a}_{\text{trial}} = \sigma_{\text{trial}} = \sigma_{\text{trial}} + R \hat{\varepsilon}_n \\
\hat{n} &= \frac{\partial \hat{\sigma}}{\partial \sigma}, \quad \hat{n}_{\text{trial}} = \frac{\partial \hat{\sigma}_{\text{trial}}}{\partial \sigma_{\text{trial}}} \\
\end{align}
The subloading surface function in the elastic trial step is expressed by the elastic trial stress and the normal-yield ratio at the elastic trial stress $R_{w+1}^{\text{trial}}$. Additionally, the normal-yield ratio in the elastic trial step is expressed by

$$R_{w+1}^{\text{trial}} = \frac{\sqrt{\frac{2}{3}} \| \mathbf{a}_{w+1}^{\text{trial}} : \mathbf{e}^t_{w+1} \|^2}{2 (F(H_w))^2 - \| \mathbf{e}^t_{w+1} \|^2}$$

(23)

### 3.2 Plastic corrector process

In the return-mapping algorithm, the elastic trial stress is adopted as updated stress when it is judged as an elastic loading process by the loading criterion. By contrast, when the elastic trial stress is judged as a plastic loading process, the plastic corrector process is applied to calculate the stress and state variables after the plastic deformation. The equilibrium equations to correct stress and state variables by an iterative convergence calculation are expressed by

$$Y_x = E^{-1} : \sigma_{w+1} - \varepsilon_{w+1}^{\text{trial}} + \Delta \lambda_{w+1} \mathbf{E}_{w+1}$$

$$Y_{\alpha} = a_{w+1} - a_{w+1} - a_{w+1} \Delta \alpha_{w+1}$$

$$Y = c_{w+1} - c_{w+1} - s_{w+1} \Delta \lambda_{w+1}$$

$$Y_{ff} = H_{w+1} - H_w - \frac{2}{3} \Delta \lambda_{w+1}$$

$$Y_{s} = f(\mathbf{\sigma}_{w+1}) - R_{w+1} F(H_{w+1})$$

(24)

Where, the unknown vector $X$ and the residual vector $Y(X)$ are introduced.

$$X \equiv (\sigma_{w+1}, a_{w+1}, c_{w+1}, H_{w+1}, \Delta \lambda_{w+1})^T$$

$$Y(X) \equiv (Y_x, Y_{\alpha}, Y, Y_{ff}, Y_{s})^T = 0$$

(25)

(26)

Additionally, the initial values of the unknown vector variables and the normal-yield ratio are expressed by the following equations.

$$\varepsilon_{w+1}^{(0)} = \varepsilon_{w+1}^{\text{trial}}, \quad a_{w+1}^{(0)} = a_{w+1}, \quad c_{w+1}^{(0)} = c_{w+1}, \quad H_{w+1}^{(0)} = H_w, \quad \Delta \lambda_{w+1}^{(0)} = 0$$

$$R_n \geq R_v : R_{w+1}^{(0)} = R_n$$

$$R_n < R_v : R_{w+1}^{(0)} = R_v$$

(27)

(28)

Where, the superscripts indicate the number of iterations in the convergence calculation.

Equation (26) is expressed by the primary approximation of the Taylor expansion. The unknown vectors are updated from iteration $k$ to $k+1$ of the convergence calculation using the Jacobi matrix. Each element of the Jacobi matrix is introduced by a direct partial differential operation, but description of that is omitted in this article.

$$Y(X^{(k+1)}) \equiv Y(X^{(k)}) + J(X^{(k)}) \cdot dX = 0$$

(29)

$$X^{(k+1)} = X^{(k)} + J(X^{(k)}) \cdot dX = X^{(k)} - \left[ J(X^{(k)})^T \right]^{-1} Y(X^{(k)})$$

(30)
The convergence calculation of the plastic corrector process continues until it satisfies the criterion expressed by Equation (31). Although they include vectors with various units, the stress dimensional vector controlling the iterative calculation converges sufficiently when the convergence criterion is satisfied.

Moreover, the consistent tangent modulus tensor is adopted to efficiently satisfy the global equilibrium condition in the static FEM analysis. In this study, it was introduced using a numerical procedure using the perturbation strain [10]. The perturbation strain was set $\Delta \varepsilon = 10 \times 10^{-8}$ in this study.

### 3.3 Initial value for normal-yield ratio in plastic corrector process

The plastic strain rate is induced even when the subloading surface contracts in the elastic trial step if it once contracts but expands larger than purely-elastic domain thereafter (Equation (17) (2) (ii) (b)). There are various stress directions in this case. However, in fact, among them are the loading processes in which the subloading surface in the elastic trial step re-expands after temporary contraction without passing the purely-elastic domain (Figure 4). In this case, Equation (28) may induce numerical error and can’t adequately express the general loading process. Then, the initial value for the normal-yield ratio in the plastic corrector process has to be applied at the transition point where the subloading surface switches from contraction to re-expansion. The calculation method for the normal-yield ratio at the transition point was introduced.

The subloading surface state in the transition point where the subloading surface switches from contraction to re-expansion is shown in Figure 5. The stress $\sigma_n^0$ and normal-yield ratio $R_{n+1}^0$ at the transition point must satisfy

$$ f(\sigma_n^0) = R_{n+1}^0 F(H_s) $$

Moreover, the elastic trial stress tangents to the subloading surface at the transition point. Therefore, the elastic trial stress and the outward-normal vector $\mathbf{n}_{n+1}^0$ of the subloading surface are intersected at right angles at the transition point. The stress at the transition point is given by the following equation based on the relationship between the stress at current step and the elastic trial stress.

![Figure 4: Inverse loading process which the elastic trial stress contracts and re-expands without passing the purely-elastic domain.](image)
Where, \( c \) is a scalar variable satisfied by Equation (32), (33) and 0 \( \leq c \leq 1 \). Additionally, the variables of the subloading surface at the transition point are expressed by

\[
\bar{\sigma}^0_{n+1} = \bar{\sigma}^0_{n} - \bar{\sigma}^0_{n} = c\Delta \sigma^{\text{trial}}_{n+1} + \hat{\sigma}_n + R^0_{n+1}\hat{e}_n \quad \text{and} \quad \bar{\alpha}^0_{n+1} = \bar{\alpha}^0_{n} - R^0_{n+1}\hat{e}_n
\]

The normal-yield ratio and scalar variable \( c \) at the transition point are expressed by

\[
\left[ \frac{1}{2} \|[c\Delta \sigma^{\text{trial}}_{n+1} + \hat{\sigma}_n + R^0_{n+1}\hat{e}_n] - R^0_{n+1}F(H_n) \| \right]^2 = 0
\]

The scalar variable \( c \) is obtained by solving the Equation (37) and (38).

\[
\Delta \sigma^{\text{trial}}_{n+1} : \Delta \sigma^{\text{trial}}_{n+1} = 2\Delta \sigma^{\text{trial}}_{n+1} : \left( \hat{\sigma}_n + R^0_{n+1}\hat{e}_n \right) \left( \hat{\sigma}_n + R^0_{n+1}\hat{e}_n \right) - \frac{2}{3} \left( R^0_{n+1}F(H_n) \right)^2 = 0
\]

Moreover, the normal-yield ratio at the transition point is expressed by substituting the scalar variable \( c \) to Equation (38).

\[
\left( S^0_{n+1} + S^0_{n} \right)^2 - S^0_{n} \left[ \left( \hat{\sigma}_n + R^0_{n+1}\hat{e}_n \right) - \frac{3}{2} R^0_{n+1}F(H_n) \right]^2 = 0
\]

\[
R^0_{n+1} = \frac{\left( S^0_{n+1} + S^0_{n} \right)^2 - S^0_{n} \left( S^0_{n+1} - S^0_{n} \right)^2 - \frac{3}{2} \left( F(H_n) \right)^2 \left( S^0_{n+1} - S^0_{n} \right) \left( S^0_{n+1} - S^0_{n} \right)}{S^0_{n+1} - S^0_{n}}
\]

Figure 5: Rigorous calculation method for initial value of normal-yield ratio in the plastic corrector process.
\[ S_{ca} = \tilde{\sigma}_{a} : \tilde{\varepsilon}_{a}, \quad S_{ae} = \tilde{\sigma}_{e} : \tilde{\varepsilon}_{e}, \quad S_{ce} = \tilde{\sigma}_{c} : \tilde{\varepsilon}_{c} \] (44)

4 NUMERICAL VERIFICATION

The proposed formulations were implemented in the FEM software ABAQUS through the user subroutine UMAT. The numerical analyses applied elastoplastic deformation using single-element model with the primary hexahedral element. Additionally, we verified the accuracy of the implicit stress integration algorithm based on the rigorous and past loading criteria. The material constants for the numerical analyses are shown in Table 1. Concisely, the isotropic and kinematic hardening are not discussed in this study.

<table>
<thead>
<tr>
<th>Table 1: Material constants</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elastic property</td>
</tr>
<tr>
<td>$E$ [GPa]</td>
</tr>
<tr>
<td>160</td>
</tr>
</tbody>
</table>

4.1 Verification with single-element model

First, the uniaxial forward and inverse loading process was performed. The forward loading process was a deformation of up to 2% of the nominal strain in the X-axis direction, and the inverse loading process was a deformation of up to 0% in the nominal strain. Numerical analysis increment was performed by four steps per process.

Stress $\sigma_a$ at the end of the forward loading process, elastic trial stress $\sigma_{b\text{trial}}$ and the subloading surface state in the elastic trial step of the beginning of the inverse loading process are shown in Figure 6 (a). The stress-strain curves and elastic trial stress in the beginning of the inverse loading process are shown in Figure 6 (b, c). There were no difference in the stress-strain curves obtained by the rigorous and past loading criteria because the forward loading process was only expansion process of the subloading surface.

Figure 6: Uniaxial forward and inverse loading process, which the subloading surface in elastic trial step of beginning of inverse loading re-expand after once contraction.
In the beginning step of the inverse loading process, the subloading surface re-expanded larger than the purely-elastic domain after it once contracted less than that domain as was similar to Figure 2. In this case, the elastic trial stress $\sigma_{\text{trial}}$ was judged as an elastic loading process by the past loading criterion, and the numerical value was calculated larger than exact value (Figure 6 (b)). On the contrary, the rigorous loading criterion judged as a plastic loading process. Thus, the plastic corrector step was applied and the elastic trial stress $\sigma_{\text{trial}}$ was corrected to the subloading surface containing the plastic deformation (Figure 6 (c)).

Next, the bi-axial forward and inverse loading process was performed to verify the accuracy of the general-loading process. The forward loading process provided a deformation of up to 2% of the nominal strain in the X-axis direction. In inverse loading process, the displacement boundary conditions in the X-axis direction were removed and the stress produced in the forward loading process gradually decreased to 0 MPa. Additionally, the deformation that was induced in the Y-axis direction was restored to 0% of the nominal strain. Thus, the stress in the X-axis direction and the strain in the Y-axis direction were controlled linearly. Numerical analysis increment was performed by three steps per process.

Stress $\sigma_c$ at the end of forward loading process, elastic trial stress $\sigma_d$ and the subloading surface state in the elastic trial step of the beginning of the inverse loading process are shown in Figure 7 (a). The subloading surface in the elastic trial step of the beginning of the inverse loading process re-expands after temporary contraction without passing to the purely-elastic domain, as can also seen Figure 4.

The stress curves in the X- and Y-axis direction of two loading criteria are shown in Figure 7 (b, c). The subloading surface in the elastic trial step of the beginning of the inverse loading process re-expands larger than the purely-elastic domain after once contracted. In this case, the elastic trial stress $\sigma_{\text{trial}}$ was judged by the past loading criterion as the elastic loading process and numerical value was calculated as larger than the exact value (Figure 7 (b)). On the contrary, the rigorous loading criterion judged it as the plastic loading process. Moreover, the normal-yield ratio of the transition point where the subloading surface switched from contraction to re-expansion was applied to the initial value for the normal-yield ratio in the plastic corrector process. Therefore, the precise numerical analyses were performed using the rigorous loading criterion regardless of the stress directions.

![Figure 7](image-url)
4.2 Verification with error map

The error map was introduced to verify the accuracy of the past and rigorous loading criteria for various strain increments and directions. The elastoplastic deformation was applied up to 1% of the nominal strain in the X-axis direction, to produce the error map. Additionally, the stress $\sigma_{\text{num}}$ was calculated using a series of strain increments corresponding to the elastic trial stress increments $\Delta\sigma_{\text{trial}}$.

$$\Delta\sigma_{\text{trial}} = \Delta\sigma_{T} + \Delta\sigma_{N}$$  \hspace{1cm} (45)

Where, $N$ and $T$ are the normal and the tangential vector. In this study, to avoid division by zero, error equation is defined as the ratio of the exact value to the initial value for normal-yield surface.

$$\text{Error} = \left( \frac{\sigma_{\text{exact}} - \sigma_{\text{num}}}{\sigma_{\text{exact}}} \right) \times 100 \, \%$$  \hspace{1cm} (46)

Where, $\sigma_{\text{exact}}$ is the exact values calculated by the sufficiently small strain increment.

The error maps are shown in Figure 8. When the subloading surface was a forward loading state from 1% of the nominal strain, there was no difference in the judgement of loading process between the past and rigorous loading criteria. However, in inverse loading process, the numerical accuracy was different depending on the loading criteria. Because the past loading criterion can’t consider the transition from contraction to expansion of the subloading surface,

![Error maps](image.png)

**Figure 8**: Error maps: numerical values in figures are error values (%).
the updated stress may be calculated as larger than the exact value. Conversely, the rigorous loading criterion can consider the process wherein the subloading surface re-expands after contraction. Therefore, the rigorous loading criterion can carry out more accurate numerical analyses compared to the past loading criterion.

5 CONCLUSIONS
- The rigorous loading criterion and the initial value calculation method for the normal-yield ratio for return-mapping were adopted to the complete implicit stress integration algorithm for the extended subloading surface model. Additionally, it has been formulated and implemented in ABAQUS through the user-subroutine UMAT.
- The rigorous loading criterion can represent that the plastic strain rate is induced when the subloading surface contracts in the elastic trial step if it once contracts but expands thereafter. The normal-yield ratio where the subloading surface switched from contraction to re-expansion is adopted to the initial value for the plastic corrector process in the general loading process. Therefore, the return-mapping with the rigorous loading criterion and the initial value calculation algorithm for normal-yield ratio express accurate cyclic loading behavior in various directions.

REFERENCES
SUBLOADING-DAMAGE MODEL AND ITS EXTENSION TO UNILATERAL DAMAGE EFFECT

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Key words: Damage, Elastoplastic deformation, Subloading surface model, Unilateral-damage.

Abstract. The elastoplastic constitutive equation with the damage is formulated incorporating the subloading surface model. Further, it is extended to describe the unilateral damage phenomenon by formulating the actual Young’s modulus tensor as the function of the signs of the principal actual damaged stresses and the damage variable. Here, we may perform the ordinary deformation analysis simply in the virtual undamaged state.

1 INTRODUCTION

The past elastoplastic-damage models [1] [2] [3] [4] have been formulated in the current damaged configuration, so that several complicated modifications of evolution rules of internal variables by incorporating the damage effect are required. In addition, they are incapable of describing cyclic loading behavior.

Further, when the material undergoes the damage, the microdefects may be partly closed leading to the reduction of the damage effect in the plane subject to the compressional normal stress in the most materials. This is more often the case for very brittle materials. The partial closure of microcracks revives the effective area which can carry the load in compression and thus the stiffness may then be partially or fully recovered in compression. It is called the unilateral microdefect closure effect or simply unilateral damaged effect by Ladeveze and Lemaitre [5]. The constitutive relations for the unilateral damage effect have been formulated in the current damaged configuration, introducing various transformation tensor of the actual damaged stress tensor to the virtual undamaged stress tensor [2] [5] [6].

The elastoplastic-damage model capable of describing the cyclic loading behavior is formulated by incorporating the subloading surface model [7] [8] [9] in this article. It is formulated in the virtual undamaged configuration, so that the elastoplastic constitutive equation in the ordinary subloading surface model itself is inherited to this model without any modification. Further, it is extended to describe the unilateral damage phenomenon by formulating the actual Young’s modulus as the function of the signs of the principal actual damaged stresses and the damage variable, in which the complicated transformation tensor is not required. Here, it is noticeable that the simple deformation analysis by the ordinary constitutive equation without the influence of the damage can be performed in the virtual undamaged configuration, provided that the actual damaged stress tensor is calculated from the...
virtual undamaged stress tensor.

2 HYPERELASTIC EQUATION

The infinitesimal strain \( \varepsilon \) is additively decomposed into the elastic strain \( \varepsilon^e \) and the plastic strain \( \varepsilon^p \) as follows:

\[
\varepsilon = \varepsilon^e + \varepsilon^p
\]

(1)

In what follows, we adopt the hypothesis of strain equivalence [10] insisting that the strain and its elastic and plastic parts in the virtual undamaged configuration are equivalent to those in the actual damaged configuration. It is based on the fact that the cracks possess infinitesimal thicknesses and various directions and thus it is assumed that the shape and the volume of the material in the actual configuration does not change from them in the virtual undamaged configuration. Mechanical quantities in the virtual undamaged configuration are specified by the symbols added the wave under them, i.e. (\( \ast \)).

The relation of the virtual Cauchy stress \( \sigma \) in the undamaged configuration and the elastic strain \( \varepsilon^e \) are given by the Helmholtz free energy function \( \psi(\varepsilon^e) \) and the Gibbs’ free energy \( \phi(\sigma) \) as follows:

\[
\sigma = \frac{\partial \psi(\varepsilon^e)}{\partial \varepsilon^e}, \quad \varepsilon^e = \frac{\partial \phi(\sigma)}{\partial \sigma}
\]

(2)

Adopting the simplest functions in the quadratic forms

\[
\psi(\varepsilon^e) = \frac{1}{2} \varepsilon^e : \varepsilon = \frac{1}{2} \frac{\sigma}{E : \varepsilon} = \phi(\sigma) = \frac{1}{2} \sigma : \varepsilon^e = \psi(\varepsilon^e)
\]

(3)

it follows that

\[
\sigma = \frac{\partial \psi(\varepsilon^e)}{\partial \varepsilon^e} = \varepsilon^e, \quad \varepsilon^e = \frac{\partial \phi(\sigma)}{\partial \sigma} = \varepsilon^e
\]

(4)

where \( E \) is the fourth-order elastic modulus tensor. If \( E \) is the constant tensor, we have the rate linear relations:

\[
\dot{\sigma} = E : \dot{\varepsilon}^e, \quad \dot{\varepsilon}^e = E^{-1} : \dot{\sigma}
\]

(5)

The elastic stiffness modulus tensor \( E \) is given for the Hooke’s law as follows:

\[
\begin{bmatrix}
E & E \\
E & E
\end{bmatrix} = \frac{1}{1 + \nu} \left[ \begin{bmatrix}
(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) + \frac{\nu}{1 - 2\nu} \delta_{ij} \delta_{kl} \\
(1 + \nu)(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) - \nu \delta_{ij} \delta_{kl}
\end{bmatrix}
\]

(6)

where \( E \) is the virtual Young’s modulus in the virtual undamaged configuration and \( \nu \) is the Poisson’s ratio which is assumed to be constant independently of the damage. Equations (2)-(4) are expressed for Eq. (6) as follows:

\[
\begin{align*}
\psi(\varepsilon^e) & = \frac{1}{2} \frac{E}{1 + \nu} \left[ \varepsilon^e_{ij} \varepsilon^e_{ij} + \frac{\nu}{1 - 2\nu} (\varepsilon^e_{kk})^2 \right] \\
\phi(\sigma) & = \frac{1}{2} \frac{E}{\nu} \left[ (1 + \nu) \varepsilon^e_{ij} \varepsilon^e_{ij} - \nu (\varepsilon^e_{kk})^2 \right]
\end{align*}
\]

(7)

\[
\sigma_{ij} = \frac{E}{1 + \nu} \left[ \varepsilon^e_{ij} + \frac{\nu}{1 - 2\nu} \varepsilon^e_{kk} \delta_{ij} \right], \quad \varepsilon^e_{ij} = \frac{1}{E} \left[ (1 + \nu) \varepsilon^e_{ij} - \nu \varepsilon^e_{kk} \delta_{ij} \right]
\]

(8)
Analogously, let the following quadratic free energy functions be adopted by taking into account of the fact that the actual elastic modulus tensor is influenced by the damage variable $D$ ($0 \leq D \leq 1$).

\[
\psi(\varepsilon^e, D) = \frac{1}{2} \varepsilon^e : \mathbf{E}(D) : \varepsilon^e = \frac{1}{2} \sigma(D) : \varepsilon^e \\
\phi(\sigma) = \frac{1}{2} \sigma : \mathbf{E}^{-1}(D) : \sigma
\]

from which one has

\[
\sigma = \frac{\partial \psi(\varepsilon^e, D)}{\partial \varepsilon^e}, \quad \varepsilon^e = \frac{\partial \phi(\sigma, D)}{\partial \sigma}
\]

Further, assume the following Hooke’s type elastic modulus tensor with the damage effect, provided that the Poisson’s ratio is not influenced by the damage.

\[
E_{ijkl}^{(D)} = E^{(D)} \left[ \frac{1}{1+v} \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) + \frac{v}{1-2v} \delta_{ij} \delta_{kl} \right]
\]

The damaged virtual stress is related to the undamaged virtual stress from Eqs. (4) and (11) as follows:

\[
\sigma = \mathbf{E}(D) : \mathbf{E}^{-1}(D) : \sigma
\]

3 SUBLOADING SURFACE MODEL IN VIRTUAL UNDAMAGED CONFIGURATION

The elastoplastic constitutive equation in the virtual undamaged configuration will be formulated based on the concept of subloading surface in this section (cf. [9]).

3.1 Normal-yield and subloading surfaces

The normal-yield surface with the isotropic and the kinematic hardening is described as

\[
f^{(\sigma)}(\sigma) = F(H)
\]

where

\[
\hat{\sigma} = \sigma - \sigma
\]

The subloading surface for the normal-yield sur-face in Eq. (16) is given as follows.

\[
f^{(\sigma)}(\sigma) = R^2 F(H)
\]

where $R (0 \leq R \leq 1)$ is the normal-yield ratio designating the ratio of the size of the subloading surface to that of the normal-yield surface and
\[ \bar{\sigma} = \sigma - \bar{\sigma} \]  

(19)

where \( \bar{\sigma} \) stands for the conjugate (similar) point to the variable \( \sigma \) in the normal-yield surface. Here, \( f(\bar{\sigma}) \) is chosen to be the homogeneous function of \( \bar{\sigma} \) in degree-one.

By letting \( \epsilon \) denote the center of similarity of the normal-yield and the subloading surfaces, i.e. the similarity-center, which is called elastic-core since the most elastic deformation behavior is induced when the stress lies on it fulfilling \( R = 0 \) as will be explained later, the following relation holds.

\[ \epsilon - \bar{\alpha} = R(\epsilon - \alpha) \]  

(20)

from which one has

\[ \bar{\sigma} = \epsilon - R \epsilon, \quad \bar{\sigma} = \sigma - R \sigma \]  

(21)

where

\[ \hat{\epsilon} = \epsilon - \alpha, \quad \hat{\sigma} = \sigma - \epsilon \]  

(22)

### 3.2 Plastic flow rule and evolution equations of internal variables

Adopt the associated flow rule for the subloading surface:

\[ \dot{\epsilon}^p = \frac{1}{\lambda} \mathbf{n} \left( \frac{\lambda}{\| \dot{\epsilon}^p \|} > 0 \right) \]  

(23)

where

\[ \mathbf{n} = \frac{\partial f(\sigma)}{\partial \sigma} / \| \frac{\partial f(\sigma)}{\partial \sigma} \| \left( \| \sigma \| = 1 \right) \]  

(24)

The rate of the isotropic hardening variable is described as

\[ \dot{H}^{(s)}(\sigma, H; \dot{\epsilon}^p) = f_{\text{in}}(\sigma, H; \mathbf{n}) \frac{\dot{\epsilon}^p}{\lambda} \]  

(25)

and the rate of the kinematic hardening variable is described as follows:

\[ \dot{\alpha} = c_k \left( \dot{\epsilon}^p - \frac{1}{b_k \lambda} \| \dot{\epsilon}^p \| \mathbf{a} \right) = c_k \dot{\mathbf{f}}_k, \quad \dot{\mathbf{f}}_k = c_k \left( \mathbf{n} - \frac{1}{b_k \lambda} \| \mathbf{a} \| \mathbf{a} \right) \]  

(26)

where \( c_k \) and \( b_k \) are the material constants.

The evolution rule of the normal-yield ratio is given by

\[ \dot{R} = U(R) \| \dot{\epsilon}^p \| \quad \text{for} \quad \dot{\epsilon}^p \neq 0 \]  

(27)

where \( U(R) \) is the monotonically-decreasing function of normal-yield ratio which is given explicitly as

\[ U(R) = \frac{u \cot \left( \frac{\pi}{2} \frac{R - R_c}{1 - R_c} \right) \}  

(28)

where \( \langle \rangle \) is the Macaulay’s bracket and \( u \) is the material parameters and \( R_c (< 1) \) is the material constant denoting the value of \( R \) below which only elastic deformation is induced practically.

### 3.3 Evolution rule of elastic-core

Let the following elastic-core surface be introduced, which always passes through the elastic-core \( \epsilon \) and maintains a similarity to the normal-yield surface with respect to the kinematic-hardening variable \( \alpha \).
\[ f'(\hat{\mathbf{e}}) = \gamma_k F(H), \text{ i.e. } \gamma_k = f'(\hat{\mathbf{e}}) / F(H) \]  \hspace{1cm} (29)

\( \gamma_k \) designates the ratio of the size of the elastic-core surface to the normal-yield surface so that let it be called the elastic-core yield ratio. Then, let it be postulated that the elastic-core can never reach the normal-yield surface designating the fully-plastic stress state so that the elastic-core does not go over the following limit elastic-core surface.

\[ f'(\hat{\mathbf{e}}) = \chi F(H) \]  \hspace{1cm} (30)

where \( \chi (\leq 1) \) is the material constant designating the limit value of the variable \( \gamma_k \).

The following evolution rule of the elastic-core is assumed [11].

\[ \dot{\mathbf{e}} = c ||E'|| \cdot \left( \frac{\chi}{R} \mathbf{\sigma} - \hat{\mathbf{e}} \right) + \frac{\hat{F}}{F} \dot{\mathbf{e}} - \frac{\hat{F}}{F} \mathbf{\tau}_{en} + \frac{\chi}{R} \mathbf{\tau}_{kn} + \frac{\chi}{R} \frac{E'}{F} \mathbf{\dot{\epsilon}} \]  \hspace{1cm} (31)

where \( c \) is the material constant and

\[ \mathbf{\tau}_{en} = c \left( \frac{\chi}{R} \mathbf{\sigma} - \hat{\mathbf{e}} \right) \]  \hspace{1cm} (32)

The time-differentiation of Eq. (21) leads to

\[ \mathbf{a} = R \dot{\mathbf{a}} + (1 - R) \mathbf{\dot{\epsilon}} - \mathbf{\dot{\mathbf{e}}} \]  \hspace{1cm} (33)

Substituting Eq. (31) into Eq. (33), one obtains

\[ \dot{\mathbf{a}} = R \dot{\mathbf{a}} + (1 - R) \left[ c ||E'|| \cdot \left( \frac{\chi}{R} \mathbf{\sigma} - \hat{\mathbf{e}} \right) + \frac{\hat{F}}{F} \dot{\mathbf{e}} - \frac{\hat{F}}{F} \mathbf{\tau}_{en} \right] - \dot{\mathbf{R}} \mathbf{\dot{\epsilon}} \]  \hspace{1cm} (34)

### 3.4 Plastic strain rate

The time derivative of Eq. (18) leads to the consistency condition for the subloading surface:

\[ \frac{\partial f(\mathbf{\sigma})}{\partial \mathbf{\sigma}} : \dot{\mathbf{\sigma}} = R F \frac{\partial f(\mathbf{\sigma})}{\partial \mathbf{\sigma}} : \dot{\mathbf{\sigma}} - \mathbf{a} \frac{\partial f(\mathbf{\sigma})}{\partial \mathbf{\sigma}} = 0 \]  \hspace{1cm} (35)

Here, one has

\[ \frac{\partial f(\mathbf{\sigma})}{\partial \mathbf{\sigma}} : \dot{\mathbf{\sigma}} = f(\mathbf{\sigma}) = R F \]  \hspace{1cm} (36)

based on the homogeneous function \( f(\mathbf{\sigma}) \) of \( \mathbf{\sigma} \) in degree-one by the Euler’s theorem. Then, it follows that

\[ \dot{\mathbf{n}} : \mathbf{\sigma} = \frac{\partial f(\mathbf{\sigma})}{\partial \mathbf{\sigma}} : \mathbf{\sigma} = \frac{R F}{\left\| \frac{\partial f(\mathbf{\sigma})}{\partial \mathbf{\sigma}} \right\|}, \quad \frac{1}{\left\| \frac{\partial f(\mathbf{\sigma})}{\partial \mathbf{\sigma}} \right\|} = \frac{\dot{\mathbf{n}} : \mathbf{\sigma}}{R F} \]  \hspace{1cm} (37)

The substitution of Eq. (37) into Eq. (35) leads to

\[ \dot{\mathbf{n}} : \dot{\mathbf{\sigma}} - \dot{\mathbf{n}} : \left[ \left( \frac{\hat{F}}{F} + \frac{\hat{F}}{F} R \right) \mathbf{\sigma} + \dot{\mathbf{a}} \right] = 0 \]  \hspace{1cm} (38)

The substitution of Eq. (34) into Eq. (38) leads to
\[
\vec{u} : \dot{\sigma} - \vec{u} : \left[ \frac{\varepsilon'}{F} \hat{\sigma} + \frac{\varepsilon}{R} \hat{\sigma} + (1-R) c \left( \frac{\varepsilon}{F} \sigma - \varepsilon \right) \right] = 0
\]  

(39)

The substitutions of Eqs. (23), (25), (26), (27) and (31) into Eq. (39) leads to

\[
\vec{u} : \dot{\sigma} - \vec{u} : \left[ \frac{\varepsilon'}{F} \bar{f}_{kn} \sigma + \frac{\varepsilon}{R} \bar{f}_{kn} + (1-R) \frac{\varepsilon}{F} \bar{E}_n + \frac{U}{R} \bar{f}_RF \sigma \right] = 0
\]

(40)

from which the plastic multiplier \( \dot{\lambda} \) and the plastic strain rate \( \dot{\varepsilon}^p \) are given as follows:

\[
\dot{\lambda} = \frac{\vec{u} : \dot{\sigma}}{\bar{M}^p}, \quad \dot{\varepsilon}^p = \frac{\vec{u} : \dot{\sigma}}{\bar{M}^p} \vec{n}
\]

(41)

where

\[
\bar{M}^p = \vec{u} : \left[ \frac{\varepsilon'}{F} \bar{f}_{kn} \sigma + \frac{\varepsilon}{R} \bar{f}_{kn} + (1-R) \frac{\varepsilon}{F} \bar{E}_n + \frac{U}{R} \bar{f}_RF \sigma \right]
\]

(42)

3.5 Stain rate vs. stress rate relations

The strain rate is given by substituting Eqs. (5) and (41) into Eq. (1) as follows:

\[
\dot{\varepsilon} = E^{-1} : \dot{\sigma} + \frac{\vec{u} : \dot{\sigma}}{\bar{M}^p} \vec{n} = \left( E^{-1} + \frac{\vec{u} \otimes \vec{n}}{\bar{M}^p} \right) : \dot{\sigma}
\]

(43)

from which the magnitude of plastic strain rate described in terms of the strain rate, denoted by \( \dot{\varepsilon}^p \) instead of \( \dot{\lambda} \), in the flow rule of Eq. (23) is given as follows:

\[
\dot{\varepsilon}^p = \frac{\vec{u} : \dot{\sigma}}{\bar{M}^p} \vec{n} = \frac{\vec{u} : \dot{\sigma}}{\bar{M}^p} \vec{n}
\]

(44)

The stress rate is given by the strain rate as follows:

\[
\dot{\sigma} = E : \dot{\varepsilon} = \vec{u} : \dot{\sigma} - \frac{\vec{u} : \dot{\sigma}}{\bar{M}^p + \vec{u} : \bar{n}} \vec{n} = \left( E - \frac{E : \vec{n} \otimes \vec{n} : E}{\bar{M}^p + \vec{u} : \bar{n}} \right) : \dot{\varepsilon}
\]

(45)

The loading criterion is given as follows [9]:

\[
\dot{\varepsilon}^p = 0 \quad \text{for} \quad \vec{u} : \dot{\sigma} > 0
\]

\[
\dot{\varepsilon}^p = 0 \quad \text{for} \quad \vec{u} : \dot{\sigma} \leq 0
\]

(46)

3.6 Improvement of inverse-reloading responses

The material parameter \( u \) is extended in order to improve the description of the inverse-reloading behavior as follows:

\[
u = \pi \exp(u_c y_n C_{\sigma})
\]

(47)

where \( \pi \) and \( u_c \) is the material constant and

\[
C_{\sigma} = \vec{u} : \vec{n} (-1 \leq C_{\sigma} \leq 1)
\]

(48)

with

\[
\vec{u}_c = \frac{\partial f(\dot{\varepsilon})}{\partial \dot{\varepsilon}} / \left\| \frac{\partial f(\dot{\varepsilon})}{\partial \dot{\varepsilon}} \right\| (\|\vec{u}_c\| = 1)
\]

(49)
4 EVOLUTION OF DAMAGE VARIABLE

The continuum damage variable $D$ is interpreted as an indirect measure of density of microvoids and microcracks [12] and its evolution rule was given as follows [13]:

$$D = \frac{(Y)^a H(\epsilon^{dp}_D - \epsilon^{dp}_B)}{1 - D} \epsilon^p$$

where $\zeta$ and $a$ are the material constants, and $\epsilon^{dp}_D$ is the threshold value of the accumulation of the deviatoric plastic strain rate, i.e. $\epsilon^{dp}_D \equiv \int \|\dot{\epsilon}^D\| dt$. $Y$ is the virtual undamaged strain energy function given by

$$Y = \frac{1}{2} \epsilon^e : \dot{\epsilon}^e = \frac{1}{2} \sigma : \dot{\epsilon}^e = \frac{1}{2} \sigma : \dot{\epsilon}^{-1}$$

5 BILATERAL DAMAGE EFFECT

The elastic modulus tensor and its inverse in the virtual undamaged configuration in Eq. (6) are expressed in the matrix form as

$$E = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1 - \nu & \nu & 0 & 0 & 0 \\ 1 - \nu & \nu & 0 & 0 & 0 \\ \nu & 1 - \nu & 0 & 0 & 0 \\ 1 - 2\nu & 0 & 0 & \text{Sym.} \\ 1 - 2\nu & 0 & & \\ \end{bmatrix}$$

and

$$E^{-1} = \frac{1}{E} \begin{bmatrix} 1 & -\nu & -\nu & 0 & 0 \\ 1 - \nu & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & \text{Sym.} \\ 1 + \nu & 0 & & \\ 1 + \nu & & & \\ \end{bmatrix}$$

Here, let the damaged Young's modulus in Eq. (12) be given by

$$E(D) = (1 - D)E$$

leading to

$$E = (1 - D)E, \quad E^{-1} = \frac{1}{1 - D}E^{-1}$$

for which the damaged current stress is related to the undamaged virtual stress by substituting Eq. (54) into Eq. (15) as follows:

$$\sigma = (1 - D)\sigma, \quad \sigma = \frac{1}{1 - D}\sigma$$

The virtual undamaged strain energy function $Y$ is given by substituting Eqs. (55) and (56) into Eq. (51) as

$$Y = \frac{1}{2} \epsilon^e : \dot{\epsilon}^e$$
5 UNILATERAL DAMAGE EFFECT

Let the principal actual damaged axial stress \( \sigma_p \) \((p=1, 2, 3)\) be given by the principal elastic axial strain \( \varepsilon_p^e \) in the uniaxial loading state as follows:

\[
\begin{align*}
\sigma_p &= E_p(D)\varepsilon_p^e \\
\varepsilon_p^e &= E_p^{-1}(D)\sigma_p
\end{align*}
\]  
(58)

Let the damaged Young’s modulus \( E_p(D) \) in Eq. (58) be given as follows:

\[
E_p = (1-H_{\sigma_p}D)E
\]  
(59)

\[
E_p = \begin{cases} 
(1-D)E & \text{for } \sigma_p \geq 0 \\
(1-h_{\sigma}D)E & \text{for } \sigma_p < 0 
\end{cases}
\]

\[H_{\sigma_p} = H(\sigma_p) + (1 - H(\sigma_p))h_{\sigma}
\]  
(60)

\(H(s)\) is the Heaviside’s step function, i.e. \(H(s)=1\) for \(s \geq 0\) and \(H(s)=0\) for \(s < 0\) (\(s\): arbitrary scalar), and \(h_{\sigma} (0 \leq h_{\sigma} \leq 1)\) is the material constant. Equation (59) is shown in Fig. 1.

![Diagram](image_url)

(a) Relation of principal actual Young’s modulus vs. principal actual damaged stress.

(b) Relation of principal actual damage stress vs. principal elastic strain

Fig. 1. Actual damaged Young’s modulus and actual damaged stress in uniaxial loading for unilateral damage phenomenon.

Extending the inverse elastic modulus tensor to the unilateral damage by adopting the damaged Young’s modulus in Eq. (59) on the premise that the elastic strain is not influenced by the lateral stresses, let the inverse elastic modulus tensor be given by the matrix form in the coordinate system with the base \(\{\bar{E}_p\}\) in the principal stress directions as follows:
The actual damaged stress is given by the virtual undamaged stress as
\[ \sigma = \mathbf{E} : \varepsilon^e = \mathbf{E} : \mathbf{E}^{-1} : \sigma = \mathbf{f} : \sigma \] (66)
where
\[ \mathbf{f} = \mathbf{E} : \mathbf{E}^{-1} = \frac{1}{\Pi} \]
(67)

The relation \( \boldsymbol{\sigma} \) to \( \varepsilon^e \) is expressed by the components in the fixed coordinate system as follows:
\[ \sigma_{ij} = Q_{Pi} Q_{Qj} Q_{Ri} Q_{Sj} \mathbf{f}_{PQRS} \sigma_{ab} \] (68)
where
\[ Q_{PQi} = \varepsilon_{ij} \]
(69)

noting
\[ \sigma_{ij} = \varepsilon_{ij} \mathbf{f}_{PQRS} \mathbf{e}_P \otimes \mathbf{e}_Q \otimes \mathbf{e}_R \otimes \mathbf{e}_S \otimes \mathbf{f}_{PQRS} \sigma_{ab} \]

Inversely, the virtual undamaged stress is given by the actual damaged stress as follows:
\[ \varepsilon = \mathbf{E} : \mathbf{E}^{-1} : \mathbf{f} : \sigma = \mathbf{e} : \sigma \] (70)
where
\[ \mathbf{E}^{-1} = \frac{1}{E} \begin{bmatrix} \Gamma_1 -\nu & -\nu & 0 & 0 & 0 \\ \Gamma_2 -\nu & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \end{bmatrix} \]
(61)
\[ \mathbf{E} = \frac{E}{\Pi} \begin{bmatrix} \Pi & 0 & 0 & 0 & 0 \\ 0 & \Pi & 0 & 0 & 0 \\ 0 & 0 & \Pi & 0 & 0 \\ 0 & 0 & 0 & \Pi & 0 \\ \end{bmatrix} \]
(62)

where
\[ \Gamma_p(D) = \frac{E_p}{E} = \frac{E}{(1 - H_{opp})E} = \frac{1}{1 - H_{opp}} \] (63)
\[ \Gamma_{PQ} = \Gamma_{PQ} = \frac{E^2_p}{E_p E_Q} \] (64)
\[ \Pi = \Gamma_{123} - \nu^2(\Gamma_1 + \Gamma_2 + \Gamma_3) - 2\nu^3 \] (65)
\[ \mathbf{J} = \mathbf{E} : \mathbf{E}^{-1} = \begin{bmatrix} (1-\nu)I_1 - 2\nu^2 & \nu(I_2 - 1) & \nu(I_3 - 1) & 0 & 0 & 0 \\ (1+\nu)(1-2\nu) & (1+\nu)(1-2\nu) & (1+\nu)(1-2\nu) & 0 & 0 & 0 \\ (1+\nu)(1-2\nu) & (1+\nu)(1-2\nu) & (1+\nu)(1-2\nu) & 0 & 0 & 0 \\ (1+\nu)(1-2\nu) & (1+\nu)(1-2\nu) & (1+\nu)(1-2\nu) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \]

(71)

noting \( \mathbf{J} \) is the non-symmetric tensor but the tensor \( \mathbf{J} : \mathbf{t} \) is the symmetric tensor for an arbitrary symmetric second-order tensor \( \mathbf{t} \).

Equation (70) is described in the component form as follows:

\[ \sigma_{ij} = Q_{PQ} Q_{QR} \mathbf{Q}_{ab} ^{\mathbf{J}_{PQRS}} \sigma_{ab} \]

(72)

because of

\[ \sigma_{ij} = \mathbf{e}_i \cdot (\mathbf{J}_{PQRS} \mathbf{e}_p \otimes \mathbf{e}_Q \otimes \mathbf{e}_R \otimes \mathbf{e}_S) : (\sigma_{ab} \mathbf{e}_a \otimes \mathbf{e}_b) \mathbf{e}_j \]

Noting

\[ \dot{E}_p = \frac{H_{\sigma P}}{E_p} \dot{E} \]

(73)

one has

\[ \dot{E}^{-1} = \begin{bmatrix} \frac{H_{\sigma 1}}{E_1} & 0 & 0 & 0 & 0 \\ \frac{H_{\sigma 2}}{E_2} & 0 & 0 & 0 & 0 \\ \frac{H_{\sigma 3}}{E_3} & 0 & 0 & 0 & 0 \\ \text{Sym.} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \]

(74)

It follows from Eq. (52) and (74) that

\[ \mathbf{E} : \dot{E}^{-1} = \mathbf{J} \dot{D} \]

(75)

where

\[ \begin{bmatrix} \frac{H_{\sigma 1}}{E_1} & 0 & 0 & 0 & 0 \\ \frac{H_{\sigma 2}}{E_2} & 0 & 0 & 0 & 0 \\ \frac{H_{\sigma 3}}{E_3} & 0 & 0 & 0 & 0 \\ \text{Sym.} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \]

(76)
It is required to calculate the virtual undamaged stress rate from the actual damaged stress rate at the boundary where the stress and its rate are given, while the virtual undamaged stress is calculated from the actual stress by Eq. (70). The virtual undamaged stress rate is given from the actual stress rate by Eqs. (70) and (75) as follows:

\[
\dot{\sigma} = \mathcal{E} : \dot{\sigma}^e = \mathcal{E} : (\mathcal{E}^{-1} : \sigma)^e = \mathcal{E} : \mathcal{E}^{-1} : \dot{\sigma} + \mathcal{E} : \dot{\mathcal{E}}^{-1} : \sigma = \mathcal{J} : \dot{\sigma} + \mathcal{J} : \sigma
\]  

(77)

or in the component description as follows:

\[
\dot{\sigma}_{ij} = \mathcal{J}_{PQRS} Q_{Pj} Q_{Qj} Q_{Ra} Q_{Sb} \sigma_{ab} + \mathcal{B}_{Qj} Q_{Qj} Q_{Ra} Q_{Sb} \mathcal{J}_{PQRS} \sigma_{ab}
\]  

(78)

noting

\[
\dot{\sigma}_{ij} = \mathcal{E} : \dot{\sigma}^e = \mathcal{E} : (\mathcal{E}^{-1} : \sigma)^e = \mathcal{E} : \mathcal{E}^{-1} : \dot{\sigma} + \mathcal{E} : \dot{\mathcal{E}}^{-1} : \sigma = \mathcal{J} : \dot{\sigma} + \mathcal{J} : \sigma
\]  

(79)

Equation (77) is rewritten by substituting Eq. (50) of the damage variable with Eq. (41) of the plastic strain rate as follows:

\[
\dot{\sigma} = \mathcal{J} : \dot{\sigma} + \left( \frac{Y}{\zeta} \right)^a \frac{H(e^{dp} - e^{dp}_0)}{1 - D} \frac{\bar{n} : \dot{\sigma}}{\bar{M}^p} \mathcal{J} : \sigma
\]  

(80)

leading to

\[
\frac{\bar{n} : \dot{\sigma}}{\bar{M}^p} = \frac{\bar{n} : \mathcal{J} : \dot{\sigma}}{\bar{M}^p - \left( \frac{Y}{\zeta} \right)^a \frac{H(e^{dp} - e^{dp}_0)}{1 - D} \bar{n} : \mathcal{J} : \sigma}
\]  

(81)

The damage variable is rewritten by substituting Eq. (81) as follows:

\[
\dot{D} = \frac{\bar{n} : \mathcal{J} : \dot{\sigma}}{\bar{M}^p \left( \frac{Y}{\zeta} \right)^a \frac{H(e^{dp} - e^{dp}_0)}{1 - D} \bar{n} : \mathcal{J} : \sigma}
\]  

(82)

Substituting Eq. (82), the rate of the virtual undamaged stress is described by the actual damaged stress and its rate as follows:

\[
\dot{\sigma} = \mathcal{J} : \dot{\sigma} + \frac{\bar{n} : \mathcal{J} : \dot{\sigma}}{\bar{M}^p \left( \frac{Y}{\zeta} \right)^a \frac{H(e^{dp} - e^{dp}_0)}{1 - D} \bar{n} : \mathcal{J} : \sigma}
\]  

(83)

where

\[
\begin{align*}
(\mathcal{J} : \sigma)_{ij} &= Q_{Pj} Q_{Qj} Q_{Ra} Q_{Sb} \mathcal{J}_{PQRS} \sigma_{ab} \\
(\bar{n} : \mathcal{J} : \sigma)_{ij} &= Q_{Pj} Q_{Qj} Q_{Ra} Q_{Sb} \mathcal{J}_{PQRS} \bar{n} : \sigma_{ab}
\end{align*}
\]  

(84)
Consider the deformation in the uniaxial loading process \((\sigma_2 = \sigma_3 = 0)\) in which the principal directions are fixed. It follows from Eq. (70) with Eq. (71) that

\[
\sigma_1 = \frac{(1 - \nu)}{(1 + \nu)(1 - 2\nu)} \sigma_1
\]

from which we have

\[
\sigma_1 = \frac{(1 + \nu)(1 - 2\nu)}{(1 - \nu)(1 - 2\nu)} \sigma_1
\]

Further, it follows from Eq. (77) with Eqs. (71) and (76) that

\[
\begin{align*}
\dot{\varepsilon}_1 &= \frac{(1 - \nu)}{(1 + \nu)(1 - 2\nu)} \dot{\sigma}_1 + \frac{1 - \nu}{(1 + \nu)(1 - 2\nu)} \frac{H_{\sigma_1}}{E_1} \sigma_1 \\
\dot{\varepsilon}_2 &= \dot{\varepsilon}_3 = \dot{\varepsilon}_4 = \dot{\varepsilon}_5 = \dot{\varepsilon}_6 = 0
\end{align*}
\]

where

\[
\dot{\lambda} = \frac{(1 - \nu)}{(1 + \nu)(1 - 2\nu)} \frac{1}{H(e^{\sigma} - e^{\sigma_0})} \left( \frac{\varepsilon}{Y} \right)^a \frac{1 - \nu}{(1 + \nu)(1 - 2\nu)} \bar{n_1} \sigma_1
\]

REFERENCES

ACCURATE PREDICTION OF SPRING-BACK PHENOMENON BY SUBLOADING SURFACE MODEL

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Abstract. The subloading surface model possesses the distinguished capability to describe the plastic strain rate for the rate of stress inside the yield surface accurately and the stress-controlling function to pull-back the stress to the yield surface even when it goes out from the yield surface in the numerical calculation. The spring-back phenomenon of the high strength steel is analyzed by the commercial software Marc implemented the subloading surface model and thus the high accuracy of the simulation is verified in this article.

1 INTRODUCTION
The subloading surface (Hashiguchi) model [1] [2] [3] [4] possesses the distinguished advantages which are not furnished in the other elastoplasticity models, i.e. the conventional elastoplasticity model and the unconventional models (cyclic elastoplasticity models), e.g. the multi surface model [5], the two surface model [6] and the superposed-kinematic hardening model [7] inheriting the yield surface enclosing purely-elastic domain from the conventional elastoplasticity model. In particular, the smooth elastic-plastic transition is always described by excluding a purely-elastic domain and the automatic controlling function to attract the stress to the yield surface is furnished in the subloading surface model. Consequently, it provides the high ability in both aspects of the accuracy for the description of physical property and the efficiency of numerical calculation. The subloading surface model has been implemented in the commercial software Marc in MSC Software Corporation [8] as the standard installation by the name “Hashiguchi model”, which can be used by all Marc users (contractors). Nowadays, the high tensile (strength) steel sheets and aluminum sheets exhibiting far larger springback than the ordinary mild steel sheets are widely used in automobile industries, etc. The springback cannot be described by the constitutive models which use the yield surface enclosing a purely-elastic domain, i.e. the conventional model and the cyclic kinematic hardening models (multi-surface, two-surface and superposed kinematic hardening models), since a plastic strain rate in the unloading process is not described appropriately by these models. The spring-back phenomenon of the high strength steel is analyzed by the Marc so that the high accuracy of the
simulation is verified in this article, illustrating several numerical results including the comparison with experimental result.

2 ADDITIVE DECOMPOSITION OF STRAIN INCREMENT AND ELASTIC STRAIN INCREMENT

The infinitesimal strain tensor \( \varepsilon \) is additively decomposed into the elastic strain tensor \( \varepsilon^e \) and the plastic strain tensor \( \varepsilon^p \) as follows:

\[
\varepsilon = \varepsilon^e + \varepsilon^p, \quad d\varepsilon = d\varepsilon^e + d\varepsilon^p
\]

(1)

First, the elastic strain \( \varepsilon^e \) and its increment are linearly related to the Cauchy stress tensor \( \sigma \) and its increment as follows:

\[
\varepsilon^e = \mathbf{E}^{-1} : \sigma, \quad d\varepsilon^e = \mathbf{E}^{-1} : d\sigma
\]

(2)

where the fourth-order tensor \( \mathbf{E} \) is the elastic modulus tensor which is given by

\[
E_{ijkl} = \frac{\nu E}{(1+\nu)(1-2\nu)} \delta_i \delta_j + \frac{E}{2(1+\nu)} (\delta_k \delta_{ji} + \delta_i \delta_{jk})
\]

(3)

\( E \) and \( \nu \) are the Young’s modulus and the Poisson’s ratio, respectively.

3. SUBLOADING SURFACE MODEL

The concept and the constitutive equation of the subloading surface model [1][4] is described concisely in this section.

3.1 Yield surface and its evolution

First, we incorporate the following Mises yield condition with the isotropic and the kinematic hardenings is adopted.

\[
f(\hat{\sigma}) = F(H)
\]

(4)

with

\[
f(\hat{\sigma}) = \sigma^{eq} = \sqrt{3/2} \| \hat{\sigma}' \|
\]

(5)

\[
\hat{\sigma} = \sigma - \alpha
\]

(6)

where \( F(H) \) is the isotropic hardening function of the isotropic hardening variable \( H \) and \( \alpha (= \alpha') \) is the kinematic hardening variable and their evolution rules are given as follows:

\[
F(H) = F_0 \{ 1 + h_1 [1 - \exp(-h_2 H)] \}, \quad F' = dF/dH = F_0 \; h_1 \; h_2 \exp(-h_2 H)
\]

(7)

\[
H = \varepsilon^{exp}, \quad dH = d\varepsilon^{exp} = \sqrt{2/3} \| d\varepsilon^{p}\|
\]

(8)

\[
d\alpha = c_k \left( d\varepsilon^p - \frac{1}{\sqrt{3/2\zeta F}} \| d\varepsilon^p \| \alpha \right)
\]

(9)

where \( \sigma^{eq} \) is the equivalent stress and \( \varepsilon^{exp} \) is the equivalent plastic strain. \( h_1, h_2, c_k \) and \( \zeta \) are the material constants.
3.2 Subloading surface

The subloading surface model is premised on the following basic concept in order to describe the plastic strain increment induced by the rate of stress inside the yield surface, renames the normal-yield surface.

Subloading surface concept: The stress approaches the yield surface when the plastic strain increment is induced, exhibiting a continuous variation of tangent modulus, but it recedes from the yield surface when only the elastic strain increment is induced.

Then, the subloading surface which passes through the current stress point and is similar to the yield surface, renamed the normal-yield surface, is introduced and the ratio of the size of the subloading surface to that of the normal-yield surface is adopted as the measure designating the degree of approaching to the normal-yield surface.

The subloading surface is given as follows (see Fig. 1).

\[ f(\bar{\sigma}) = RF(H) \]

where

\[ \bar{\sigma} \equiv \sigma - \bar{\alpha} \]

\( \bar{\alpha} \) stands for the conjugate (similar) point in the subloading surface to the point \( \alpha \) in the normal-yield surface. The function \( f(\bar{\sigma}) \) is given explicitly conforming to Eq. (5) as follows:

\[ f(\bar{\sigma}) = \sqrt{3/2} \| \bar{\sigma}' \| \]

By letting \( \mathbf{c} \) denote the center of similarity of the normal-yield and the subloading surfaces, i.e. the similarity-center, which is called elastic-core since the most elastic deformation behavior is induced when the stress lies on it fulfilling \( R = 0 \) as will be explained later, the following relation holds (see Figure 1).

\[ \mathbf{c} - \bar{\alpha} = R(\mathbf{c} - \alpha) \]

which yields

\[ \bar{\alpha} = \mathbf{c} - R \hat{\mathbf{c}} \]

\[ \bar{\sigma} = \sigma + R \hat{\sigma} \]

where

\[ \begin{cases} \hat{\mathbf{c}} \equiv \mathbf{c} - \alpha \\ \hat{\sigma} \equiv \sigma - \mathbf{c} \end{cases} \]
The evolution rule of the normal-yield ratio is given by

$$dR = U(R) \| \Delta \varepsilon_p \| \quad \text{for} \quad \Delta \varepsilon_p \neq \mathbf{0}$$

(17)

where

$$U(R) = u \cot \left( \frac{\pi}{2} \frac{R - R_e}{1 - R_e} \right)$$

(18)

The evolution rule of the kinematic hardening rule is given by

$$d\alpha = c_k \left( \Delta \varepsilon_p - \frac{1}{\sqrt{3}} \frac{1}{2 \xi^2} \| \Delta \varepsilon_p \| \alpha \right)$$

(19)

Now, let the following elastic-core surface (see Fig. 1) be introduced, which always passes through the elastic-core \( \mathbf{c} \) and maintains a similarity to the normal-yield surface with respect to the kinematic-hardening variable \( \alpha \).

$$f'(\hat{\mathbf{c}}) = \mathcal{H}_e F(H), \quad \text{i.e.} \quad \mathcal{H}_e = \frac{f'(\hat{\mathbf{c}})}{F(H)}$$

(20)

where \( \mathcal{H}_e \) designates the ratio of the size of the elastic-core surface to that of the normal-yield surface and thus let it be called the elastic-core yield ratio. The function \( f'(\hat{\mathbf{c}}) \) is given for Eq. (5) by

$$f'(\hat{\mathbf{c}}) = \sqrt{3/2} \| \hat{\mathbf{c}} \|$$

(21)

The translation rule of elastic-core is given by

$$d\mathbf{c} = c \left( \Delta \varepsilon_p - \frac{R_e}{\xi^2} \| \Delta \varepsilon_p \| \hat{\mathbf{n}}_e \right)$$

(22)

where \( \xi (<1) \) is material constant, \( c \) is a material parameter and
The increment form of Eq. (14) leads to
\[ d\tilde{\alpha} = Rd\tilde{\alpha} + (1-R)d\mathbf{c} - d\mathbf{R} \hat{c} \tag{26} \]
Substituting Eqs. (17), (19) and (22) into Eq. (26), one obtains
\[ d\tilde{\alpha} = c_k R \left( \mathbf{c} \mathbf{R}^p - \frac{1}{b_h} || \mathbf{c} \mathbf{R}^p || \mathbf{a} \right) + c \left( 1-R \right) \left( \mathbf{c} \mathbf{R}^p - \frac{R_c}{\kappa} || \mathbf{c} \mathbf{R}^p || \hat{\mathbf{c}} \right) - U(R)\hat{c} || \mathbf{c} \mathbf{R}^p || \tag{27} \]

The increment of Eq. (10) leads to the consistency condition of the subloading surface:
\[ \frac{\partial f(\boldsymbol{\sigma})}{\partial \sigma} : d\sigma - \frac{\partial f(\boldsymbol{\sigma})}{\partial \boldsymbol{\sigma}} : d\tilde{\sigma} - RdF - dRF = 0 \tag{28} \]

### 3.3 Plastic strain increment

Adopt the associated flow rule for the subloading surface:
\[ d\mathbf{c}^p = \mathbf{n} d\tilde{\lambda} \quad (d\tilde{\lambda} = ||d\mathbf{c}^p|| > 0) \tag{29} \]
where \( d\tilde{\lambda} \) is the plastic multiplier and
\[ \mathbf{n} = \frac{\partial f(\boldsymbol{\sigma})}{\partial \sigma} / || \frac{\partial f(\boldsymbol{\sigma})}{\partial \boldsymbol{\sigma}} || = \frac{\boldsymbol{\sigma}'}{|| \boldsymbol{\sigma}'||} = \mathbf{n}' \quad (||\mathbf{n}'|| = 1) \tag{30} \]
Substituting Eq. (29) into Eqs. (7), (17), (19) and (22), one has
\[ dF = F'dH = F'_{kH} || \mathbf{c} \mathbf{R}^p || \tag{31} \]
\[ dR = U(R)d\tilde{\lambda} \tag{32} \]
\[ d\alpha = d\tilde{\lambda} \tilde{f}_{kn} \tag{33} \]
\[ d\mathbf{c} = d\tilde{\lambda} \tilde{f}_{cn} \tag{34} \]
where
\[ f_{H} = \sqrt{\frac{2}{3}} \tag{35} \]
\[ \tilde{f}_{kn} = c_k \left( \mathbf{n} - \frac{1}{\sqrt{3/2} \xi} \mathbf{a} \right) \tag{36} \]
\[ \tilde{f}_{cn} = c \left( \mathbf{n} - \frac{R_c}{\xi} || \mathbf{c} \mathbf{R}^p || \hat{\mathbf{c}} \right) \tag{37} \]
The substitutions of Eqs. (31), (32), (33) and (34) into Eq. (28) leads to
\[
\mathbf{n} : d \sigma - \mathbf{n} : \left[ \left( \frac{2}{3} \frac{F'}{F} d \mathbf{\bar{\lambda}} \mathbf{\bar{\sigma}} + R \mathbf{\bar{f}}_{kn} d \mathbf{\bar{\lambda}} + (1 - R) \mathbf{\bar{f}}_{cn} d \mathbf{\bar{\lambda}} + \frac{U}{R} d \mathbf{\bar{\gamma}} \mathbf{\bar{\sigma}} \right) \right] = 0
\]  
(38)
rom which the plastic multiplier \( d \mathbf{\bar{\lambda}} \) and the plastic strain increment \( d \varepsilon^p \) are given as follows:
\[
d \mathbf{\bar{\lambda}} = \frac{\mathbf{n} : d \sigma}{\mathbf{M}^p}, \quad d \varepsilon^p = \frac{\mathbf{n} : d \sigma}{\mathbf{M}^p} \mathbf{n}
\]  
(39)

where
\[
\mathbf{M}^p = \mathbf{n} : \left[ \left( \frac{2}{3} \frac{F'}{F} \mathbf{\bar{\sigma}} + R \mathbf{\bar{f}}_{kn} + (1 - R) \mathbf{\bar{f}}_{cn} + \frac{U}{R} \mathbf{\bar{\sigma}} \right) \right]
\]  
(40)

### 3.4 Stain increment vs. stress increment relations

The strain increment is given by substituting Eqs. (2) and (39) into Eq. (1) as follows:
\[
d \varepsilon = \mathbf{E}^{-1} : d \sigma + \frac{\mathbf{n} : d \sigma}{\mathbf{M}^p} \mathbf{n} = \left( \mathbf{E}^{-1} + \frac{\mathbf{n} \otimes \mathbf{n}}{\mathbf{M}^p} \right) : d \sigma
\]  
(41)

from which the plastic multiplier described in terms of the strain increment, denoted by \( d \mathbf{\bar{\lambda}} \) instead of \( d \mathbf{\bar{\lambda}} \), in the flow rule of Eq. (29) is given as follows:
\[
d \mathbf{\bar{\lambda}} = \frac{\mathbf{n} : \mathbf{E} : d \varepsilon}{\mathbf{M}^p + \mathbf{n} : \mathbf{E} : \mathbf{n}}, \quad d \varepsilon^p = \frac{\mathbf{n} : \mathbf{E} : d \varepsilon}{\mathbf{M}^p + \mathbf{n} : \mathbf{E} : \mathbf{n}}
\]  
(42)

The stress increment is given from Eq. (41) with Eq. (42) as follows:
\[
d \sigma = \mathbf{E} : d \varepsilon - \frac{\mathbf{n} : \mathbf{E} : d \varepsilon}{\mathbf{M}^p + \mathbf{n} : \mathbf{E} : \mathbf{n}} \mathbf{E} : \mathbf{n} = \left( \mathbf{E} - \frac{\mathbf{E} : \mathbf{n} \otimes \mathbf{n} : \mathbf{E}}{\mathbf{M}^p + \mathbf{n} : \mathbf{E} : \mathbf{n}} \right) : d \varepsilon
\]  
(43)

The loading criterion is given as follows (Hashiguchi, 2000, 2017):
\[
\begin{cases}
    d \varepsilon^p \neq \mathbf{0} & \text{for } \mathbf{n} : \mathbf{E} : d \varepsilon > 0 \\
    d \varepsilon^p = \mathbf{0} & \text{for } \mathbf{n} : \mathbf{E} : d \varepsilon \leq 0
\end{cases}
\]  
(44)

### 4 IMPLEMENTATION OF SUBLOADING SURFACE MODEL TO IMPLICIT NONLINEAR FE A CODE

The subloading surface constitutive model innovated by Hashiguchi has rich functionalities describing plasticity phenomena such as isotropic hardening, kinematic hardening, marasing effect, stagnation, tangential plasticity and so on in addition to the most beneficial scheme of smooth transition description of elastic to elastoplastic region. In order to implement these full functionalities of subloading surface model, stress integration is performed explicitly so-called forward Euler integration method. With the conventional explicit integration scheme for nonlinear finite element analysis such as explicit creep analysis, program can not take large time step size due to stability limit. This is critical disadvantage of explicit integration method in general. Therefore, we tried to invent new solution scheme using explicit stress integration method for the implementation of subloading surface model into Marc general purpose finite element code mainly used statically loaded nonlinear analysis.
4.1 Forward Euler stress integration

The stress calculation phase occurs twice in nonlinear finite element software, internal force calculation before matrix solution phase for incremental displacement calculation and stress recovery phase after incremental displacement calculation. Total stress is calculated using incremental strain converted with incremental displacement in case of additive decomposition based large displacement finite element analysis. In case of large time step is taken for speed performance purpose, stress integration based on forward Euler fails due to excessive incremental strain, this characteristic called stability problem in explicit time step integration scheme. In order to resolve this stability limit problem, we developed a scheme that incremental strain is subdivide into small enough incremental strain then total incremental stress calculated using multiple sub-steps, hereafter called SSM Strain Subdivided Method. This logic requires multiple stress calculation steps within a single global stiffness matrix solution step that consumes lots of calculation time and also difficult to parallelize efficiently. In the other hand, element stiffness calculation and stress recovery phase can be easily parallelized by Domain Decomposition Method, hereafter called DDM, or OpenMP based multi-threading.

Fig. 2 illustrates the FEA model used for numerical experiment in order to investigate the required minimum subdivided strain increment for SSM. Model consists of single cubic element with 1mm edge length.

The material is elastic-plastic with material constants of Young’s modulus, Poisson’s ratio and initial yield stress used here are 170000 MPa, 0.3 and 510 MPa, respectively. The hardening coefficients, evolution of normal-yield ratio are defined as follows;

\[
\begin{align*}
\text{Isotropic hardening parameter:} & \quad h_1=0.61, \ h_2=170 \\
\text{Kinematic hardening parameter:} & \quad C_k=5200 \text{ MPa}, \ \zeta=0.2 \\
\text{Evolution of normal-yield ratio:} & \quad \bar{\sigma}=60, \ \bar{u}_c=5, \ \bar{R}_e=0.5
\end{align*}
\]

The face loads are applied on the top face of the mesh. The amplitude of the load is 830 MPa with pulsating cyclic history as shown in Fig. 3.

The three different limit strain cases were tested, case1 with limit strain of 1.0d-3, case2 with limit strain of 1.0d-4 and case3 with limit strain of 1d-5. Fig. 4 shows the numerical experiment result. From this numerical experiment result for limit strain impact to analysis stability and accuracy, limit strain of 1.0d-3 is too large and showed different result from other two cases and limit strain of 1.0d-4 and 1.0d-5 cases showed acceptable result. 1.0d-3 of strain is similar level of elastic limit of steel material and applying this level of strain in single stress calculation step is obviously causes accuracy problem. We selected limit strain of 1/20 of initial elastic strain obtained by Young’s modulus and initial yield stress.
4.2 Mid-point tangential stiffness evaluation

With the SSM program work flow, tangential stiffness matrix is evaluated multiple times since incremental strain is subdivide and stress integration calculation occurs multiple times.
within a Newton Raphson iteration. We conducted a series of numerical experiments to find the best tangential stiffness evaluation timing, beginning of the increment, mid-point of the increment or end of the increment using the same FEA model in the previous section and selected mid-point tangential stiffness evaluation scheme that gives accuracy and stability.

5 SPRINGBACK ANALYSES

The metal forming analyses are of importance in the industrial production. The analysis of the springback by use of the subloading surface model will be described in here.

The high strength steel sheets and aluminum sheets exhibiting far larger springback than ordinary mild steel sheets are widely used in automobile industries. The springback cannot be described by the constitutive models which use the yield surface enclosing a purely-elastic domain, i.e. the conventional model and the cyclic kinematic hardening models (multi-surface, two-surface and superposed kinematic hardening models), since a plastic strain rate in the unloading process is not described appropriately by these models. The schematic illustration of the draw-bending (so-called hat-bending) is shown in Fig. 5.

![Fig. 5. Schematic illustration of the set-up of hat-bending](image)

Fig. 6 illustrates the comparison of measured stress-strain curve and the reproduced stress-strain curve with subloading surface model using the following values of material parameters. Material constants :

- Initial yield stress: $F_0 = 402\text{MPa}$
- Elastic moduli: $E = 200,000\text{MPa}$, $\nu = 0.3$,
- $h_1 = 0.75$, $h_2 = 15$,
- $c_k = 250\text{MPa}$, $\zeta = 1.0$,
- $\bar{E} = 300$, $u_c = 5$.

The good agreement is observed in Fig. 6 unlike Fig. 7 that illustrates the comparison of measured one and reproduced one with conventional combined hardening model. Conventional combined hardening model in Marc uses the ratio of isotropic hardening part and kinematic hardening part, 80% for isotropic hardening and 20% for kinematic hardening were used in this case.
Fig. 6 Measured stress-strain curve and reproduced stress-strain curve with subloading surface model.

Fig. 7 Measured stress-strain curve and reproduced stress-strain curve with conventional combined hardening model.

The calculation results of the shapes of the sheet after the springback are shown in Fig. 8, which was analyzed with the subloading surface model in the commercial software Marc (MSC Software, Ltd.). The enough springback is predicted, which is caused by the plastic deformation in the forming process by virtue of the advantage of the subloading surface model describing the plastic strain rate due to the rate of stress inside the yield surface.
In contrast, the springback, shown in the Fig. 9, is predicted slightly by the conventional elastoplastic model which is realized by using the combined hardening model in Marc. The major reason seems to be lack of accurate reproduction of Bauschinger effect during reverse yielding stage with conventional plasticity model and it is obvious that some part of material is subjected to reverse yielding situation in this type of forming process since initially bended portion, partially tensile yielding state and partially compressive yielding state, will be stretched in the later forming stage, all stretched yielding state. Then, the importance is recognized for the introduction of the rigorous elastoplastic model, i.e. the subloading surface model capable of describing the plastic strain rate in the stress-reducing process appropriately. Hereinafter, it is desirable that the prediction of springback behavior will be executed by the pertinent analysis exploiting the subloading surface model, aiming at the epochal improvement of the prediction of the springback behavior in industries.
5 CONCLUSIONS
The subloading surface elastoplastic constitutive model innovated by Hashiguchi was implemented in Marc general purpose nonlinear finite element commercial software. Implementation of forward Euler based stress integration formulation, that has full functionality to describe plasticity phenomena such as the Masing effect, stagnation and so on, into implicit static software is not easy since typical incremental strain is much larger than the stability limit of Eulerian integrator. In order to preserve unconditionally stable characteristic, we used Strain Subdivide Method as stress integration scheme that subdivide the incremental strain into acceptably small size for stress integrator. During the implementation, several numerical tests were carried out in order to confirm the speed performance and also accuracy using typical industrial problem such as tensile test of dumbbell specimen.

The springback simulation for sheet metal forming of high strength steel material is performed and the result was compared against the measured result of physical experiment. Throughout this numerical experiment it is confirmed that springback phenomena which has strong dependency on Bauschinger effect can be predicted with subloading elastoplastic constitutive model and the conventional elastoplastic constitutive model has limitation in accuracy for the prediction of springback due to lack of accurate reproduction capability of Bauschinger effect.

REFERENCES
LONG-TERM RELIABILITY EVALUATION OF FLUORORESIN GASKET FOR ELECTRODE OF AUTOMOTIVE LITHIUM-ION BATTERY USING SIMULATION

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Key words: Fluororesin, Gasket, Sealing Pressure, Maximum Principal Strain, Elasto-Plastic and Creep Properties, Finite Element Method.

Abstract: In this paper, we proposed a simulation method based on the finite element method using an elasto-plastic model and a creep model to evaluate the changes in fluororesin properties with time. The validity of the proposed simulation method was verified by comparing the simulation results with the experiment results for the compression set of fluororesin PFA (Perfluoroalkoxy Copolymer). Furthermore, with the proposed simulation method, we evaluated the long-term reliability of PFA gaskets for the electrodes of automotive lithium-ion batteries.

1 INTRODUCTION

In recent years, in order to prolong life of automotive lithium-ion (Li-ion) batteries for electric vehicles, fluororesin such as PFA (Perfluoroalkoxy Copolymer), which has excellent electrolyte resistance, electrical insulation properties, climate resistance and low moisture permeability, is being used as a material for gaskets around electrodes [1]. Since the reliability such as sealing performance and strength properties of automotive Li-ion battery gaskets must be guaranteed for 10 years or more, the long-term reliability evaluation of fluororesin gaskets has become an important issue.

In this paper, we proposed a simulation method based on the finite element method (FEM) using a combined material model, which is composed of an elasto-plastic model and a creep model, to evaluate the changes in fluororesin properties with time. We verified the validity of the simulation method by comparing the simulation results with the experiment results for the compression sets of fluororesin PFA. Moreover, we clarified that it is possible to quickly
evaluate the long-term reliability of gaskets for electrodes of automotive Li-ion batteries when shapes of the gaskets, electrodes and lids change without relying on prototype tests, and realize an optimum gasket structure design in a short time.

2 PERFORMANCE REQUIREMENTS FOR AUTOMOTIVE Li-ION BATTERY GASKETS

Figure 1 shows a schematic diagram of a prismatic-type automotive Li-ion battery. Gaskets used in Li-ion batteries act as seals to prevent electrolyte from leaking out and moisture in the air from infiltrating the battery. The gaskets also provide electrical insulation to prevent the positive and negative electrodes from making contact and causing short circuits. To ensure the safety and life-span of the batteries, sealing and insulation functions of automotive Li-ion battery gaskets must be guaranteed for 10 years or more. Battery gaskets must also possess restoring force to maintain the shape of the seal under adverse conditions, such as high temperatures and long-term stresses, which can cause creep deformation. When a gasket is tightened, the restoring force generated by tightening creates seals between the gasket and the electrode and between the gasket and the lid. In designing automotive Li-ion battery gaskets, it is an important task to evaluate the long-term reliability of gaskets to ensure the required sealing pressure while suppressing the maximum strain in gaskets.

Battery gaskets have traditionally been made of rubbers. For many years, it was not considered possible to produce the gaskets from other polymers. Fluoro resin like PFA, however, possesses excellent electrolyte resistance, electrical insulation and climate resistance in addition to low moisture permeability. The material wedges into the concavities on metal surfaces, and can form seals, even on rough surfaces without the use of treatment agents or adhesives. Even at a low temperature of \(-40^\circ\text{C}\) or when exposed to a long-term high temperature of \(65^\circ\text{C}\), the PFA retains its restoring force and maintains its sealing performance. In addition, the amount of swelling of PFA in response to electrolyte is less than one-tenth that of rubbers. Therefore, deterioration of material properties of PFA due to swelling is small, and long-term reliability improvement of its gaskets can be expected.

3 MATERIAL PROPERTIES OF FLUORORESIN PFA

In this paper, we assumed that the time dependence of the mechanical properties of PFA can be represented by a combined material model, which is composed of an elasto-plastic

![Figure 1: Schematic diagram of a prismatic-type automotive Li-ion battery showing gaskets](image-url)
model and a creep model. The elasto-plastic model is assumed to meet the von Mises yield criteria and isotropic hardening rule, and is approximated by multiple lines, and the creep model is characterized by the modified time hardening creep model [2]. In particular, the elasto-plastic model of PFA is prepared based on the tensile stress-strain diagrams at a normal temperature of 23°C and a high temperature of 65°C, and the creep model of PFA is created based on the results of compression creep tests with different stress levels at the corresponding temperatures. The modified time hardening creep model is shown in the following equation (1).

\[ \varepsilon_{\text{crep}} = C_1 \sigma^2 t^{C_3} + e^{-C_4/T}/(C_3+1) \]  

where, \( \varepsilon_{\text{crep}} \) is creep strain, \( \sigma \) is stress, \( T \) is temperature and \( C_1, C_2, C_3, C_4 \) are parameters identified from the compression creep experiment results. In particular, the values of the parameters \( C_1, C_2, C_3 \) are identified by fitting the compression creep experiment results at the normal temperature and the high temperature to the equation (1), with the parameter \( C_4 \) representing the temperature dependency of the creep characteristic set to 0.

3.1 Compression set test for PFA

In this paper, we verify the validity of the combined material model by comparing simulation results of the compression sets of PFA over time with the experiment results.

The compression set [3] of a material is the permanent deformation remaining after removal of a force that was applied to it. The term is normally applied to soft materials such as elastomers, and is considered as an important property for gasket materials. Compression set is normally measured in two ways: compression set under constant force in air (A) and compression set under constant deflection in air (B).

In compression set B, the specimen is compressed to 75% of its original height for a set time and at a set temperature. Compression set B is defined as the percentage of original specimen thickness after it has been left in normal conditions for 30 minutes. \( C_B \), the compression set B is given by

\[ C_B = \left[ (t_o - t_i)/(t_o - t_n) \right] \times 100 \]  

where, \( t_o \) is the original specimen thickness, \( t_i \) is the specimen thickness after testing and \( t_n \) is the spacer thickness or the specimen thickness during the test.

In this paper, we expand and apply the method of compression set test B to fluororesin PFA to evaluate its permanent deformation characteristics. Figure 2 shows the detailed procedure of the compression set test for fluororesin PFA.

1) Compress the cylindrical specimen by 25% using a jig at a normal temperature of 23°C and hold it for 30 minutes.
2) Place the specimen in a furnace at a high temperature of 65°C and hold it for a set time.
3) Remove the specimen from the furnace after the set time and cool it naturally at the normal temperature for 3 hours.
4) Release the specimen from the jig and leave it at the normal temperature for another 30 minutes, then measure the thickness of the specimen.
5) Calculate the compression set from the change in the thickness of the specimen using the equation (2).
3.2 Verification of the combined material model

Figure 3 shows the compression set results of simulations and experiments for the specimens of fluororesin PFA. The simulation results are obtained by FEM based on the combined material model and the experiment conditions described above. A good correlation was found between the compression set results of simulations and experiments over 50,000 hours (about 5.7 years). Since the simulation results and the experiment results are in good agreement, we can conclude that the proposed simulation method and the combined material model are valid and effective for evaluating time-dependent deformation behaviors of fluororesin PFA.

By using the proposed simulation method and the combined material model, it is possible to evaluate the long-term reliability of fluororesin PFA gaskets having different shapes and structures quickly without relying on experiments.

![Diagram of compression set test](image)

**Figure 2:** Procedure of the compression set test for fluororesin PFA

![Graph of compression set results](image)

**Figure 3:** Compression set results of simulations and experiments for fluororesin PFA
4 SIMULATING GASKET RELIABILITY

In general, a gasket with a uniform cross-sectional thickness is used. In order to reduce variations in tightening of gasket and to increase the sealing pressure, it is common to make protrusions on the tightening members. Because it takes a lot of time to create and test physical prototypes, little research had been done on the effects of changing protrusion shapes and distances between the protrusions, and the limits of physical testing mean that we had to rely on trial-and-error methods to improve gasket designs.

In this section, we use the above-described simulation method and the proposed combined material model of fluoro resin PFA to obtain a better understanding of the effects of age-related change and to learn how changing the protrusion shapes and distances between protrusions could improve efficiency and life expectancy of PFA gaskets.

4.1 Effects of protrusion shapes

Figure 4 shows a schematic half cross-sectional shape of a gasket structure for an electrode of a Li-ion battery. Here, the dimensions of the gasket are referred to the reference [4]. In this paper, we assumed that the gasket, the lid and the electrode have geometrical axial symmetry, and there is a protrusion on the lid, and the protrusion tip has an arc shape. Based on these assumptions, the simulations of the gasket tightening process and sealing performance change over time after the gasket tightening can be performed by a two-dimensional axisymmetric finite element model.

In the simulation, the lid and the electrode are assumed to be rigid because they have remarkably higher rigidity than the gasket. In the tightening process of the gasket, it is assumed that the electrode is completely fixed, and the reinforced displacement in the axial direction is applied to the lid. The maximum axial reinforced displacement of the lid is the same as the height of the protrusion. Moreover, the friction coefficients of the contact surfaces between the gasket and the lid, between the gasket and the electrode are set to 0.2. FEM code ANSYS is used in the simulations.

In this section, we show the aging changes of sealing performance of fluoro resin PFA gaskets obtained by using the simulation method. The gaskets are tightened at the normal temperature (23°C) and moved to a furnace (65°C) an hour later.

Figure 4: Cross-sectional shape of a gasket structure with a protrusion on the lid
The changes with time in the maximum gasket sealing pressure on the electrode side and the lid side are shown in Fig. 5 in the case where the protrusion height is 0.18mm and the width is 0.36mm (h0.18; w0.36). According to these results, it is obvious that a larger sealing pressure is generated on the lid side with a protrusion than on the electrode side without protrusion. It is also found that the sealing pressure on both the lid side and the electrode side greatly decrease after the gasket was moved to the furnace, but the differences in the sealing pressures between the lid side and the electrode side become smaller. In addition, the maximum sealing pressures after 90,000 hours (about 10.3 years) on the electrode side and the lid side are 3.2MPa and 8.6MPa, respectively, which are sufficient for sealing the electrodes of the automotive Li-ion batteries where required sealing pressure is 1MPa.

The distributions of the sealing pressures with time on the lid side and the electrode side are shown in Fig. 6. Judging by these results, it is seen that the distribution shapes of the sealing pressures do not change with time, but the maximum sealing pressures decrease with time. It is also found that the maximum sealing pressures on the lid side are generated slightly inside the protrusion, not directly below the protrusion, and the maximum sealing pressures on the electrode side occur inside the protrusion as well. In addition, it should be noted that the sealing pressure distributions shown at the end of Fig.6 are the results when the internal pressure of 1MPa is applied to the Li-ion battery after 90,000 hours. In this case, the maximum sealing pressures on the electrode side and the lid side are 3.2MPa and 8.8MPa, respectively, which are sufficient for sealing pressures for the automotive Li-ion batteries.

Figure 7 shows the changes with time in the maximum first principal mechanical strain, creep strain and total strain of the gasket when the protrusion height is 0.18mm and the width is 0.36mm. Here, the true strain is used and the maximum first principal total strains are calculated by the following equation (3). Based on these results, it is clear that the mechanical strains and the creep strains increase with time. It is also found that the strains do not change significantly after the gasket is moved to the furnace. This is caused by the fact that the gasket is tightened and cannot deform freely. The maximum first principal strain of the gasket is about 0.83 after 90,000 hours, it is much less than 1.61 of PFA breaking strain.

\[
\varepsilon_{total} = \ln[\exp(\varepsilon_{mech}) + \exp(\varepsilon_{crep}) - 1] \tag{3}
\]

Figure 5: Changes with time in the gasket sealing pressures on the electrode side and the lid side (h0.18; w0.36)
Figure 6: Distributions of sealing pressures with time on the lid side and the electrode side (h0.18; w0.36)
Figure 8 shows the changes in the sealing pressures of the gasket after 90,000 hours due to the differences in the protrusion shapes \((h/w)\) and the tightening ratios \((h/H)\), and Fig. 9 shows the corresponding maximum first principal strains. Here, the vertical axis in Fig. 8 represents:

![Figure 7: Changes with time in the maximum first principal strain of the gasket \((h0.18; w0.36)\)](image)

![Figure 8: Sealing pressures of gaskets after 90,000 hours with a protrusion on the lid](image)

![Figure 9: Maximum first principal strains of gaskets after 90,000 hours with a protrusion on the lid](image)
the smaller of the maximum sealing pressures on the lid and the electrode side, the vertical axis in Fig. 9 means the total strains which are calculated by the equation (3). Based on these results, it is found that the gasket can secure the required sealing pressures while suppressing the maximum strains even after 90,000 hours if the h/w and h/H are in the range of 0.1 to 0.7, and in the range of 0.1 to 1.0.

4.2 Effects of distances between protrusions

Figure 10 shows a schematic half cross-sectional shape of a gasket structure which has one protrusion on the lid and one on the electrode. In this section, the cross-sectional shape of the protrusion is assumed to be semicircular, and the simulation conditions are the same as above. Now, we show the effects of the distances between the protrusions on the aging changes of the sealing performance of fluororesin PFA gaskets obtained by using the simulation method.

Figure 11 shows the changes in the sealing pressures of the gasket after 90,000 hours (about 10.3 years) due to the differences in the distances between protrusions (d/H) and the tightening ratios (2h/H), and Fig. 12 shows the corresponding maximum first principal strains. As mentioned in the above section, the vertical axis in Fig. 11 represents smaller values of the maximum sealing pressures on the lid and the electrode side, and the vertical axis in Fig. 12 means the total strains calculated by the equation (3). According to these results, it is observed that the sealing pressures after 90,000 hours decrease as the tightening ratios (2h/H) increase in the range of 0.1 to 0.5. It is considered that this is because the stress relaxation of the PFA increases rapidly as the tightening ratio increases. However, the sealing pressures increase again when the tightening ratios is greater than 0.5. On the other hand, it is found that the maximum strains after 90,000 hours increase as the tightening ratios increase in the range of 0.1 to 0.8. It is revealed that the sealing pressures and maximum strains after 90,000 hours fluctuate greatly if d/H is in the range of 1 or less and 2h/H in the range of 0.5 or more.

It is also confirmed that the sealing pressures and the strains approach nearly constant values when d/h is greater than 1.5, especially for the tightening ratios in the range of 0.1 to 0.7. Therefore, it is concluded that if d/H is in the range of 1.5 or more and 2h/H is in the range of 0.1 to 0.7, the sealing pressures and the maximum strains after 90,000 hours can be maintained at appropriate values, which are suitable for sealing automotive Li-ion batteries.

Figure 10: Cross-sectional shape of a gasket structure with protrusions on the lid and the electrode
5 CONCLUSIONS

- A Simulation method based on the finite element method using a combined material model which is composed of an elasto-plastic model and a creep model is established to evaluate the changes in fluoro resin PFA properties with time. The elasto-plastic properties are modeled with a multilinear isotropic-hardening elastic-plastic model meeting the von Mises yield criteria, and creep properties are modeled with the modified time-hardening creep model.

- The validity of the simulation method and the combined material model for PFA is verified by comparing the simulation results of compression sets over 5 years with the experiment results.

- Based on the established simulation method, the influence of protrusion shapes and distances between protrusions on the long-term reliability of the PFA gasket is clarified, and PFA gasket structures that can maintain the required sealing pressures while reducing the maximum principal strains are revealed.

- Using the established simulation method, it is possible to quickly evaluate the long-
term reliability of PFA gaskets for automotive Li-ion batteries when shapes of gaskets, electrodes and lids change without relying on experiments, and realize an optimum gasket design in a short time.

REFERENCES
COUPLED PORO-INELASTIC RESPONSE OF SOILS USING A NEW INTERPOLATION RULE THROUGH THE GENERALIZED PLASTICITY THEORY WITHIN THE UBCSAND MODEL

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Abstract. During numerical computations, when the stress is updated in the constitutive relationship, it is of major necessity to distinguish the soil behavior under cyclic or transient loads from that of monotonic ones. The cyclic plasticity models developed to simulate the mechanism of soil failure, require accurate predictions of irreversible strains computed through a flow rule in both virgin loading and stress reversals. In multi-surface type models, such as UBCSAND, plastic modulus is calculated using a hardening rule where the location of the current stress tensor is related to its projection on the bounding surface through an interpolation rule.

In this study, the plastic hardening modulus \( (H_L) \) that is calculated using the Generalized Plasticity Theory, is adapted in the current formulation of the UBCSAND hardening rule in terms of deviatoric plastic strains. Hence, the UBCSAND model is modified to serve with the generalized plasticity framework to evaluate the cyclic behavior of sands. This way of calculating the plastic modulus is based upon an interpolation rule that typically exists in the bounding surface theory with the value of \( H_L \) on the bounding surface. Such a concept is very well applicable to clay soils also.

Firstly, a number of strain and stress-controlled cyclic triaxial tests are simulated in order to validate the current constitutive formulation. Secondly, the effects of the new interpolation rule on the cyclic behavior of granular soils is investigated with a number of parametric studies which are performed to examine the effect of \( H_L \) on the overall cyclic response. Finally, the new formulation is implemented in an in-house finite element code developed to solve the coupled equations of the partially dynamic (PD) Biot formulation used to analyse a soil-column problem under harmonic surface excitation. Results are obtained in terms of solid displacement, pore pressure and effective stress variation in temporal and spatial domains.
1 INTRODUCTION

Elasto-plastic response of soils are evaluated based upon the valid assumption that the constitutive behavior of soils is inherently nonlinear under applied loads beyond a certain strain level. Such a phenomenon becomes particularly important when the coupled flow and deformation response of soils is taken into consideration in solution of related geomechanics problems, hence the theory of poro-inelasticity. Therefore, one should adopt a coupled mathematical formulation, such as that of Biot’s theory for porous media, and make use of a nonlinear elasto-plastic model governing essentially the effective stress-strain relationship. While such a process is applicable to all soils and geomechanics problems, this is by no means a trivial process. That is, finding a constitutive model that is capable of capturing the most essential features of soil dynamic behavior under cyclic loading caused by earthquakes or ocean waves and yet keeping the theory as simple as possible is the most challenging task of all. In this study, such an objective is set with the idea of enhancing a well-known constitutive model, UBCSAND, which is used to model the cyclic response of loose sands through the basic notions of another simple theory called the Generalized Plasticity Theory (GPT). A simple hardening interpolation rule is proposed to calculate the plastic hardening modulus with an analogy to bounding surface plasticity concept. GPT was proposed to encompass the existing theories in a unified manner acting as a more general theory which allows the inclusion of main features of other frameworks (Pastor et al., 1985; Pastor et al., 1990). This property of the GPT comes from the fact that it is a very flexible theory leading to a model that captures observed fundamental behavior under static and dynamic loading. It requires only the loading/unloading directions, a plastic flow direction, a plastic hardening modulus in loading/unloading, and an elasticity matrix. These main properties of the theory are adapted to work within UBCSAND to enhance its capability towards modeling undrained cyclic triaxial behavior of sands. A number of strain and stress-controlled undrained cyclic triaxial tests are simulated in order to validate the current constitutive formulation. Then the effects of the new interpolation rule on the liquefaction behavior of loose sands is investigated in a few parametric studies which are performed to examine the effect of hardening modulus on liquefaction. Finally, the new formulation is implemented in a new finite element code developed to solve the coupled equations of the partially dynamic (PD) Biot formulation used to analyse a soil-column problem under harmonic surface excitation.

2 UBCSAND MODEL

The formulation of the original UBCSAND model is based on classical plasticity theory. In order to model the behavior of sandy soils in static and dynamic conditions, UBCSAND model was first developed by Puebla et al. (1997) and later Beaty and Byrne (1998) at the University of British Columbia (UBC). In this initial version of the model, mathematical formulation is implemented to work for the plane stress state. Then Tsegaye (2010) extended the model to work for three-dimensional (3-D) problems which was termed the UBC-PLM model. Also, Petalas and Galavi (2012) and Petalas et al. (2013) made some improvements to the model to better explain the soil behavior under dynamic loading. Below summarizes the fundamentals.
2.1 Mathematical formulation

Elastic behavior

The elastic behavior within the yield surface is governed by a non-linear rule as a function of mean effective stress. Two parameters that control the nonlinear elastic behavior are the elastic bulk modulus, $K$ and shear modulus, $G$ calculated using the following relations:

$$K = k_B^e A P_A (p'_A)_{me}$$

(1)

$$G = k_G^e A P_A (p'_A)_{ne}$$

(2)

where $k_B^e$ and $k_G^e$ are the elastic bulk and shear moduli at the reference stress level, $P_A$ which is the atmospheric pressure, $p'$ is the effective stress, $me$ and $ne$ are the model parameters.

Yield function

UBCSAND model uses the well-known Mohr-Coulomb yield function generalized in 3-D principal stress space given as:

$$f_m = \frac{\sigma'_{\text{max}} - \sigma'_{\text{min}}}{2} - \left( \frac{\sigma'_{\text{max}} + \sigma'_{\text{min}}}{2} + c' \cot \phi_p \right) \sin \phi_m$$

(3)

where $\sigma'_{\text{max}}$ and $\sigma'_{\text{min}}$ are the maximum and minimum effective stresses, $c'$ is the effective cohesion of the soil, $\phi_p$ is the peak friction angle and $\phi_m$ is the mobilized friction angle during hardening. The yield surface defined in terms of the principal stresses can be written in terms of stress invariants, including shear stresses without departing from the actual theory:

$$f (\sigma, \sin \varphi_m) = \bar{\sigma} - M I = 0$$

(4)

where $\bar{\sigma} = \sqrt{3 J_2}$, $I = I_1/3$ with $I_1$ being the first invariant of stress and $J_2$ is the second deviatoric stress invariant. $M$ determines the position of the yield surface and depends on the third stress invariant, $J_3$, Lode’s angle ($\theta$) and the hardening parameter, $\sin \varphi_m$. Thus we have:

$$M = \frac{6 \sin \varphi_m}{3 - \sin \varphi_m \sin 3\theta}$$

(5)

and the $\theta$:

$$\theta = \frac{1}{3} \sin^{-1} \left( -\frac{3\sqrt{3}}{2} \frac{J_3}{J_2^{3/2}} \right), \quad -\frac{\pi}{6} \leq \theta \leq \frac{\pi}{6}$$

(6)
**Elasto-plastic behavior**

When the stress vector reaches the yield surface, plastic deformations begin to occur. In the model, a non-associated flow rule is considered for the calculation of the plastic deformations using the plastic potential function defined as:

\[ g(\sigma) = \sigma - M^* I = 0 \]  \hspace{1cm} (7)

Here, \( M^* \) depends on the mobilized dilation angle, \( \psi_m \), calculated similar to (5) as:

\[ M^* = \frac{6 \sin \psi_m}{3 - \sin \psi_m \sin 3\theta} \]  \hspace{1cm} (8)

with

\[ \sin \psi = \sin \phi_m - \sin \phi_{cv} \]  \hspace{1cm} (9)

where \( \phi_{cv} \) is the critical friction angle. Flow rule is written in a classical fashion as:

\[ d\epsilon^p = d\lambda \frac{\partial g}{\partial \sigma} \]  \hspace{1cm} (10)

where \( d\lambda \) is the plastic multiplier which defines plastic deformation amount and \( \frac{\partial g}{\partial \sigma} \) describes the direction of the plastic deformation vector. Hardening law is defined by the hyperbolic relationship between the plastic shear strain and the mobilized friction angle which acts as the hardening parameter as per Puebla et al. (1997):

\[ d\sin \phi_m = G^* d\lambda d\text{dev} \left( \frac{\partial g}{\partial \sigma} \right) \]  \hspace{1cm} (11)

where \( G^* \) is the plastic shear modulus given as:

\[ G^* = k_G^p \left( \frac{I}{P_A} \right)^{np-1} \left( 1 - \frac{\sin \phi_m}{\sin \phi_p} \right)^2 \]  \hspace{1cm} (12)

Here \( k_G^p \) is the plastic shear modulus number, \( np \) is the model parameter, \( P_A \) is the atmospheric pressure and \( R_f = \frac{n_f}{n_{ult}} \) is the failure ratio generally ranging from 0.5 to 1.0 with \( n_f \) being the stress ratio at failure and \( n_{ult} \), the ultimate stress ratio (Petalas et al., 2012).

**Stress-strain relationship**

The strain decomposition in an incremental form is written as:

\[ d\xi = d\epsilon^e + d\epsilon^p \]  \hspace{1cm} (13)

where \( d\epsilon^e \) and \( d\epsilon^p \) are the elastic and plastic strain increments, respectively. Taking the elastic strains from this relation and using in the stress-strain relationship, we get:
\[ d\sigma = D^e (d\varepsilon - d\varepsilon^p) \]  
(14)

where \( D^e \) is the elastic constitutive matrix. Using the consistency condition with the inclusion of the hardening term gives:

\[ \left( \frac{\partial f}{\partial \sigma} \right)^T D^e (d\varepsilon - \lambda \frac{\partial g}{\partial \sigma} + d\lambda \frac{\partial f}{\partial \sin \phi_m} G^* \sqrt{\text{dev} \frac{\partial g}{\partial \sigma} \text{dev} \frac{\partial g'}{\partial \sigma}} = 0 \]  
(15)

which is used to derive the final stress-strain relationship in incremental form as,

\[ d\sigma = D^e \left( I - \frac{\frac{\partial g}{\partial \sigma} \left( \frac{\partial f}{\partial \sigma} \right)^T}{\frac{\partial f}{\partial \sigma}} D^e \right)^T d\varepsilon \]  
(16)

where the plastic modulus is:

\[ H_L = -\frac{\partial f}{\partial \sin \phi_m} \frac{\partial \sin \phi_m}{\partial \varepsilon^p} \sqrt{\text{dev} \frac{\partial g}{\partial \sigma} \text{dev} \frac{\partial g'}{\partial \sigma}} \]  
(17)

The tensor in (16) linking stress increments to strains is the 4th order elastoplastic matrix, \( D^{ep} \).

**Verification of the static behavior**

Analyses are performed using a fully explicit forward Euler integration method for a representative soil element. Figure 1 shows the comparison of triaxial tests (Eliadorani, 2000) and the simulation results. Comparisons are made in terms of shear stress-axial strain relationships as well as stress path plots for fully undrained and partially drained tests. Partial drainage condition is defined as; \( \varepsilon_d = \varepsilon_p \) where \( \varepsilon_p \) is the total volumetric strain. Figure 2 presents the results for the fully drained condition obtained by Tatlıoğlu, (2018), which are compared with the tests of Tsegaye, (2010). Overall the presented formulation of the model is capable of capturing the main features of sand behavior under monotonic loading for three drainage conditions.

**Figure 1:** Simulation of undrained and partially drained triaxial test (Tatlıoğlu, 2018; data of Eliadorani, 2000)
2.2 Formulation for cyclic behavior using GPT

UBCSAND cyclic model

In the UBCSAND model, two different surfaces are defined: the primary and the secondary yield surface. The primary yield surface is active during the primary loading when it expands following the isotropic hardening rule until it reaches the maximum stress ratio. The secondary yield surface moves with a simplified kinematic hardening rule and is active after one loading-unloading step (Petalas et al., 2012). The same yield surface definition is used for both surfaces. However, a different hardening rule is defined for each surface through the hardening parameter, \( \sin \varphi_m \). The difference between the hardening rules used on these yield surfaces is due to the parameter, \( k_p^G \) used in \( G^* \) calculated as:

\[
G^* = k_p^G \left( \frac{I}{P_A} \right)^{p-1} \left( 1 - \frac{\sin \varphi_m R}{\sin \varphi_p} \right)^2
\]

where \( k_p^G \) is taken constant during isotropic hardening. When the stress vector is on the secondary yield surface during stress reversals, \( k_p^G \) is a function of the number of cycles of loading;

\[
k_p^G = k_p^G \left( 4 + \frac{n}{2} \right) k_d \ast \delta_d
\]

Here \( n \) is the number of stress reversals, \( k_d \) is the correction factor for loose soils calculated as below and \( \delta_d \) is a material parameter; \( k_d = \min(1, \max(0.5, 0.1 N_{i,60})) \) (Petalas et al., 2012).

Formulation of stress reversals using GPT

Generalized Plasticity Theory (GPT), capture the stress-strain relationship as observed in laboratory tests through minimum possible complexity. This means, the model is able to capture the actual behavior of soils by keeping the number of model parameters at a minimum (Ülker, 2016). Generalized Plasticity Model (GPM) is flexible enough to be used together with other models. In this study, it is aimed to improve the UBCSAND soil model with the
contribution of some of the features of GPM to better explain the dynamic behavior of sands.

In GPT, unit vector definition is used to decide loading and unloading steps in terms of $f$:

$$n = \frac{\partial f}{\partial \sigma} / \left| \frac{\partial f}{\partial \sigma} \right|$$  \hspace{1cm} (20)

The direction of plastic flow is also calculated with unit vectors using the $g$ surface through:

$$n_g = \frac{\partial g}{\partial \sigma} / \left| \frac{\partial g}{\partial \sigma} \right|$$  \hspace{1cm} (21)

The following conditions are checked to decide the loading and unloading steps (Pastor et al., 1985; Pastor et al., 1990) in the case of hardening behavior:

$$d \sigma : n > 0 \rightarrow \text{loading} , \ d \sigma : n < 0 \rightarrow \text{unloading} , \ d \sigma : n = 0 \rightarrow \text{neutral loading}$$  \hspace{1cm} (22)

Finally, the stress-strain relationship is obtained in the same way as in equation (16):

$$d \sigma = \left( D' - \frac{D' n_g n^T D'}{H_L + n^T D' n_g} \right) d \varepsilon$$  \hspace{1cm} (23)

where the plastic hardening modulus is obtained with a reference to a consistency condition:

$$H_L = -\left[ \frac{df}{d \varepsilon^p} \frac{d \sin \phi_m}{d \varepsilon^p} \frac{dg}{d \sigma} / \left| \frac{df}{d \sigma} \right| \frac{dg}{d \sigma} \right]$$  \hspace{1cm} (24)

**New interpolation rule for the plastic hardening modulus**

In order to improve the simulation of dynamic behavior of sandy soils, plastic hardening modulus ($H_L$) that is calculated in its original form in the GPT, is now adapted in the current formulation of the hardening rule of UBCSAND using deviatoric plastic strains. When the stress vector lies on the secondary yield surface, the interpolation rule ensures the calculation of plastic modulus from primary loading. The following simple relation is proposed:

$$H_{L_{\text{sec}}} = H_{L_{\text{prim}}} \left( \frac{\sigma_U}{\sigma} \right)^\gamma$$  \hspace{1cm} (25)

where $H_{L_{\text{prim}}}$ is the value of the plastic modulus on the primary yield surface, $\sigma$ is the current stress, $\sigma_U$ is the stress value at the time of unloading and $\gamma$ is the material parameter taken in this study as a function of accumulated plastic deviatoric strain, $\varepsilon^p_s = \int |d \varepsilon^p|$ , defined as:

$$\gamma = \gamma_0 \exp \left( -D \varepsilon^p_s \right)$$  \hspace{1cm} (26)

where $D > 0$ is a proportionality constant and $\gamma_0$ is the initial value of $\gamma$.

**2.3 Simulation of cyclic behavior**

In this study, UBCSAND soil model with given interpolation rule of GPT is implemented in a
computer program which is verified with a number of cyclic undrained triaxial tests. Figure 3 shows a strain-controlled test simulation. Except for the primary loading, the actual cyclic trend leading to a decrease in the mean stress is well captured. This is also the case for plastic deviatoric strains used to update the hardening parameter. Figure 4 presents the stress-controlled triaxial test. Simulations are compared with the ones from Pastor et al. (1985). Hardening material parameters are taken as; $D=300$ and $\gamma_0=20$ for both simulations which seem to be the optimum values to obtain convergence for both of the analyses. As a result of these simulations, this simply modified UBCSAND model is in a better position to simulate undrained cyclic triaxial tests, particularly the liquefaction of loose sand which has been an issue for the original formulation of this model (Beaty and Byrne, 1998).

![Figure 3: Simulation of strain-controlled undrained cyclic triaxial test as compared to Pastor et al. (1985)](image)

### 3 IMPLEMENTATION INTO FINITE ELEMENT METHOD

#### 3.1 PD formulation of Biot poroelasticity

The dynamic behavior of loose sands requires the solution of coupled flow and deformation equations proposed by Biot (1941, 1955, 1962). These equations are derived from the conservation of momentum and mass as well as the inclusion of a valid constitutive law for the stress-strain relationship of the solid skeleton of the soil. D’Arcy’s law is also
added to govern the pore water flow. By ignoring the inertial forces associated with the pore water, the equations can be written in the Partially Dynamic (PD) form as follows:

\[
\sigma_{ij,j} + \rho g_i = \rho \ddot{u}_i \tag{27}
\]

\[-p_{,i} + \rho_w g_i = \rho_w \ddot{w}_i + \frac{\ddot{w}_i}{k_i} \rho_w g_i \tag{28}
\]

\[
\dot{\epsilon}_{ii} + \ddot{w}_{ij} = -\frac{n}{K_f} \dddot{p} \tag{29}
\]

where for the material parameters; \( \rho \) is total density of soil, \( \rho_w \) is density of the water, \( n \) is porosity, \( K_f \) is bulk modulus of the pore water, \( g \) is the gravitational acceleration and \( k_i \) is the permeability coefficient. As for variable unknowns, \( \sigma_{ij,j} \) is the divergence of total stress, \( u \) is solid part’s displacement, \( w \) is the relative fluid displacement, \( p \) is the pore fluid pressure, \( \ddot{u}_i \) is the acceleration of solid skeleton and \( p_{,i} \) is the gradient of pore pressure, finally \( \dot{\epsilon}_{ii} \) is the rate of change of volumetric strain of the solid part.

**Figure 4:** Simulation of two way stress-controlled undrained cyclic triaxial test, data of Pastor et al. (1985)
3.2 Finite element formulation

Finite element (FE) formulation of the nonlinear dynamic analysis of coupled soil medium can be written using the Newton-Raphson iterative method and the Newmark time integration scheme. If we write the nonlinear equation of motion in matrix-vector form, we get:

\[
\begin{bmatrix}
\mathbf{M}_s & 0 \\
\mathbf{M}_f & 0
\end{bmatrix}
\begin{bmatrix}
\dot{\mathbf{U}} \\
\dot{\mathbf{P}}
\end{bmatrix}_{n+1} +
\begin{bmatrix}
\mathbf{0} & \mathbf{0} \\
\mathbf{C}_f & \mathbf{C}_f
\end{bmatrix}
\begin{bmatrix}
\mathbf{P} \\
\mathbf{P}
\end{bmatrix}_{n+1} +
\begin{bmatrix}
-\mathbf{C} \\
\mathbf{0}
\end{bmatrix}
\begin{bmatrix}
\mathbf{U} \\
\mathbf{P}
\end{bmatrix}_{n+1} +
\begin{bmatrix}
\mathbf{R}^{\text{int}} \\
\mathbf{R}^{\text{int}}
\end{bmatrix}_{n+1} =
\begin{bmatrix}
\mathbf{R}^{\text{ext}} \\
\mathbf{R}^{\text{ext}}
\end{bmatrix}_{n+1}
\tag{30}
\]

where \( \mathbf{M}_s \) and \( \mathbf{M}_f \) are the mass matrices of the solid phase and the coupled system, \( \mathbf{C}_f \) is the coupling matrix, \( \mathbf{C}_f \) is the fluid compressibility matrix. \( \mathbf{R}^{\text{int}} \) is the internal force of the solid part, and \( \mathbf{R}^{\text{int}} \) is the internal force based on flow of fluid part, \( \mathbf{R}^{\text{ext}} \) and \( \mathbf{R}^{\text{ext}} \) are the external load vectors associated with the solid and the fluid part, hence water. The nonlinear equation of motion is written in general form as below:

\[
\mathbf{M}_s \ddot{\mathbf{X}}_{n+1} + \mathbf{C}_f \dot{\mathbf{X}}_{n+1} + \mathbf{K} \mathbf{X}_{n+1} + \mathbf{R}^{\text{int}}_{n+1} = \mathbf{R}^{\text{ext}}_{n+1}
\tag{31}
\]

\( \mathbf{X} \) is the vector involving both solid and fluid part’s degree of freedoms namely, displacement, \( \mathbf{U} \) and pore pressure, \( \mathbf{P} \). Nonlinear formulation of the coupled system yields:

\[
\begin{bmatrix}
\frac{1}{\beta \Delta t^2} M + \frac{\gamma}{\beta \Delta t} C + \hat{\mathbf{k}}^{\text{tan}}\n\end{bmatrix}_{n+1} \partial \mathbf{X}^{i+1}_{n+1} =
\begin{bmatrix}
\mathbf{R}^{\text{ext}}_{n+1} - \hat{\mathbf{k}}^{\text{tan}}\n\end{bmatrix}_{n+1} -
\frac{1}{\beta \Delta t^2} M + \frac{\gamma}{\beta \Delta t} C
\begin{bmatrix}
\mathbf{X}^{i}_{n+1} - \mathbf{X}_{n}\n\end{bmatrix}

\left[
\begin{array}{c}
\frac{1}{\beta \Delta t^2} M + \frac{\gamma}{\beta \Delta t} C \\
\frac{1}{\beta \Delta t} M + \frac{1}{2 \beta} \frac{\gamma - \beta}{\beta} \mathbf{X}_{n} + \Delta \left[ \frac{\gamma - \beta}{\beta} \mathbf{X}_{n} \right]
\end{array}
\right]
\right]
\tag{32}
\]

where \( \hat{\mathbf{k}}^{\text{tan}} \) is the tangent stiffness matrix including the phase stiffness matrices and \( \mathbf{C} \). In (32), \( \gamma \) and \( \beta \) are the Newmark parameters, \( i \) is the iteration number and \( n \) is the load step. (32) is solved for \( \partial \mathbf{X}^{i+1}_{n+1} \) at \( N \) number of iterations used to update incremental values as:

\[
\Delta \mathbf{U}^{N}_{n+1} = \sum_{i=1}^{N} \partial \mathbf{U}^{i}_{n+1}
\tag{33}
\]

A residual force is calculated to check for convergence against a specified tolerance:

\[
\left( \mathbf{R}^{\text{ext}} \right)^{i+1}_{n+1} = \mathbf{R}^{\text{ext}}_{n+1} - \left( \mathbf{R}^{\text{int}} \right)^{i+1}_{n+1} - M \dot{\mathbf{U}}^{i+1}_{n+1} - C \ddot{\mathbf{U}}^{i+1}_{n+1} \leq \mathbf{TOL}
\tag{34}
\]

3.3 FE Results

In this section, dynamic response of a 10m high soil column is analysed under harmonic load through the updated UBCSAND model. A computational FE model is developed and nonlinear finite element analyses are performed on a saturated porous sand soil using the coupled flow and deformation theory. The model parameters are obtained from Pastor et al. (1985). Figure 5 shows the variation of displacement, pore pressure and effective stress in
time for various depths. Though the pore pressures seem to rise unboundedly, failure seem to occur due to liquefaction in a short amount of time.

Figure 5: FE analysis results for a sandy soil column under surface harmonic excitation, $T=0.1s$, $k=1e^{-4}m/s$

4 CONCLUSIONS

In this study, cyclic response of loose sand is studied through elastoplastic analyses using the finite element method. First the UBCSAND constitutive model is evaluated generating results that are compared with available static and cyclic triaxial tests used to calibrate the model. Next, the calculation of plastic hardening modulus is updated using a proposed interpolation rule. The new rule accounts for the relative location of the current stress vector on the secondary surface acting as a yield surface in comparison to its value on the primary surface acting now as a bounding surface in the model. Then, the Generalized Plasticity Theory is adapted in the current formulation of the UBCSAND in terms of the deviatoric hardening rule using deviatoric plastic strains. Furthermore, the model is modified to serve with the generalized plasticity framework to evaluate the cyclic behavior of sands. Such an inclusion
of the theory led to better verification with corresponding undrained triaxial test results as opposed to its original formulation. Finally the latest update of the model is implemented into a newly developed 1-D finite element code and the harmonic response of a sandy soil column which is governed by the Biot’s poroelasticity theory, is evaluated. A set of poro-elastoplastic analyses conducted indicate the effectiveness of the proposed interpolation rule along with the effect of the inclusion of basic definitions of the GPT which is found to be quite useful.

REFERENCES


**COUPLED THM ANALYSIS OF LONG-TERM ANISOTROPIC CONVERGENCE IN THE FULL-SCALE MICRO TUNNEL EXCAVATED IN THE CALLOVO-OXFORDIAN ARGILLITE**

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Key words: in situ testing; numerical modelling; convergence measurements; anisotropy.

**Abstract.** The main purpose of this paper is to analyse the convergence measurements of the ALC1604 in situ heating test carried out in the Callovo-Oxfordian claystone formation (COx) in the Meuse/Haute-Marne underground research laboratory (MHM URL). The concept of the test consists of horizontal micro-tunnel, equipped with a steel casing. The micro-tunnel is excavated in the direction of the horizontal principal major stress ($\sigma_H$). In situ observations showed anisotropic convergence with the maximum and minimum values in the horizontal and vertical directions, respectively. Coupled THM numerical analyses have been carried out to provide a structured framework for interpretation, and to enhance understanding of THM behaviour of Callovo-Oxfordian claystone. However, a special mechanical constitutive law is adopted for the description of the time-dependent anisotropic behaviour of the COx. The simulation of the test using this enhanced model provides a satisfactory reproduction of the THM long-term anisotropic convergence results. It also provides a better understanding of the observed test response.

1 INTRODUCTION

The construction of the M/HM URL was initiated by the French National Radioactive Waste Management Agency (Andra) in 2000 with the main objective of demonstrating the feasibility of geological repository of radioactive waste in the Callovo-Oxfordian claystone formation. It has indeed very favourable characteristics for radioactive waste disposal like low permeability, significant retardation properties for radionuclide migration, no economic value and often exhibits a significant capacity of hydraulic self-sealing of fractures. A network of experimental drifts has been excavated in the directions of the horizontal principal stresses. Micro-tunnels were excavated from these experimental drifts to test the feasibility of disposal cells for packages of high-level radioactive waste and their impact on the surrounding rock.

The HA-ALC1604 is an in situ heating test conducted in the M/HM URL at the main 490 m deep level (Armand et al. 2017). The concept of the test consists of horizontal micro-tunnel approximately 25 m long and 0.7 m in diameter which has been excavated in the direction of the major horizontal stress. The excavation rate of the micro-tunnel was around 0.3-0.5 m hr$^{-1}$ and the
excavation was completed in seven days. A non-alloy steel casing was placed in the cell body while the cell head was sustained by a metal sleeve called the Insert. Figure 1 shows the concept of the experiment, with the 25m long micro-tunnel and surrounding boreholes for THM observations. Five heaters (H1 to H5), each 3 m long and 0.5 m in diameter, have been installed in the body section. The power applied in the deepest 15m was constant and equal to 220 W/m, in order to reach around 85 °C in two years.

2 MAIN FEATURES OF THE NUMERICAL MODEL

The coupled THM formulation employed herein to the solution of the analyzed boundary value problem is a particular case of the general formulation presented in Olivella et al. (1994). However, a special mechanical constitutive law is adopted for the description of the stress-strain behaviour of the Callovo-Oxfordian claystone. It has been presented in more detail in (Mánica; et al. (2016a) and Mánica et al. (2016b)). The model was developed within the framework of elastoplasticity and includes a number of features that are relevant for a satisfactory description of COx hydromechanical behaviour: anisotropy of strength and stiffness, behaviour nonlinearity and occurrence of plastic strains prior to peak strength, significant softening after the peak, time-dependent creep deformations and permeability increase due to damage (Gens 2011). Both saturated and unsaturated conditions are considered. The mesh and main boundary conditions (BC) are illustrated in Figure 2. The model includes the host rock domain, the steel casings and the gap between the casings, the container and the COx. For computational purposes, the gap will be dealt with as a continuous medium provided with the bi-linear elastic model to represent opening and closing responses. According to the experimental set-up, the casing is supported at the bottom of...
the excavation. Thus, container, gaps and casing are eccentric with respect to the centerline of the micro-tunnel. The specific parameters used in the analysis are listed in Table 1-3.

![Finite element mesh and boundary conditions.](image)

**Figure 2** Finite element mesh and boundary conditions.

| Table 1 Callovo-Oxfordian claystone parameters used in the 2D THM analysis. |
| --- | --- | --- |
| properties | Parameter | Orientation* | Value |
| Physical | Porosity, φ | - | 15 |
| Thermal | Thermal Conductivity, λ: W/m/K | Parallel | 2.05 |
| | | Perpendicular | 1.33 |
| | Specific Heat of Solid, cs: J/kg/K | - | 800 |
| Hydraulic | Intrinsic Permeability, k | Parallel | 6•10-20 |
| | | Perpendicular | 3•10-20 |
| Mechanical | Young’s Modulus, E: MPa | Parallel | 5200 |
| | | Perpendicular | 4000 |
| | Poisson ratio, ν | Parallel | 0.25 |
| | | Perpendicular | 0.35 |
| | Solid compressibility, βs | - | 2.5•10-5 |
| HM coupling | Biot Coefficient, b | - | 0.6 |
| TM coupling | Linear Thermal expansion coefficient of the rock, αT: K-1 | - | 1.4•10-5 |
| | Linear Thermal expansion coefficient of the solid grain, bs: K-1 | - | 1.4•10-5 |
Table 2 Steel casing properties adopted in the 2D THM analysis.

<table>
<thead>
<tr>
<th>properties</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal</td>
<td>Thermal Conductivity, $\lambda$ : (W/m/K)</td>
<td>80</td>
</tr>
<tr>
<td></td>
<td>Specific heat of solid (J/kg/K)</td>
<td>550</td>
</tr>
<tr>
<td></td>
<td>Linear Thermal expansion coefficient, $\alpha_T$: K$^{-1}$</td>
<td>$1.4\times10^{-5}$</td>
</tr>
<tr>
<td>Mechanical</td>
<td>Young’s Modulus, $E$: MPa</td>
<td>0.005</td>
</tr>
<tr>
<td></td>
<td>Poisson’s ratio, $\nu$(-)</td>
<td>0.3</td>
</tr>
</tbody>
</table>

Table 3 Air-gap element properties adopted in the 2D THM analysis.

<table>
<thead>
<tr>
<th>properties</th>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal</td>
<td>Thermal Conductivity, $\lambda_{dp}$ : (W/m/K)</td>
<td>0.035</td>
</tr>
<tr>
<td></td>
<td>Thermal Conductivity, $\lambda_{sat}$ : (W/m/K)</td>
<td>0.6</td>
</tr>
<tr>
<td>Hydraulic</td>
<td>Intrinsic permeability, $k_0$ : (m2)</td>
<td>$10^{16}$</td>
</tr>
<tr>
<td></td>
<td>Porosity, $\phi$ (-)</td>
<td>0.8</td>
</tr>
<tr>
<td></td>
<td>Parameter for van Genuchten model, $\lambda$ (-)</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>$P_f(\phi) = P_o \exp[\alpha (\phi_0 - \phi)]$, $P_o$(MPa)</td>
<td>0.001</td>
</tr>
<tr>
<td></td>
<td>Parameter for van Genuchten model, $a$ (-)</td>
<td>10</td>
</tr>
<tr>
<td>Mechanical</td>
<td>Young’s Modulus, $E_c$: MPa</td>
<td>1000</td>
</tr>
<tr>
<td></td>
<td>Young’s Modulus, $E_o$: MPa</td>
<td>1.0</td>
</tr>
<tr>
<td></td>
<td>Strain limit, $\varepsilon_{\text{limit}}$ (-)</td>
<td>0.005</td>
</tr>
<tr>
<td></td>
<td>Poisson’s ratio, $\nu$(-)</td>
<td>0.3</td>
</tr>
</tbody>
</table>

3 NUMERICAL SIMULATION AND INTERPRETATION

3.1 Excavation damage zone

The experiments have revealed that excavation operations induce damage and fracturing around the galleries (Armand et al. 2014), creating a zone known as the excavation damaged zone (EDZ), where significant changes in flow and transport properties take place (Tsang et al. 2005). The observed configuration of the EDZ depends on the orientation of the excavation with respect to the anisotropic in situ stress state. The EDZ is identified as one of the key issues affecting the long-term behaviour of the tunnel near-field (Blümling et al. 2007). Major efforts have been made to simulate these experimental excavations (Seyedi and Gens 2017) and to gain insights into the design of the actual repository. As stated above, the ALC1604 cell is parallel to the major horizontal stress $\sigma_H$ has a nearly isotropic stress state in the plane normal to the tunnel axis. However, the EDZ extends further in the horizontal direction (Figure 3a), suggesting strong anisotropic characteristics of the rock mass. An estimate of the configuration of the excavation damaged zone can be obtained by plotting contours of the cumulative plastic multiplier as it is directly related to the magnitude of irreversible strains (Figure 3b). The lateral extent of the shear fractures zone for smaller opening is almost equal to 1 diameter of the opening (Armand et al. 2014). Model results suggest that a plastic zone of up to 0.7 m away from the micro-tunnel wall is formed. In the zones of the higher plastic multiplier, greater mechanical effects will be noticed on the deformability of rock and hydraulic diffusion. It can be seen that the configuration of the damaged zone is similar to that observed in the previous micro-tunnels with the same orientation, extending more in the horizontal direction (Armand et al. 2014, 2017).
3-1- Convergence Measurements

*Figure 5* shows the overall evolution of convergence measurement in steel casing section 9, at a depth of 7 m, and insert sections 11 and 12, at respective depths of 4 and 2 m in the cell (note that the sensors were connected 48 days after the excavation of the micro-tunnel). Although the in-situ stress field is isotropic in the section of a micro-tunnel parallel to $\sigma_H$, measurements exhibit an anisotropic load. This behaviour is consistent with the convergence anisotropy measurements reported by Morel et al. (2013) and Armand et al. (2013).

With regard to the steel casing, three loading stages can be distinguished in *Figure 5a*. In the first one, the load is localized in the horizontal direction, corresponding to the maximum extension of the excavation-induced fracture network. It can be observed that immediately after emplacement, the casing starts to converge in the horizontal direction, meaning that the theoretical initial annular space, which is about 3 per cent of the excavation diameter, is totally consumed in this direction in less than 25 days. This loading results in the radial bending of the casing and decrease in diameter. The heating phase strongly increases the casing convergence rate and thus the casing deformation, until contact with the micro-tunnel vault occurs. In this step, the ovalization of the casing continues until it reaches the rock wall in the vertical direction. Once the annular space is closed in the vertical direction, the mechanical load remains anisotropic with no impact on the casing convergence.

The second loading step is followed by a third one, corresponding to a progressive decrease of the load anisotropy, resulting in a decrease of the ovalization. After one year heating, convergence rate is less than $5 \times 10^{-11} \text{s}^{-1}$, which is the same order of magnitude as convergence rate of 5 m in diameter, drifts having the same orientation (Armand et al. 2013). *Figure 5b, 5c* present the horizontal and vertical convergence of Insert sections 11 and 12. A similar short-term mechanical loading of the casing is observed also at the insert. However, after 5 years of measurements, the convergence of the insert is not stabilized, which means that we are still in the first loading step as defined before. The behaviour of the insert sections does not show any significant heating impact (the sections were 8 and 6 meters behind the heated zone). On both sections, the loading schema is the reverse of that seen for the sleeve and consists of vertical convergence and noticeably
equivalent horizontal divergence. Given that, the annular space is much smaller at the insert level (initially 12 mm at the radius, compared with 25 mm around the casing), this behaviour could be caused by the insert being in contact with the rock in the vertical and horizontal planes. As the mechanical strength of the rock was lower horizontally due to the damage generated during excavation, the insert tended to diverge horizontally. For both sections, the loading direction is rotated with respect to the previous one and characterized by a vertical convergence and noticeably equivalent horizontal divergence. A comparison between the results of the analysis and observations, in terms of diameter variations (measured on the casing at the depth of 7 m and on the insert at a depth of 4 and 2 m) are presented in Figure 5. It is apparent that the evolution and maximum convergence is reasonably well captured with the formulation and parameters used.

**Figure 4** Diameter variations measured on the sleeve at a depth of 7 m and on the insert at a depth of 4 and 2 m (negative values = convergence)
5-2- Mechanical signatures

The strain gauges were glued on the casing previously to its installation and connected 27 days after the cell was excavated. For each section, the gauges are spread out into six sectors, two in the horizontal plane and the other four at 45° angles on either side of it. Figure 5 presents the evolution of the circumferential strain ($\varepsilon_{\theta\theta}$) around the inner face of the casing at different times and at 18 m depth (section 4) with the computed results from the analysis. These evolutions tend towards a stabilized curve, which represents the mechanical signature of the applied load. Indeed casing does not evolve significantly after the second year of heating. By comparison with the numerical results, the maximum load direction corresponds to an inclination of $30^\circ$ with respect to the horizontal.

Figure 5 Evolution of circumferential strain at 18m depth for (a) 17/06/2013 (b) 11/08/2014 (c) 16/02/2015 (d) 16/07/2016 (e) 18/09/2017 observations.

4 CONCLUSIONS

The HA-ALC1604 in situ heating test performed by Andra was modelled using the finite-element code Code_Bright. The mechanical behaviour of the material has been described by a constitutive model that explicitly developed for this type of material. It is of interest to note that the predicted damaged zone appears to be quite consistent with the test observations. Overall, the theoretical formulation adopted and the analysis performed have been able to provide a satisfactory reproduction of in situ test observations, even from a quantitative point of view.

We analysed convergence measurements in HA-ALC1604 test in Callovo-Oxfordian claystone, with the axis following the direction of the major initial principal horizontal stress. The first convergence measurement was made several days after the end of excavation and thus the analysis of the recorded data mainly focused on the time-dependent behaviour of the rock formation. The in situ measurements showed an anisotropic closure of the walls that evolved over time. The analysis of in situ deformation as measured in the full-scale test has led to the definition of the short-term mechanical load applied by the rock. Three loading steps can be distinguished for casing parallel to the major horizontal stress:

1) The localized load applied along the horizontal direction;
2) Significant anisotropic load with no impact on the convergence once the casing reaches the vault of the borehole;

3) Progressive decrease of the load anisotropy.

The applied load remains anisotropic after more than 5 years. This phenomenon is explained by the specific elliptic shape of the excavation-induced fracture network, which governs the convergence of the cell wall. Figure 3 presented qualitatively the extension of this damaged zone around an uncased full-scale cell. The heating effect has been highlighted concerning the duration of the first loading step. Indeed steps 2 and 3 have only been reached on the steel casing (after one year) in the heated zone. At insert sections, the insert remains in the first loading step after 5 years of measurements. The bending stiffness is the same for both, casing and insert this difference is mainly related to heating phase in step 2 as shown in Figure 4. Strain gauges measurements performed on ALC1604 cell have shown anisotropic loading applied by the rock, which is almost horizontal.

REFERENCES


UNIFIED DESCRIPTION OF DRY AND FLUID FRICTIONS
BY SUBLOADING-OVERSTRESS FRICTION MODEL

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Key words: Dry and Fluid Frictions, Subloading-overstress Friction Model, Rate-sensitivity

Abstract. The subloading-overstress friction model is formulated for the unified description of the dry and the fluid frictions which exhibit the negative and the positive rate dependences, i.e. the decrease and the increase, respectively, of friction resistance. The validity of this model will be verified by the comparisons with test data in this article.

1 INTRODUCTION

The dry friction without a lubrication exhibits the decrease of friction resistance with the sliding velocity, which is called the negative rate-sensitivity. On the other hand, the fluid friction exhibits the increase of friction resistance with the sliding velocity, which is called the positive rate-sensitivity. The generalized friction model, called the subloading-overstress friction model [1], is formulated based on the subloading surface model [2] [3] [4], which is capable of describing the dry and the fluid frictions by the unified formulation.

The validity of the subloading-overstress friction model is examined by the comparisons with test data in this article. Then, the capability of describing both the dry and the fluid frictions is verified by these comparisons.

2 SLIDING DISPLACEMENT AND CONTACT TRACTION VECTORS

The sliding displacement vector \( \mathbf{u} \), which is defined as the sliding displacement of the counter (slave) body to the main (master) body, is orthogonally decomposed into the normal sliding displacement vector \( \mathbf{u}_n \) and the tangential sliding displacement vector \( \mathbf{u}_t \) to the contact surface as follows:

\[
\mathbf{u} = \mathbf{u}_n + \mathbf{u}_t
\]  

where...
The sliding displacement vector $\mathbf{u}$ can be exactly decomposed into the elastic sliding displacement $\mathbf{u}^e$ and the viscoplastic sliding displacement $\mathbf{u}^{vp}$ in the additive form even for the finite sliding displacement, i.e.
\[
\mathbf{u} = \mathbf{u}^e + \mathbf{u}^{vp}
\]
(4)

\[
\begin{cases}
\mathbf{u}^e = \mathbf{u}_n^e + \mathbf{u}_f^e \\
\mathbf{u}^{vp} = \mathbf{u}_n^{vp} + \mathbf{u}_t^{vp}
\end{cases}
\]
(5)

where
\[
\begin{cases}
\mathbf{u}_n^e = (\mathbf{u}^e \cdot \mathbf{n})\mathbf{n} = (\mathbf{n} \otimes \mathbf{n})\mathbf{u}^e = -\mathbf{n}^e \mathbf{n} \\
\mathbf{u}_f^e = \mathbf{u}^e - \mathbf{u}_n^e = (1 - \mathbf{n} \otimes \mathbf{n})\mathbf{u}^e \\
\mathbf{u}_n^{vp} = (\mathbf{u}^{vp} \cdot \mathbf{n})\mathbf{n} = (\mathbf{n} \otimes \mathbf{n})\mathbf{u}^{vp} \\
\mathbf{u}_t^{vp} = \mathbf{u}^{vp} - \mathbf{u}_n^{vp} = (1 - \mathbf{n} \otimes \mathbf{n})\mathbf{u}^{vp}
\end{cases}
\]
(6)

setting
\[
\mathbf{n}^e \mathbf{n} = -\mathbf{n} \cdot \mathbf{u}^e
\]
(7)

The minus sign is added for $\mathbf{n}^e \mathbf{n}$ to be positive when the counter body approaches the main body. The plastic sliding displacement $\mathbf{u}^{vp}$ is derived by the unloading to the contact traction-free state along the hyperelastic constitutive equation which will be formulated in Section 3. The viscoplastic sliding flow rule will be formulated to fulfill $\mathbf{u}_n^{vp} = \mathbf{0}$ in Section 4.

The contact traction vector $\mathbf{f}$ acting on the main body is additively decomposed into the normal traction vector $\mathbf{f}_n$ and the tangential traction vector $\mathbf{f}_t$ as follows (see Figure 2):
\[
\mathbf{f} = \mathbf{f}_n + \mathbf{f}_t = -\mathbf{f}_n \mathbf{n} + \mathbf{f}_t \mathbf{t}_f
\]
(9)

where
The minus sign is added for $f_n$ to be positive when the compression is applied to the main body by the counter body.

The contact traction vector $f$, $f_n$ and $f_t$ are calculated from the Cauchy stress $\sigma$ applied to the contact surface by virtue of the Cauchy’s fundamental theorem as follows:

$$f = \sigma n$$

$$f_n = (n \cdot \sigma n)n = (n \otimes n)\sigma n$$

$$f_t = (I - n \otimes n)\sigma n$$

(12)

Figure 2 Coulomb-type normal- and subloading-sliding surfaces

3 HYPERELASTIC SLIDING EQUATION

Let the contact traction vector $f$ be given by the hyperelastic relation with the elastic sliding displacement energy function $\varphi(\vec{u}^s)$ as follows:

$$f = \frac{\partial \varphi(\vec{u}^s)}{\partial \vec{u}^s}$$

(13)

The simplest function $\varphi(\vec{u}^s)$ is given by the quadratic form:

$$\varphi(\vec{u}^s) = \vec{u}^s \cdot \tilde{E} \vec{u}^s / 2$$

(14)
where the second-order symmetric tensor \( E \) is the elastic contact tangent modulus tensor fulfilling the symmetry \( E = E^T \). The substitution of Eq. (14) into Eq. (13) leads to
\[
f = E \mathbf{u}^e
\] (15)
The inverse relation of Eq. (15) is given by
\[
\mathbf{u}^e = E^{-1} f
\] (16)
The elastic contact tangent modulus tensor \( E \) is given for the isotropy on the contact surface as follows:
\[
E = \alpha_n n \otimes n + \alpha_t (I - n \otimes n)
\]
\[
E^{-1} = \frac{1}{\alpha_n} n \otimes n + \frac{1}{\alpha_t} (I - n \otimes n)
\] (17)
where \( \alpha_n \) and \( \alpha_t \) are the normal and tangential contact elastic moduli, respectively. Their values are quite large usually as \( 10^2 - 10^5 \text{ GPa/mm}^3 \) for metals because the elastic sliding is caused by elastic deformations of the surface asperities. Equations (15) and (16) with Eq. (17) leads to
\[
f = \alpha_t \mathbf{u}_t^e + \alpha_n \mathbf{u}_n^e
\]
\[
\mathbf{u}^e = \frac{1}{\alpha_t} f_t + \frac{1}{\alpha_n} f_n
\] (18)
Now, introduce the normalized rectangular coordinate system \((\hat{e}_1, \hat{e}_2, \hat{e}_3) = (\hat{n}, \hat{t}, \mathbf{n})\) fixed to the contact surface, which changes with the rotation of the contact surface. The elastic sliding displacement and the contact traction are described as follows:
\[
f = f_t \hat{e}_1 + f_2 \hat{e}_2 + f_n \mathbf{n}
\]
\[
\mathbf{u}^e = \mathbf{u}_t^e \hat{e}_1 + \mathbf{u}_n^e \hat{e}_2 + \mathbf{u}_n^e \mathbf{n}
\] (19)
Hence, Eq. (15) is described in the simple form as follows:
\[
\begin{bmatrix}
f_1 \\
f_2 \\
f_n
\end{bmatrix}
= \begin{bmatrix}
\alpha_t & 0 & 0 \\
0 & \alpha_t & 0 \\
0 & 0 & \alpha_n
\end{bmatrix}
\begin{bmatrix}
\mathbf{u}_t^e \\
\mathbf{u}_n^e \\
\mathbf{u}_n^e
\end{bmatrix}
= \begin{bmatrix}
1/\alpha_t & 0 & 0 \\
0 & 1/\alpha_t & 0 \\
0 & 0 & 1/\alpha_n
\end{bmatrix}
\begin{bmatrix}
f_t \\
f_2 \\
f_n
\end{bmatrix}
\] (20)
The sliding velocity vector \( \mathbf{u} \) is the objective vector, since it is not an absolute velocity vector but the mutual velocity vector between surface points on the master and the counter bodies. Therefore, it is not necessary to use a corotational velocity vector but we only have to use the time derivative for the sliding velocity vector. Further, note that one does not need to adopt a corotational rate but one has only to use the time derivative for the contact traction vector \( f \) by the fact: The contact traction \( f \) is calculated from the hyperelastic equation with the substitution of the elastic displacement \( \mathbf{u}^e \) which is obtained by subtracting the plastic displacement vector \( \mathbf{u}^{pl} \) from the displacement vector \( \mathbf{u} \).
4 NORMAL-SLIDING YIELD AND SUBLOADING-SLIDING SURFACES

Assume the following sliding-yield surface with the isotropic hardening/softening, which describes the sliding-yield condition.

\[ f(\mathbf{f}) = \mu \]  

(21)

\( \mu \) is the isotropic hardening/softening function denoting the variation of the size of the sliding-yield surface. The friction-yield stress function \( f(\mathbf{f}) \) for the Coulomb friction law is given by

\[ f(\mathbf{f}) = f_n / f \]  

(22)

for which \( \mu \) specifies the coefficient of friction.

Then, in order to introduce the measure of approaching degree to the sliding-yield surface, renamed the normal sliding-yield surface, let the following subloading-sliding surface passing through the current contact stress and maintaining a similarity to the normal sliding-yield surface be introduced, which plays the general measure of approaching degree of the contact stress to the normal sliding-yield surface (see Figure 2).

\[ f(\mathbf{f}) = r \mu \]  

(23)

where \( r (0 \leq r \leq 1) \) is the ratio of the size of the subloading surface to that of the normal sliding-yield surface and called the normal sliding-yield ratio, playing the role of the measure of the approaching degree of the contact stress to the normal sliding-yield surface.

The evolution rule of the isotropic hardening/softening function \( \mu \) in Eq. (21) is extended as follows:

\[ \dot{\mu} = -\kappa \left( \frac{\mu}{\mu_k} - 1 \right) \| \dot{\mathbf{u}}^{vp} \| + \xi \left( 1 - \frac{\mu}{\mu_s} \right) \]  

(24)

The viscoplastic sliding rate is given as follows:

\[ \dot{\mathbf{u}}^{vp} = \bar{\mathbf{F}} \mathbf{n}_t \ (\bar{\mathbf{F}} \geq 0) \]  

(25)

where \( \bar{\mathbf{F}} \) and \( \mathbf{n}_t \) are the magnitude and direction, respectively, of the plastic sliding velocity as shown below.

\[ \mathbf{n}_t = \left( \frac{\partial f(\mathbf{f})}{\partial \mathbf{f}} \right)_t / \left( \| \frac{\partial f(\mathbf{f})}{\partial \mathbf{f}} \|_t \right) \quad (\| \mathbf{n}_t \| = 1, \ \mathbf{n} \cdot \mathbf{n}_t = 0) \]  

(26)

with

\[ \left( \frac{\partial f(\mathbf{f})}{\partial \mathbf{f}} \right)_t = \frac{\partial f(\mathbf{f})}{\partial \mathbf{f}} - (\mathbf{n} \cdot \frac{\partial f(\mathbf{f})}{\partial \mathbf{f}}) \mathbf{n} = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n}) \frac{\partial f(\mathbf{f})}{\partial \mathbf{f}} \]  

(27)

\[ \bar{\mathbf{F}} \equiv \frac{1}{\mu_v} \left( r - r_s \right)^n \begin{cases} 0 & \text{for } r < r_m \\ \rightarrow \infty & \text{for } r \rightarrow r_m \end{cases} \]  

(28)

or

\[ \bar{\mathbf{F}} \equiv \frac{1}{\mu_v} \left( \exp[n(r - r_s)] - 1 \right) \begin{cases} 0 & \text{for } r < r_m \\ \rightarrow \infty & \text{for } r \rightarrow r_m \end{cases} \]  

(29)
where $\bar{\mu}$, $n \geq 1$ and $r_m \geq 1$ are the material parameters, while $r_m$ is the maximum value of $r$, and

$$\dot{r}_s = \begin{cases} \bar{U}(r_s) \| \dot{\bar{u}}^{vp} \| \text{ under } \dot{\bar{u}}^{vp} \neq 0 \text{ for } r_s < r \\ 0 \text{ for } \dot{\bar{u}}^{c} = 0 \text{ under } \dot{\bar{u}}^{vp} = 0 \text{ for } r_s = r (r_s = \dot{r}) \\ < 0 \text{ for } \dot{\bar{u}}^{c} \neq 0 \end{cases}$$

(30)

with

$$\bar{U}(r_s) = \bar{\mu} \cot \left( \frac{\pi}{2} r_s \right).$$

(31)

Here, $r (0 \leq r < r_m)$ in Eq. (23) is renamed as the dynamic sliding-loading ratio and $r_s (0 \leq r_s \leq r \leq 1)$ is called the static normal sliding-yield ratio because it designates the normal sliding-yield ratio which evolves under the virtual quasi-static elastoplastic sliding process. The viscoplastic sliding velocity is induced by the overstress $f(f^{*}) - r_s \mu$ from the subloading friction surface:

$$f(f^{*}) = r_s \mu, \text{ i.e. } r = r_s$$

(32)

so that a smooth elastic–viscoplastic transition is described.

The sliding rate and its inverse relation are given by Eqs. (4), (15) and (25) as follows:

$$\begin{align*}
\dot{\bar{u}} &= E^{-1} \dot{f} + \bar{f} n_t \\
\dot{f} &= E \dot{\bar{u}} - \bar{f} n_t
\end{align*}$$

(33)

which is represented in the incremental form as follows:

$$\begin{align*}
\begin{bmatrix} d\bar{u} \\ d\bar{f} \end{bmatrix} &= E^{-1} \begin{bmatrix} df \\ \Gamma n_t \end{bmatrix} dt \\
\begin{bmatrix} d\bar{u} \\ d\bar{f} \end{bmatrix} &= E \begin{bmatrix} \bar{u} - \dot{\bar{u}}^{vp} \\ \bar{f} n_t \end{bmatrix} dt
\end{align*}$$

(34)

5 CALCULATION PROCEDURE

The calculation by the subloading-overstress friction model may be performed by the following procedure.

1. $d\bar{u}^{vp}$ is calculated by the input of $dt$ into Eq. (25), and then its accumulation leads to $\bar{u}^{vp}$.
2. $d\mu$ and $dr_s$ are calculated by inputs of $d\bar{u}^{vp}$ into Eqs. (24) and (30), and their accumulations lead to $\mu$ and $r_s$.
3. The elastic sliding displacement $\bar{u}^e$ is calculated by $\bar{u}^e = \bar{u} - \bar{u}^{vp}$.
4. $f$ is calculated by $f = E \bar{u}^e$.
5. $r$ is calculated by $r = (f_t / f_n) / \mu$. 
These calculation processes are repeated for the further sliding.

6 COMPARISON WITH TEST DATA

The comparison of the simulation by the subloading-overstress friction model with the test data [5] for the dry friction is shown in Figure 3. The test curve for sliding between roughly polished steel surfaces under the quite low sliding velocity $\dot{u}_t \leq 0.0002 \text{ mm/s}$ is simulated well enough by the present model, where the material parameters are selected as follows:

$$\mu_s = 0.58, \mu_k = 0.38, \kappa = 35 \text{ mm}^{-1}, \xi = 0.001/\text{s}$$

$$\ddot{u} = 1500 \text{ mm}^{-1}, \mu_v = 150, r_n = 2.0, n = 3$$

$$\alpha_n = \alpha_i = 10000 \text{ N/mm}^3$$

under the condition

$$f_n = 10 \text{ MPa}, \dot{u}_t = 0.0002 \text{ mm/s}$$


The comparison of the simulation by the present model with the test data [6] for the fluid friction is shown in Figure 4. The test plate is the galvannealed steel sheet which is sandwiched by the steel SKD-11 plates. The normal contact stress is 5.56 MPa. The friction surfaces were coated with the anti-rust oil prior to the tests. The drawing velocity of the test plate is set at the five levels 1, 10, 50, 100, 200 mm/min. The simulation of the test result using the exponential function in Eq. (29) is shown by the solid lines, using the following values for the material constants.
Comparison with test data for fluid friction.

REFERENCES


A MONOLITHIC FORMULATION OF FLUID-STRUCTURE INTERACTION FOR THE CO-SIMULATION: APPLICATION TO THE PISTON PROBLEM

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Abstract. This extended abstract presents a coupling method for the Fluid-Structure Interaction (FSI) problem, which aim is to be conservative and to use classical spatio-temporal discretization methods on each sub-domains; fluid and structure. In this way, the coupling is based on a monolithic formulation and solved by a co-simulation algorithm. The structural sub-domain is spatially discretized by finite elements method and temporally discretized by Newmark implicit scheme. While the fluid sub-domain is discretized by finite volumes method and Runge-Kutta order 2 explicit scheme. The long-term objective is to couple two existing commercial softwares. The proposed method is validated using the one-dimension piston test case.

1 INTRODUCTION

There are various fields of application for the FSI simulation, aerospace [1], bio-medical [10], civil engineering [13]... The three past decades the research have been really active and numerous coupling methods have been developed. Several classifications and definitions are used, here the classification used is based on the formulation of the problem.
Thus, in terms of formulation, the FSI problems are divided into two main categories; the partitioned coupling treats the problem in a uncoupled way while the monolithic coupling treats the sub-domain fluid, the sub-domain structure and the FSI-interface as a single system, see Fig. 1. The partitioned methods have the advantage to be easy to implement but lacks accuracy due to the time-lag involved by the methods itself. The monolithic methods are better in term of accuracy and stability but also are difficult to implement and not easily generalizable.

![Diagram: Partitioned formulation versus Monolithic formulation](image)

In order to guarantee the energy conservation, the method presented here is based on a monolithic formulation. Nevertheless, to avoid the difficulties of implementation and generalization, the algorithm used is based on the GC coupling method [4] [5], which has initially been introduced for the coupling problems of structural sub-domains. This method allows the construction of an algorithm, predictor/corrector like, without time lag between the two sub-domains, using the Lagrange multiplier method. This coupling method has been extended to the FSI problems, and has already shown promising results. As an instance, Casadei [3] has proposed an explicit coupling method for finite elements and finite volumes vertex centered. Li has coupled finite elements and SPH particles [7]. More recently, Meduri has proposed a coupling method fully Lagrangian of finite elements fluid and structure [8].

The aim here is to extend this coupling method to more classical spatio-temporal discretization methods for both physics in order to use an existing and efficient commercial solvers. Thus, the structural sub-domain uses a Lagrangian formulation and is discretized thanks to the finite elements in space and thanks to an implicit Newmark scheme in time. The fluid is written using an Arbitrary Lagrangian Eulerian (ALE) formulation, discretized by the means of finite volumes method (cell-centered and vertex-centered) and an explicit second order Runge-Kutta scheme. Finally each sub domain uses its own time step. In this way the global integration method is heterogeneous and asynchronous.

In a first step, the discretization methods of each sub-domain are briefly recalled. Then the coupling method is presented. Finally, this one is validated using the 1D piston test case.

## 2 CONSTITUTIVE EQUATIONS

The domain $\Omega \times [0, T]$ closed, spatially partitioned, without overlap, by a fluid sub-domain $\Omega_f$ and a structural one $\Omega_s$, such as $\Omega_f \cap \Omega_s = \emptyset$, is considered. The external fluid
sub-domain boundary is called $\Gamma_f$, respectively $\Gamma_s$ for the structural sub-domain. Finally $\Gamma_{FSI}$ is the boundary between the two sub-domain, see Fig. (2).

![Figure 2: Geometry of the fluid-structure interaction problem](image)

The fluid considered is compressible, inviscid and submit to the perfect gas law. The sub-domain structure is considered homogeneous, continuous and isotropic. It is considered linear elastic, under small displacement. The small perturbations hypothesis is assumed.

### 2.1 Structural sub-domain

The structural sub-domain $\Omega_s$ is spatially discretized because of the finite element method. This one is based on a Lagrangian formulation and the weak formulation of the equation of motion. Thus, under the hypotheses and the boundaries conditions, the discretized admissible state vector $U_s(t) = [d_s, v_s, a_s]^T(t)$ is sought. Where $d_s$, $v_s$, $a_s$ are the discretized fields of displacement, velocity and acceleration respectively:

$$M_s a_s(t) + K_s d_s(t) = F_s(t) \quad \forall t \in [0, T] \quad (1)$$

Where in the semi-discretized equation (1), $M_s$ is the mass matrix, $K_s$ is the stiffness matrix and $F_s$ is the vector of the external force.

Finally the implicit Newmark scheme is used as temporal discretization. This one is second order and unconditionally stable. Thus the discretized structural state vector at
the instant $t^{(n+1)}$ is written as:

$$a_s^{(n+1)} = \tilde{M}_s^{-1}(F_s^{(n+1)} - K_s d_{\text{pred}}^{(n+1)})$$

(2)

$$v_s^{(n+1)} = v_s^{(n)} + \frac{\Delta t}{2} a_s^{(n)} + \frac{\Delta t}{2} a_s^{(n-1)}$$

(3)

$$d_s^{(n+1)} = d_s^{(n)} + \Delta t v_s^{(n)} + \frac{\Delta t^2}{4} a_s^{(n)} + \frac{\Delta t^2}{4} a_s^{(n-1)}$$

(4)

where $\tilde{M}_s = (M_s + \frac{\Delta t^2}{4} K_s)$.

### 2.2 Fluid sub-domain

Regarding the hypotheses, the Euler equations (mass, momentum and energy conservation) are used over the fluid sub-domain. Thus, the quantity of interest is the vector of the conservative variables

$$U_f = [\rho_f, \rho_f v_f, E_f]^T$$

admissible on $\Omega_f \times [0, T]$.

The Euler equations are traditionally written using the Eulerian Formulation for the fluid problem. In other words, the laboratory referential, fixed over the time, is used. Nevertheless, dealing here with FSI problems without overlap, a dynamic referential has to be used to fit at each instant at the boundary $\Gamma_{\text{FSI}}$. The Lagrangian formulation being not really well adapted for fast transient fluid problems, the ALE formulation is used. The ALE grid is defined thanks to its velocity $w$. This one is Lagrangian at the domain’s boundaries; defined by the boundaries conditions on $\Gamma_f$ and by the velocity continuity condition on $\Gamma_{\text{FSI}}$. On $\|\Omega_f\|$, the interior fluid domain, $w$ is arbitrary defined using any desired law, under the CFL condition. Thus the continuous ALE formulation of the Euler equations is:

$$\frac{\partial JU_f}{\partial t} + J \nabla \cdot (F_f - w U_f) = 0$$

(5)

Where $J$ is the Jacobian of the frame transformation of the Eulerian space to ALE space, and $F_f$ the flux vector define as $F_f = [\rho v, \rho v \otimes v + p I, (E + p) v]^T$. We also introduce the following notation $\tilde{F}_f = F_f - w U_f$.

Using the integral form of the equation (5) and the finite volumes method cell centered, the semi-discretized Euler equations are written over one finite volumes $V_i$ with boundary $\Gamma_{V_i}$ as:

$$\frac{\partial \Delta V_i(t) U_{f_i}(t)}{\partial t} = - \sum_{\forall \Gamma_{ia} \in \Gamma_{V_i}} s_{ia}(t) \tilde{F}_{f_{ia}}(t) \quad \forall i \in [1, ..., n_{\text{cell}}], \quad \forall t \in [0, T]$$

(6)

Where $n_{\text{cell}}$ is the number of cells over the sub-domain $\Omega_f$. $\Delta V_i$ is the volume of the $i^{th}$ cell and $s_{ij}$ the area of the boundary between the $i^{th}$ and the $j^{th}$ neighbourhood cell,
these two values being variable due to the use of the ALE formulation. Finally, $\tilde{F}_{ij}$ is the numerical flux between the actual cell $i$ and the adjacent cell $j$ defined here using the Roe flux difference splitting method [12].

The explicit second order Runge-Kutta scheme is used for the temporal discretization of the equation (6).

$$\Delta V_i^{(n+\frac{1}{2})} U_i^{(n+\frac{1}{2})} = \Delta V_i^{(n)} U_i^{(n)} - \frac{\Delta t}{2} \sum_{\forall \Gamma_{ih} \in \Gamma_{V_i}} s_{ih}^{(n)} \tilde{F}_{fh}^{(n)}$$  \(7\)

$$\Delta V_i^{(n+1)} U_i^{(n+1)} = \Delta V_i^{(n)} U_i^{(n)} - \Delta t \sum_{\forall \Gamma_{ih} \in \Gamma_{V_i}} s_{ih}^{(n+\frac{1}{2})} \tilde{F}_{fh}^{(n+\frac{1}{2})}$$  \(8\)

The finite volumes cell centered method, defines the vector of the conservative variables at the center of each cell. In this way, to compute the numerical flux at the boundary of the fluid sub-domain, it is necessary to use ghost cells, defined by extrapolation. Hence, the variables at the interface $\Gamma_{FSI}$ are not exactly known, which induces an approximation for the velocities continuity condition.

To avoid this problem, the fluid equations are also written using the finite volumes method vertex centred and the same temporal discretization. Thus the velocity at the boundaries will be computed instead of being extrapolated. The equations are written in the same way as the equations (7) and (8) except that they are written for $i \in [1, ..., n_{\text{vertex}}]$ where $n_{\text{vertex}}$ is the number of vertex.

3 COUPLING METHOD

3.1 Multi-time step monolithic formulation

The GC coupling method is based on a dual formulation of the Schur complement, that ensures the velocities continuity through the interface $\Gamma_{FSI}$. In this way, the Lagrangian multiplier method is used. Thus the cinematic condition is written as :

$$L_s v_s(t) + I_f v_{f_{\text{vertex}}}(t) = 0$$  \(9\)

Where $L_s$ is the row selection vector of the finite elements nodes being at the fluid-structure interface, its size being the number of nodes. In the same way, the operator $I_f$ is the row selection vector of the vertex of the finite volume included in $\Gamma_{FSI}$. When the discretized grids of the fluid and the structural sub-domain are compatible, these operators are Boolean.

Finally, based on the energy method, the semi-discretized balance equations of fluid and structural sub-domains are written using Lagrange multipliers, thus the condition of ve-
locities continuity is ensured:

\[
M_s a_s(t) + K_s d_s(t) = F_s(t) - L_T^T \Lambda(t) \quad (10)
\]

\[
\frac{\partial \Delta V_i(t) U_{f_i}(t)}{\partial t} = - \sum_{\forall V_i \in \Gamma} (s_{ih}(t) \tilde{F}_{f_{ih}}(t) + L_{f_{ih}}^T \Lambda_{ih}(t)) \quad (11)
\]

The Lagrange multipliers represent the interaction force between the two sub-domains. \(L_f\) is a \((n_{\text{vertex}} \times 3)\) matrix, where the first and the last columns are zeros vector and the second columns is the transpose of the selection vertex vector \(l_f\). In this way, the matrix \(L_f = [0, l_f^T, 0]\), allows taking into account the interaction force for the cells with one or more vertex included inside \(\Gamma_{FSI}\), in the momentum conservation equation. Thus the equations (9), (10) and (11) are the semi-discretized monolithic system.

Concerning the temporal discretization, the choice is to use a proper temporal scale on each sub-domain. Regarding the hypotheses and the temporal discretization schemes, the fluid sub-domain is discretized using a micro time scale while the structural sub-domain is discretized using a macro time scale. Let’s calling \(\Delta t\) the micro time step between the instants \(t^{(j-1)}\) and \(t^{(j)}\), and \(\Delta T\) the macro-time step between the instants \(t^{(0)}\) and \(t^{(m)}\) such as \(\Delta T = m \Delta t\). Finally, applying these time-scales to the discretization methods presented in the previous sections (equations (2), (3), (4), (7) and (8)) for the equations (10) and (11) and selecting the velocity continuity at the micro-time step for the equation (9), the following discretized system is obtained:

\[
\begin{align*}
(M_s + \frac{\Delta T^2}{4} K_s)a_s^{(m)} &= -K_s d_{s_{\text{pred}}}^{(m)} - L_s^T \Lambda^{(m)} \\
\Delta V_i^{(j-\frac{1}{2})} U_{f_i}^{(j-\frac{1}{2})} &= \Delta V_i^{(j-1)} U_{f_i}^{(j-1)} - \Delta t \sum_{s_{ih}} (s_{ih}^{(j-1)} \tilde{F}_{f_{ih}}^{(j-1)} + L_{f_{ih}}^T \Lambda_{ih}^{(j-\frac{1}{2})}) \\
\Delta V_i^{(j)} U_{f_i}^{(j)} &= \Delta V_i^{(j-1)} U_{f_i}^{(j-1)} - \Delta t \sum_{s_{ih}} (s_{ih}^{(j-\frac{1}{2})} \tilde{F}_{f_{ih}}^{(j-\frac{1}{2})} + L_{f_{ih}}^T \Lambda_{ih}^{(j)}) \\
L_s v_s^{(j)} + l_f v_{f_{\text{vertex}}}^{(j)} &= 0 \quad (j = 1, \ldots, m)
\end{align*}
\]

3.2 Co-simulation algorithm

To solve the system (12), several tricks are used. First, the discretized structural velocities at the interface are defined at the Runge-Kutta mid-step and at the micro-time step. A simple linear interpolation is used, such as:

\[
L_s v_s^{(j-\frac{1}{2})} = (1 - \frac{j-\frac{1}{2}}{m}) L_s v_s^{(0)} + \frac{j-\frac{1}{2}}{m} L_s v_s^{(m)} \quad (13)
\]

\[
L_s v_s^{(j)} = (1 - \frac{j}{m}) L_s v_s^{(0)} + \frac{j}{m} L_s v_s^{(m)} \quad (14)
\]

The same kind of interpolation is used to define the Lagrange multipliers.

The second trick is to split the fluid and the solid variables into a part called "free", which is equivalent to the predictor state, without interaction at the interface, and a part
called "link" representing the corrected state taking into account the interaction force from the interface. Thus the structural sub-domain is re-written as:

\[
\begin{align*}
    a^{(m)}_{s_{\text{free}}} &= M_s^{-1}(F^{(m)} - K_s d^{(m)}_{\text{pred}}) \\
    v^{(m)}_{s_{\text{free}}} &= v^{(m)}_{\text{pred}} + \frac{\Delta T}{2} a^{(m)}_{s_{\text{free}}} \\
    d^{(m)}_{s_{\text{free}}} &= d^{(m)}_{\text{pred}} + \frac{\Delta T^2}{4} a^{(m)}_{s_{\text{free}}} \\
    a^{(m)}_{s_{\text{link}}} &= -M_s^{-1} L_s A^{(m)} \\
    v^{(m)}_{s_{\text{link}}} &= \frac{\Delta T}{2} a^{(m)}_{s_{\text{link}}} \\
    d^{(m)}_{s_{\text{link}}} &= \frac{\Delta T^2}{4} a^{(m)}_{s_{\text{link}}}
\end{align*}
\]

Following the same idea on \( \Omega_f \):

\[
\begin{align*}
    (\Delta VU)^{(j-\frac{1}{2})}_{f_{\text{free}}} &= \Delta V^{(j-1)}_{i_f} - \frac{\Delta t}{2} \sum s_{ih}^{(j-1)} \tilde{F}^{(j-1)}_{f_{ih}} \\
    (\Delta VU)^{(j)}_{f_{\text{free}}} &= \Delta V^{(j-\frac{1}{2})}_{i_f} - \Delta t \sum s_{ih}^{(j)} \tilde{F}^{(j-\frac{1}{2})}_{f_{ih}} \\
    (\Delta VU)^{(j-\frac{1}{2})}_{f_{\text{link}}} &= -\frac{\Delta t}{2} \sum L^{T}_{f_{ih}} A^{(j-\frac{1}{2})}_{ih} \\
    (\Delta VU)^{(j)}_{f_{\text{link}}} &= -\Delta t \sum L^{T}_{f_{ih}} A^{(j)}_{ih}
\end{align*}
\]

Let's recall that the first and the last columns of the selection operator are zero vectors, in this way \((\Delta V\rho)_{f_{\text{link}}} = 0\) and \((\Delta VE)_{f_{\text{link}}} = 0\).

Using the relation \(U_s = U_{s_{\text{free}}} + U_{s_{\text{link}}}\) respectively \(U_f = U_{f_{\text{free}}} + U_{f_{\text{link}}}\), \(A\) is defined as:

\[
(\mathbf{H}_s + \mathbf{H}^{(j)}_f)A^{(j)} = L_s v^{(j)}_{s_{\text{free}}} + l_f v^{(j)}_{\text{vertex}_{f_{\text{free}}}}
\]

The equation (17) is written in the same way at the half micro-time step \(t^{(j-\frac{1}{2})}\).

Then, we define:

\[
\begin{align*}
    \mathbf{H}_s &= \frac{1}{2} \Delta T L_s M_s^{-1} L_s^T \\
    \mathbf{H}^{(j-\frac{1}{2})}_f &= \frac{1}{2} \Delta t l_f M^{(j-\frac{1}{2})}_f^{-1} l_f^T \\
    \mathbf{H}^{(j)}_f &= \Delta t l_f M^{(j)}_f^{-1} l_f^T
\end{align*}
\]

Where the mass fluid matrix \(M_f\) is defined as a diagonal matrix \((n_{\text{vertex}} \times n_{\text{vertex}})\) with \(M_{fi} = (\Delta V\rho)_{f_i}\).

Finally the last trick is to keep the conservative variable and the cell volumes grouped. After the computation of \((\Delta V\dot{U})_f\), the fluid velocity at the interface taking into account the structural interaction is known using the following relation:

\[
V_{f_{\text{vertex}}} = \frac{(\Delta V\rho V)_{f_{\text{vertex}}}}{(\Delta V\rho)_{f_{\text{vertex}}}}
\]
The monolithic coupling algorithm for finite elements / finite volumes vertex centred, is then completely defined. For the coupling method, using the finite volume cell centered, we need to define the fluid velocity at the boundary $\Gamma_{FSI}$. A simple first order extrapolation from the interior cells is used.

The complete algorithm is defined on the fig. (3). The global idea is the following; the free structural variable are computed at the macro time-step, the free fluid variables are computed at the half micro time-step, then the structural velocity at the interface is interpolated at the half micro-time step. Using the free velocities (fluid and solid) the Lagrange multiplier is computed, using it the link fluid state is known and finally the total fluid state at the half-micro time step. The process is repeated at each micro-time step until $j = m$. Then, at the macro-time step, the link structural state is computed in addition to the fluid one.

![Figure 3: Multi time-step algorithm](image)

### 4 NUMERICAL TEST CASE

To validate the method presented below, the piston test case is used. This one has been introduced by Piperno in 1995 [11]. Later, it has often been used to validate new FSI methods [2], [6]. It is really simple, an aero-elastic problem in one dimension. The set of parameters used here are the same as those proposed by Michler [9].
4.1 Presentation

The problem is considered in 1D. A gas is enclosed inside a cavity closed at the left side by a wall and at the right side by a mass-spring system. Its length is 1m. The fluid domain $\Omega_f$ is composed of air (specific heat ratio $\gamma_{air} = 1.4$ and celerity $c_{air} = 340 \text{m.s}^{-1}$). Thus the fluid is considered a perfect gas compressible and inviscid. Moreover the thermal exchanges are neglected. The structure domain $\Omega_s$ is a simple mass-spring system, with a mass of $m_s = 0.8 \text{Kg}$ and a stiffness of $k_s = 7991 \text{N.m}^{-1}$.

At the beginning of the simulation, the piston is at rest. The pressure inside the cavity is $p_f(0) = 10^5 \text{Pa}$, the atmospheric pressure. The velocity $v_f(0)$ of the fluid is zero and its density is $\rho_f(0) = 1.3 \text{Kg.m}^{-3}$. The velocity of the structure $v_s(0)$ system is initially zero and a displacement of $d_s(0) = 0.01 \text{m}$ is imposed on it.

![Figure 4: Piston au pas de temps initial](image)

4.2 Results

First, the results obtained for the monolithic coupling method mono time step for finite element/finite volumes vertex centered are presented. The Fig. (4.2) shows the position of the interface $\Gamma_{FSI}$ during time. The amplitude is globally constant, it seems that there is no significant loss or gain of energy. However a slight loss of amplitude, around 0.01% after 20 cycle, is noticed. Nevertheless, this error could be correlated to the error induced by the simulation of the same fluid domain alone, where the right side is closed by a moving wall governing by the same mass-spring system (this simulation is equivalent to the one-way coupling of the piston problem). In this way the error is induced by the fluid discretization methods, not by the coupling method.

Moreover the relative error to the velocities continuity is also studied. We define $err = \frac{|L_v\nu_f^{(n)} - L_v\nu_s^{(n)}|_{\text{max}(\nu_{FSI})}}{\text{max}(\nu_{FSI})}$. This one is of the order of $10^{-16}$ what is satisfying, see Fig.(6).

Considering the coupling finite elements / finite volumes cell centered, the interface position is globally the same, nevertheless a little gain of amplitude is remarked over 0.03% after 20 cycles. Moreover this error cannot be correlated to the fluid model alone. The relative velocity error between fluid and structure is here more important.
Figure 5: Interface position according time

Figure 6: Relative error of the velocities continuity at the interface, left coupling of finite volume vertex centred, right coupling of finite volume cell centered

around $10^{-9}$. Let’s recall that this coupling method introduced an approximation; the free fluid velocities at the interface are extrapolated. In this way, we can make the following hypothesis; improving this extrapolation would improve the FSI results too.

Finally, the multi time-step method has also been studied for the finite elements / finite volumes vertex centred coupling. The results seem to be really promising because the quality is a few degraded even when the ratio between the micro and the macro time-step increased. For instance, we have remarked previously that for $m = 1$ (mono time-step case) the relative error of velocities was around $10^{-16}$. For $m = 100$, this error remains is the same magnitude.
5 CONCLUSION

To conclude, the presented method allows a co-simulation coupling and ensures the energy conservation and the velocity continuity through the interface, for a mono time step coupling of finite volumes vertex centered and finite elements. The results are weakly defaced for a coupling using finite volumes cell centered instead of vertex centered which is involved by the extrapolation of the fluid velocity from the cell center to the fluid-structure interface, useful for the coupling condition. Nevertheless this error remains limited. Finally the multi time-step coupling finite volumes vertex centred / finite elements have been studied. This one shows good results, the results deterioration is limited despite the ratio increase between the fluid and the structural time step.

The next step is to study the coupling of finite volumes cell centered and finite elements in 2D and using multi time-step. Even if the coupling using finite volumes vertex centered has shown better results, we will use finite volumes cell centered because the aim is to use the commercial software Fluent to compute the fluid sub-domain, this one is based one finite volumes cell centered method. The velocity continuity condition at the interface could be improved, using more complex extrapolation of the fluid variables.

REFERENCES


A STATE-SPACE PARTITIONED TIME INTEGRATION ALGORITHM FOR REAL-TIME HYBRID SIMULATION WITH NONLINEAR NUMERICAL SUBDOMAINS

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Key words: Hybrid Simulation; Partitioned Time Integration; State-Space Model; Seismic Isolation.

Abstract. This paper describes a state-space partitioned algorithm for real-time hybrid simulation. The state-space modeling is proposed to represent nonlinear numerical substructures. The effectiveness of the proposed method is demonstrated for a virtual bridge case study equipped with seismic isolation devices.

1 INTRODUCTION

Hybrid simulation (HS) merges structural testing and numerical modelling into a unique dynamic simulation paradigm, which has been extensively used to investigate the seismic response of civil structures [1]. In detail, a time stepping analysis algorithm solves for the coupled equation of motion of a prototype structure made of numerical and physical subdomains (NS and PS, respectively), which are assembled in a finite element (FE) fashion. On the PS side, servo-controlled actuators equipped with load cells impose displacement trials to the tested component and measure corresponding restoring forces. The NS is typically instantiated in a structural analysis software. In order to minimize actuator control errors, when the PS restoring force is rate independent, pseudodynamic- (PSD-) HS is performed, which means that the wall-clock duration of HS scales up with respect to the duration of the virtual excitation and velocities scale down of the same amount. If not, real-time- (RT-) HS is
performed. In both cases, PS testing is conducted by reproducing boundary and loading conditions as experienced within the prototype structure when subjected to a realistic excitation. Data from experiments is intended support model validation and calibration for tested structural components.

Most of developments related to HS consist on adaptations of existing FE analysis codes to accommodate so-called experimental elements, which incorporate a digital interface to the testing equipment. However, complexity of FE software, which trades off between modularity and computational performance, struggles with the deterministic execution scheduling imposed by RT-HS (i.e., evaluation of the NS response with a constant sampling period of 1÷10 msec). In our opinion, the state-space approach, which is quite popular in the control community, offers a computationally cheaper alternative to FE for modelling nonlinear NS. This paper describes a state-space partitioned time integration algorithm for RT-HS. The dual-coupling strategy of the modified-PH method [2] allows for assembling state-space equations of PS and NS in a FE fashion. HSs of a virtual two-pier reinforced concrete bridge equipped with friction pendulum bearings are presented as proof-of-concept example.

1 STATE-SPACE PARTITIONED ALGORITHM FOR HYBRID SIMULATION

In order to facilitate the assembly of nonlinear NSs simulated with well-known differential models (e.g. Mostaghel [3] hysteretic springs), the HS framework presented in this section relies on a newly conceived parallel partitioned algorithm tailored to state-space systems. The Monolithic-Generalized-\(\alpha\) (MG-\(\alpha\)) time stepping scheme proposed by Brüls and Arnold [4] is used as basic solver for the Partitioned-Generalized-\(\alpha\) (PG-\(\alpha\)) method, which adopts the coupling scheme of the modified PH method conceived by Brun and co-workers [2]. Both algorithms solve the system of equations of motion re-casted in state-space form that, for a generic nonlinear mechanical system, reads,

\[
\mathbf{M}\dot{\mathbf{Y}} + \mathbf{R}(\mathbf{Y}) = \mathbf{F}(t) \tag{1}
\]

where,

\[
\mathbf{Y} = \begin{bmatrix} \mathbf{u} \\ \mathbf{v} \\ \mathbf{s} \end{bmatrix}, \quad \mathbf{M} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & m & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \mathbf{R} = \begin{bmatrix} -\mathbf{v} \\ \mathbf{r}(\mathbf{u}, \mathbf{v}, \mathbf{s}) \\ \mathbf{g}(\mathbf{u}, \mathbf{v}, \mathbf{s}) \end{bmatrix}, \quad \mathbf{F}(t) = \begin{bmatrix} 0 \\ \mathbf{f}(t) \\ 0 \end{bmatrix} \tag{2}
\]

In detail, \(\mathbf{u}, \mathbf{v}\) and \(\mathbf{s}\) are displacement, velocity and additional state vectors, respectively. The former two always appear as a pair in second-order mechanical systems, while the latter is used to model nonlinearities endowed with memory (e.g., hysteresis). In particular, \(\mathbf{r}(\mathbf{u}, \mathbf{v}, \mathbf{s})\) is the nonlinear restoring force vector while the nonlinear function \(\mathbf{g}(\mathbf{u}, \mathbf{v}, \mathbf{s})\) comprises the evolution of the additional state vector \(\mathbf{s}\). Moreover, \(\mathbf{m}\) is the mass matrix and \(\mathbf{f}(t)\) is the external time varying load while \(\mathbf{I}\) and \(\mathbf{0}\) are identity and zero matrices, respectively. When the system is linear, velocities and displacements only characterize the system state, which does not include additional variables. As a result, the restoring force reduces to,
with \( \mathbf{k} \) and \( \mathbf{c} \) stiffness and damping matrices, respectively. For simplicity time dependency is omitted and hereinafter, \( \mathbf{M}, \mathbf{K}, \mathbf{R} \) and \( \mathbf{F} \) are referred to as generalized mass, stiffness, restoring force and external loading. First, the MG-\( \alpha \) is presented; successively, the PG-\( \alpha \) is described for coupling one PS and one NS.

### 1.1 The Monolithic G-\( \alpha \) time integration algorithm

The original MG-\( \alpha \) algorithm proposed by Jansen and co-workers [5] applied to integrate (1) from \( t_n \) to \( t_{n+1} \) with a time integration step \( \Delta t = t_{n+1} - t_n \), reads,

\[
\mathbf{M} \dot{\mathbf{Y}}_{n+\alpha_m} + \mathbf{R} \left( \mathbf{Y}_{n+\alpha_f} \right) = \mathbf{F}_{n+\alpha_f}
\]

where,

\[
\dot{\mathbf{Y}}_{n+\alpha_m} = (1 - \alpha_m) \dot{\mathbf{Y}}_n + \alpha_m \dot{\mathbf{Y}}_{n+1}
\]

\[
\mathbf{Y}_{n+\alpha_f} = (1 - \alpha_f) \mathbf{Y}_n + \alpha_f \mathbf{Y}_{n+1}
\]

\[
\mathbf{Y}_{n+1} = \mathbf{Y}_n + \dot{\mathbf{Y}}_n (1 - \gamma) \Delta t + \dot{\mathbf{Y}}_{n+1} \gamma \Delta t
\]

Parameters \( \alpha_f, \alpha_m \) and \( \gamma \) define the setting of the algorithm. They are expressed as function of the infinity spectral radius \( \omega_\infty \) parameter as,

\[
\alpha_m = \frac{3 - \rho_\infty}{2(1 + \rho_\infty)}, \quad \alpha_f = \frac{1}{1 + \rho_\infty}, \quad \gamma = \frac{1}{2} + \alpha_m - \alpha_f
\]

The resulting algorithm is second order accurate. In detail, if \( \omega_\infty \) is chosen to be zero, the method annihilates the components of the system response whose frequencies are high compared to the sampling frequency. If \( \omega_\infty = 1 \), then, \( \alpha_m = \alpha_f = \gamma = 1/2 \) and the MG-\( \alpha \) method is equivalent to the trapezoidal rule, which does not introduce algorithmic dissipation.

### 1.2 The Partitioned G-\( \alpha \) time integration algorithm

The PG-\( \alpha \) method is a parallel partitioned time integration algorithm that couples two monolithic time integration processes based on the MG-\( \alpha \) algorithm following a dual assembly approach. In detail, two parallel time integration processes are coupled at the coarse time step, where the compatibility of NS and PS is forced by a dual assembly procedure. The corresponding coupled system of equations of motion reads,

\[
\begin{align*}
\mathbf{M}^N \dot{\mathbf{Y}}^N_{n+1} + \mathbf{R}^N (\mathbf{Y}^N_{n+1}) &= \mathbf{L}^N \mathbf{A}_{n+1} + \mathbf{F}^N_{n+1} \\
\mathbf{M}^P \dot{\mathbf{Y}}^P_{n+1} + \mathbf{R}^P \left( \mathbf{Y}^P_{n+1} \right) &= \mathbf{L}^P \mathbf{A}_{n+1} + \mathbf{F}^P_{n+1} \\
\mathbf{G}^N \dot{\mathbf{Y}}^N_{n+1} + \mathbf{G}^P \dot{\mathbf{Y}}^P_{n+1} &= \mathbf{0}
\end{align*}
\]
where, $M$, $R$ and $F$ are defined in Eq. (2) while signed Boolean collocation matrices $L$ and $G$ localize interface forces and define compatibility equations, respectively. In line with Eq. (7), time steps $\Delta t^N$ and $\Delta t^P$ refer to simulation time, which is a virtual time axis defined by the time integration process. As an example, the seismic ground motion is expressed as function of the simulation time. In particular, $\Delta t^N$ is the coarse time step adopted for the NS while $\Delta t^P$ is the fine time step used to calculate the PS response. In order to guarantee a sufficient accuracy, $\Delta t^N = 1 \text{ msec}$ is typically considered. The testing time scale $\lambda$ defines the ratio between wall-clock and simulation time speeds. In particular, when $\lambda = 1$ the test is conducted in real-time. Conversely, when $\lambda > 1$, the simulation time is extended in comparison with the wall-clock time and the test is conducted in a pseudodynamic regime. When the response of the PS does not depend on the rate of loading, $\lambda$ usually ranges between 50 and 200. This approach reduces control tracking errors. Moreover, an extended simulation time scale $\lambda$ reduces the destabilizing effect of actuator delay, which is typically of the order of $10 \div 20 \text{ ms}$. On the other hand, $\Delta t^S = \lambda \Delta t^N$ and $\Delta t^C = \lambda \Delta t^P$ refer to the wall-clock time, which is the real time flow measured in the laboratory. In particular, $\Delta t^S$ defines the maximum solving time that can be allocated to compute the NS response while $\Delta t^C$ is the actuator controller time step, which typically ranges between 1 and 2 $\text{ msec}$ to guarantee smooth displacement trajectories. In principle, at each simulation step displacement and velocity solutions of Eq. (7) split into free and link components. The former are calculated discarding coupling conditions, which are used to compute the latter by means of a linearized Steklov-Poincaré operator. The coupled solution is the sum of both free and link contributions. Both free and link solutions are solved based on the MG-$\alpha$ algorithm, which provides tunable algorithmic damping to the coupled scheme.

2 THE VIRTUAL TWO-PIER BRIDGE

2.1 Description of the case study

In order to verify the proposed computational framework, we conceived a two-pier bridge case study that we used to benchmark three alternative seismic isolation schemes. The virtual bridge prototype depicted in Figure 1 is characterized by a three-span reinforced concrete deck with two independent roadways, sustained by two twin cantilever rectangular hollow cross-section RC piers. Cross sections of deck and pier are depicted in Figure 2. As depicted in Figure 1, a pair of seismic isolation devices was interposed between deck and piers and deck and abutments.

Three alternative seismic isolation devices were tested, namely, double and triple concave sliding bearing (D- and T-CSB, respectively) and lead rubber bearing (LBR). All devices were dimensioned to keep the maximum transversal shear force applied to each pier below $370 \text{ kN}$ and the corresponded transversal displacement below $3 \text{ mm}$. 
Due to the limited length of the paper, only the T-CSB device is described. Figure 3 depicts a schematic of a generic T-CSB device, for which a detailed mechanical model can be found in [6].

The REXEL software [7] was used to select a single ground motion record corresponding to a seismic scenario characterized by moment magnitude $M = 5 \div 7$, epicentral distance $D = 0 \div 30$ km and soil type B, which was scaled to different values of peak ground acceleration (PGA). In detail a PGA value of $0.12$ g was assigned to the serviceability limit state (SLS) while a PGA value of $0.30$ g was selected for the ultimate limit state (ULS) based on a comprehensive analysis of the bridge response based on a nonlinear FE model. The horizontal seismic excitation was orthogonal to the main axis of the bridge deck.
2.2 Substructuring scheme

Figure 4 depicts the partitioning of the virtual bridge prototype into PSs and NSs, which are colored in red and blue, respectively. In detail, nonlinear springs represent piers and seismic isolation device pairs, while the continuous line is the deck. The latter was obtained via static condensation of a linear FE model based on Bernoulli beam elements, by retaining transversal displacements of Nodes #1, #6, #11 and #16, that is, connection points to piers and abutments.

As can be appreciated from Figure 4, one pair of T-CSB devices was tested in the laboratory while all other substructures were simulated numerically. In order to reproduce the hysteretic response of the T-CSB on the NS, a state-space model inspired to Mostaghel's work [3] was developed. In this regard, Figure 5 shows both the spring-slider idealization and the entailing hysteretic loop.

![Figure 4: Plan views of the substructured virtual bridge prototype.](image)

![Figure 5: T-CSB state-space model: a) spring-slider idealization; b) hysteretic loops.](image)

The state-space model of the restoring force $r$ is described as,

$$\dot{r} = \dot{r}_0 + \dot{r}_1 + \dot{r}_2$$

$$\dot{r}_0 = \left(k_0 \left(\bar{N}(v)\bar{M}(s_0 - \delta_0) + M(v)N(s_0 + \delta_0)\right)\right)v$$

$$\dot{r}_1 = \left(k_1 \left(\bar{N}(v)\bar{M}(s_1 - \delta_1) + M(v)N(s_1 + \delta_1)\right)\right)v$$

$$\dot{r}_2 = k_2 v$$

(8)
where slip displacements of equivalent sliders read,

\[ s_1 = \frac{r_1}{k_1} \]
\[ s_2 = \frac{r_2}{k_2} \]  \hspace{1cm} (9)

and functions \( N, M, \bar{N} \) and \( \bar{M} \) read,

\[ N(w) = 0.5 \left( 1 + \text{sgn}(w) \right) \left( 1 + \left( 1 - \text{sgn}(w) \right) \right) \]
\[ M(w) = 1 - N(w) \]
\[ \bar{N}(w) = M(-w) \]
\[ \bar{M}(w) + N(-w) \]  \hspace{1cm} (10)

Values of model parameters identified for the maximum velocity peak of 0.1 m/s read,

\[ k_0 = 6.67e7 \text{ N/m}, \delta_0 = 1.5e - 3 \text{ m}, \]
\[ k_1 = 1.15e6 \text{ N/m}, \delta_1 = 0.07 \text{ m}, \]
\[ k_2 = 5e5 \text{ N/m} \]

The developed model was validated against experimental data. In this respect, Figure 6 compares emulated and measured hysteretic loops and dissipated energy histories. As can be appreciated, the developed model accurately reproduces the response of the tested T-CSB device.

![Figure 6: Validation of the D-CSB model against experimental measurements at \( v = 0.1 \text{ m/s} \): a) hysteretic loop; b) dissipated energy.](image)

3 HYBRID SIMULATION OF THE VIRTUAL BRIDGE

3.1 Architecture of the implementation

In order to simulate the virtual bridge prototype, the HS framework of Figure 7, which relies on the PG-\( \alpha \) algorithm described in Section 1, was implemented at the Experimental Laboratory of EUCENTRE, Pavia, Italy. A Windows-based HOST-PC runs the MATLAB-SIMULINK...
computational environment [8], which implements both the PG-α algorithm and the NS of the substructured system. The C-code automatically generated by SIMULINK is compiled and uploaded to the XPC-TARGET that executes the software in real-time. The XPC-TARGET is provided with DAQ boards that communicate with the Bearing Testing System (BTS) controller, which controls a servo-hydraulic loading system specifically conceived for testing bearings. At each simulation step of the PG-α algorithm, the XPC-TARGET sends displacement commands to the physical D-CSB, and the related restoring force is fed back to the PG-α algorithm that solves the system of coupled equations of motion. In order to enable fast-time testing i.e., $\lambda = 2 \div 20$, the delay compensation algorithm proposed by Wu and co-workers [9], was adopted.

The BTS of the Experimental Laboratory of EUCENTRE has been specifically designed to impose realistic boundary conditions to full-scale seismic isolation devices [10]. In this regard, Figure 8 shows the BTS setup and provides a close-up view of the restoring force measuring system. In detail, the specimen is positioned on a self-equilibrating vertical reaction structure; the bottom plate of the specimen is connected to a 6-DoF shake table, driven by vertical and horizontal actuators and connected to an additional horizontal reaction structure, which can be operated in mixed force-displacement control. The maximum vertical and horizontal load capacities of the BTS are $50 \, MN$ and $2.8 \, MN$, respectively. The allowed horizontal displacement range is $\pm 495 \, mm$ with a velocity peak of $2200 \, mm/s$. During standard characterization tests, the load cells of the horizontal actuators measure the raw restoring force of the specimen, which is post-processed offline to remove machine inertia and friction. In order to skip this task during HS, a force measuring system is developed. It is based on a steel plate sliding on a Teflon layer and surrounded by 8 ring pre-stressed load cells, which measure the specimen restoring force in two orthogonal plane directions.

Figure 7: Block diagram of the HS framework.
Since energy dissipation in seismic isolation devices mainly relies on friction or damage mechanisms, they are easily biased when devices are scaled. Accordingly, full-scale devices are considered in this testing campaign. It is worthy to note that the interaction between displacement controlled actuators and stiff specimens easily triggers dynamic instability. This situation is very likely to occur on elements subjected to axial deformation, where small displacement perturbations generate large feedback forces. In order to overcome this problem, the common practice consists on excluding vertical degrees-of-freedom from the HS loop and impose nominal loads in force control. Accordingly, the nominal vertical load owing to the self-weight of the bridge deck is kept constant and applied to the tested seismic isolation device in force control. In addition, a single bearing per pair is physically tested and the measured restoring force feedback to the HS algorithm is doubled. This latter simplification was preliminary verified with numerical simulations, which prove that deck overturning moment is negligible and does not affect the transversal response of the bridge.

3.2 Results of experiments

The HS campaign started on February 2015 and ended in April 2017. Experiments were conducted by scaling the reference ground motion record up to a PGA value of 0.85 g. Figure 9 compares the hysteretic loops of the restoring forces of tested isolation devices, which show similar forces and displacement ranges. This trend confirms that the investigated isolation schemes highlight similar performances.
4 CONCLUSIONS

This paper presented a state-space partitioned time integration algorithm for real-time hybrid simulation. State-space modeling simplifies the implementation of nonlinearities on the numerical substructures, which can be incorporated with a lower computational cost compared to the finite-element modeling paradigm. The effectiveness of the proposed method is demonstrated for a virtual two-pier bridge case study equipped with friction pendulum bearings.

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6 REFERENCES


Prestressed Vibrations of Partially Filled Tanks Containing a Free-Surface Fluid: Finite Element and Reduced Order Models

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Abstract. In linear vibration analysis of partially filled elastic tanks [1], even if the tank is submitted by a gaz or a liquid pressure, the reference configuration is generally used without the effect of static loads. In the case of very thin structures or soft material, the static state is considered as prestressed, due to geometrical nonlinearities of the deformed tank. The global stiffness of the structure may change in function of the fluid volume amount [2, 3, 4]. The aim of the paper is to quantify the prestressed effects on the linearized dynamic behavior of the fluid-structure system. The chosen methodology is the following: (i) A quasi-static solution is computed from an empty to a fully filled state of the tank, by considering geometrical nonlinearities and hydrostatic follower forces [5] (no volumetric mesh of the fluid is needed for this step); (ii) after a volumetric remeshing of the fluid at each states, a linearized hydroelastic displacement-pressure formulation around the prestressed state, without gravity effects, is established; (iii) a reduced basis of the hydroelastic problem is generated by using prestressed dry modes to minimize the computation of the added mass matrix. Numerical examples are given to illustrate the proposed approaches.
1 INTRODUCTION

For geometrical simple fluid-structure systems such as cylinders, relevant of semi-analytical analysis, the problem has been solved by using, as a projection basis, the structural dry modes (i.e. modes in vacuo).

For complex structures, it is known that the presence of an added mass operator may lead to prohibitive computational times and memory (computation of a Schur complement matrix). An alternative formulation, for partially filled structures, using the computation of the added mass for a limited number of filled structures, has been presented in [1]. In the paper, the aim is to evaluate here the approach using only dry-structural modes, but prestressed, in order to reduce future computational times.

1.1 Definition of the emptying rate

We consider an elastic tank partially filled by an internal fluid. We denote by $V_t$ the initial volume tank and $V_f$ the current fluid volume corresponding to various level of liquid in the tank. We define the emptying rate $\tau$ such that

$$\tau = \frac{V_t - V_f}{V_t}$$

The main objective of the study is to estimate the influence of this parameter on the prestressed dynamic behavior of the fluid-structure system. We make the assumption that the frequency range of interest is high enough ($f > 5$ Hz) compared to the evolution of the emptying rate, so the evolution of the fluid volume is supposed to be quasi-static in our study. Thereby, at each emptying rate the fluid-structure system vibrations are computed around a quasi-static equilibrium state.

1.2 Fluid-structure-hypotheses

Structure - In the numerical examples, the structure is supposed to be isotropic, homogeneous, elastic and prestressed. At the equilibrium, the displacements of the structure are high enough to take into account the prestressed effect on the dynamic behavior due to an hydrostatic or a gas pressurization. The linear vibrations are computed around each prestressed configurations. Three states of the structural domain, described in Fig. 1, are considered. At first, the reference configuration $\Omega_0$ is the domain occupied by the solid without any external forces. The associated position vector is noted $X_0$. Then, the current "quasi-static" $\Omega_q$ is the domain occupied by the structure considering finite deformations. The position of the prestressed state is associated with $x_q = X_0 + u_q$. Finally, we denote $\Omega_s$ the current "dynamic" configuration under the assumption of harmonic excitations and the position vector $x_s = x_q + u_s$. In the following, $\Omega_s$ and $\Omega_q$ coincide because $\|u_s\|$ is very small compared the thickness $t$ of the elastic tank. All the domains are bounded of $\mathbb{R}^3$. 

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Free-surface fluid hypotheses - At the equilibrium, the horizontal free-surface fluid is supposed to be at rest, homogeneous, inviscid, incompressible and without surface tension. We neglect, as usually done in hydroelastic linear vibrations, the gravity effect (sloshing). Consequently, the pressure fluctuation is null on the free-surface Γ and written as

\[ p = 0 \text{ on } \Gamma \]  \hspace{1cm} (2)

Finally, we denote by Σ the fluid-structure interface on the current configuration. The Fig. 2 recapitulates the methodology such that:

- Phase 1: Computation of the quasi-static deformation in finite deformation;
- Phase 2: Coincident re-meshing of the fluid and the structure around the prestressed state;
- Phase 3: Prestressed hydroelastic vibrations

Only Phase 3 will be presented in the current paper.

**Figure 1:** (a) Reference configuration for a dry structure; (b) Current "quasi-static" configuration in finite deformation; (c) Linearized "structural" dynamic configuration around the prestressed state.

**Figure 2:** (a) Phase 1: Prestressed state computed with follower forces (due to a gas or liquid pressure); (b) Phase 2: Current configuration of the structure Ωq around a quasi-static equilibrium and the fluid domains Ωf at rest; (c) Phase 3: Hydroelastic vibrations around the prestressed state with an excitation f and a pressure fluctuation p = 0 on the free surface Γ
2 Discretized added mass prestressed hydroelastic formulation

In this section, the nodal finite element displacement $U_q$ of a deformed elastic structure, related to the quasi-static finite deformation, is supposed to be known. We denote by $U_s$ the fluctuation of displacement vector around the prestressed state. The structure is supposed to be clamped at $\partial \Omega_0 = \partial \Omega_s$.

2.1 Symmetric eigenvalue problem with added mass matrix

We will use an intermediate discrete variable called the fluid displacement potential, denoted by $\varphi$, related to the pressure fluctuation vector $P$ by $P = \rho \omega^2 \varphi$ (with $\varphi = 0$ on $\Gamma$). Using the condition of $P$ or $\varphi$, the discretized variational approach of the FSI problem leads to a pure structural eigenvalue problem written as

$$\begin{bmatrix} K_{\text{tan}} - \omega^2 (M + M_a) \end{bmatrix} U_s = 0$$

where $\omega$ is the natural angular frequency of the system. The eigenvalues and eigenvectors of the system Eq. (3) are respectively the prestressed hydroelastic natural angular frequencies $\omega_\alpha$ and the structural part of the hydroelastic modes $U_\alpha$. Due to the fluid incompressibility and geometric considerations from the fluid-structure interface displacements, the potential of displacement part is then deduced, for each hydroelastic modes, with the following equations:

$$H_s \varphi_\alpha = -C_s^T U_\alpha$$

where $\rho_f$ is the fluid density, $\star$ corresponds to the matrices which take into account $\varphi = 0$ on $\Gamma$ and:

- $K_{\text{tan}}$ is the tangent stiffness matrix which is symmetric and supposed to be positive-definite. The tangent matrix is a contribution of the geometrical, material and load contribution to the stiffness of the prestressed structure, respectively denoted by $K_g$, $K_m$ and $K_f$, such that:

$$K_{\text{tan}} = K_g + K_m + K_f$$

- $M$ is the positive-definite mass matrix of the structure;
- $M_a$ is the added mass matrix which is positive-definite, symmetric and full in the columns and the lines related to the fluid-structure interface displacements degrees of freedom;
- $H$ is a fluid operator related to the kinetic energy of the displaced fluid induced by the displacement of the fluid-structure interface;
- $C$ is the coupling matrix at the fluid-structure interface.

We shall note that $K_{\text{tan}}$, $M$, $C$ and $H$ depend on the known quasi-static displacement $U_q$. The eigenvalues and eigenvectors of the system Eq. (3) are respectively the prestressed hydroelastic natural angular frequencies $\omega_\alpha$ and the structural part of the hydroelastic modes $U_\alpha$. Due to the fluid incompressibility and geometric considerations from the fluid-structure interface displacements, the potential of displacement part is then deduced, for each hydroelastic modes, with the following equations:

$$H_s \varphi_\alpha = -C_s^T U_\alpha$$
Due to the matrix inverse computation $H^{-1}$ in Eq. (4), the computational time might become prohibitive.

3 PROJECTION ON PRESTRESSED DRY MODES

The projection of the coupled problem on the dry modes is presented in three steps:

**Step 1:** We compute $N$ eigenvectors by solving the linearized eigenvalue problem of the structure *in vacuo*:

$$[K_{\text{tan}} - \omega^2 M] U_s = 0 \quad (7)$$

**Step 2:** For each deformed shapes $U_\beta$, we solve a linear system to compute the associated fluid potential displacement [1] expressed as:

$$H_\beta \varphi_\beta = -C^T U_\beta \quad (8)$$

where $\varphi_\beta$ is the associated fluid potential displacement ($\varphi_\beta = 0$ on the discretized free surface $\Gamma$). We introduce the following notations:

$$B = \begin{bmatrix} U_1 & \ldots & U_N \end{bmatrix}, \quad \Phi = \begin{bmatrix} \varphi_1 & \ldots & \varphi_N \end{bmatrix} \quad \text{and} \quad \kappa = \begin{bmatrix} \kappa_1 \\ \vdots \\ \kappa_N \end{bmatrix} \quad (9)$$

where $B$ and $\Phi$ are the rectangular matrices containing respectively each structural eigenvectors (normalized by the mass matrix $M$) and the associated potential of displacements on the fluid for each mode. $\kappa$ is the generalized unknown coordinates vector. We suppose that $N$ is high enough such that $U_s \simeq B\kappa$.

**Step 3:** The induced pressure associated with the $\beta$th dry mode is written in the following form:

$$P_\beta = -\omega^2 \rho_\ell \varphi_\beta \kappa_\beta \quad (10)$$

We take into account each pressure contribution of the fluid, induced by the structural dry modes displacements such that an external load appear in the right side of Eq. (7) written as:

$$[K_{\text{tan}} - \omega^2 M] B \kappa = \omega^2 \rho_\ell C^T \Phi \kappa \quad (11)$$

Finally by multiplying Eq. (11) by $B^T$ in the left, we obtain the following reduced eigenvalue equation:

$$[\Omega - \omega^2 (I + r_a)] \kappa = 0 \quad (12)$$

where $\Omega = B^T K_{\text{tan}} B$, $I = B^T M B$ and $r_a = \rho_\ell B^T C^T \Phi$. We shall denote the following remarks:
• The resulting reduced matrix problem is very small due to the fact that \( N \) is supposed to be very small compared to the displacement structural degree of freedom;

• All the matrices are symmetric, according to Eq. (8), \( r_a = \rho_f B^T C H^{-1} C^T B \), except that no matrix inversion have been computed for \( r_a \) but only \( N \) linear system of equations;

• If \( N \) is high enough, the \( K \) first eigenvalues of this reduced problem (with \( K \leq N \)) converge to the \( K \) first one of the hydroelastic with the full added mass matrix;

• The \( N \) linear system of equations can be done in parallel.

4 Numerical examples

The objective of the numerical examples is to compare the hydroelastic dynamic behavior computed with (i) classical added mass formulation and (ii) the coupled problem projected on the dry mode. Two cases are presented, one with prestressed effects and one without.

4.1 Example without prestressed effects of a partially filled cylinder

The first case concerns the computation of a partially filled elastic clamped cylinder with a rigid bottom (see Fig. 3 for the geometry and the mesh parameterization). The material properties are the Young modulus \( E = 200 \times 10^9 \) Pa, the Poisson ratio \( \nu = 0.33 \), the structural mass density \( \rho_s = 7.8 \times 10^3 \) kg/m\(^3\) and \( \rho_f = 1.0 \times 10^3 \) kg/m\(^3\).

![Figure 3](image-url)

Figure 3: (a) Geometry of the partially filled elastic clamped cylinder with rigid bottom with \( t = 6 \) mm, \( L = 6 \) m and \( R = 2 \) m; (b) Mesh parameterization, with 20 hexaedral elements, where \( n_\theta = 1 \) and \( n_z = 4 \) are fixed.

The objective of this example consist to show the convergence of the problem projected on the dry modes toward the classic added mass formulation involving the computation of an inverse matrix. Three cases are analyzed:
• An empty cylinder $\tau = 0$ with $n_\theta = 10$, $n_z = 10$, $n_f = 0$;
• A half filled cylinder $\tau = 0.5$ with $n_\theta = 10$, $n_z = 5$, $n_f = 5$;
• A fully filled cylinder $\tau = 1$ with $n_\theta = 10$, $n_z = 0$, $n_f = 10$.

The hydroelastic analysis, done with the added mass formulation are given in Fig. 4. As expected, the natural hydroelastic frequencies rises when $\tau$ decreased.

![Representation of the circumferential and the longitudinal wave numbers $n$ and $m$.](image)

**Figure 4:** Representation of the circumferential and the longitudinal wave numbers $n$ and $m$. (a) Hydroelastic frequencies with $\tau = 1$; (b) Hydroelastic frequencies with $\tau = 0.5$; (c) Natural frequencies in vacuo

A convergence analysis of the $K = 20$ first hydroelastic natural frequencies is presented in Fig. 5 and Fig. 6 for $\tau = 1$ and $\tau = 0.5$. For both cases the hydroelastic natural frequencies computed with the projection on $N$ dry modes are done with $N = 20$, $N = 50$, $N = 100$ and $N = 150$:

• the proposed method based on the projection of the coupled problem on $N$ dry modes converge toward the classic added mass formulation when $N$ increases;
the maximum error within the $K = 20$ hydroelastic frequencies, decreases, but not continuously. In fact, it depends on the contribution of a specifics number of modes. It means that the number of linear system of equation could be reduced if the modal contribution could be known \textit{a priori}.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure5.png}
\caption{Value natural hydroelastic frequencies for the 20 first $K$ modes in dashed blue (added mass formulation) and hydroelastic frequencies computed with the projection on $N$ dry modes in red ($N = 20$, $N = 50$, $N = 100$ and $N = 150$); (a) $\tau = 1$; (b) $\tau = 0.5$.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure6.png}
\caption{Evolution of the maximum error on the $K = 20$ first hydroelastic modes between the two approaches in function of the number of dry modes. The added mass formulation with the full matrix is the reference.}
\end{figure}

A comparison between computational times is done for the fully filled cylinder $\tau$, considering various mesh parameterizations which increase the number of fluid degrees of freedom (see Tab. 1). Two computational times are considered:
• the time needed to compute $H_\ast^{-1}$;
• the time needed to solve $N$ linear system form Eq. (8).

<table>
<thead>
<tr>
<th>$(n_\theta,n_\ell)$</th>
<th>(5, 5)</th>
<th>(10, 10)</th>
<th>(15, 15)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n_{\text{elem-s}}$ (structure)</td>
<td>100</td>
<td>400</td>
<td>900</td>
</tr>
<tr>
<td>$n_{\text{elem-f}}$ (fluid)</td>
<td>500</td>
<td>2600</td>
<td>6975</td>
</tr>
<tr>
<td>$n_{\text{dof-s}}$ (structure)</td>
<td>2100</td>
<td>8400</td>
<td>18900</td>
</tr>
<tr>
<td>$n_{\text{dof-f}}$ (fluid)</td>
<td>2260</td>
<td>11020</td>
<td>29280</td>
</tr>
</tbody>
</table>

Table 1: Number of elements and number of degrees of freedom for the structure and the fluid in function of the mesh parameterization

In Fig. 7, two graphs are proposed (one for $N = 20$ and the other for $N = 150$) in which the computational time is plotted in function of the number of degrees of freedom on the fluid.

![Figure 7](image)

**Figure 7**: Computational time in function of the number of pressure degrees of freedom (in red a matrix inversion is computed, in blue $N$ linear system is computed one by one and in dashed blue line $N$ linear system is done in parallel with 12 cores).

• As expected, if the number of degrees of freedom is to high, the computation time needed to inverse the matrix is prohibitive (more than 2000 second for 29280 fluid degrees of freedom);
In the proposed approach with the projection on dry modes, $N$ linear system of equations are computed. Except for very coarse systems, the computational time of the projection on dry modes is lower than the matrix inversion (it depend on the fluid degree of freedoms and the number $N$ of linear system). Even if those systems can be solved in parallel, among the $N$ contributions, it seems that only a few of them contributes to the convergence. The number of linear systems could be even more reduced.

### 4.2 Validation with prestressed effects

The projection on prestressed dry mode have been performed in a clamped elastic bottom based on an experiment done in [2]. The problem consists in computing the hydroelastic angular frequencies of the prestressed elastic circular plate in function of the fluid height. Geometrical nonlinearities are taken into account and have been computed before the dynamic analysis. The geometrical and mesh parameters are exposed in Fig. 8. The material parameters are $E = 5.47 \times 10^9$, $\nu = 0.38$, $\rho_s = 1.4 \times 10^3$ kg/m$^3$ and $\rho_f = 1.0 \times 10^3$ kg/m$^3$.

![Figure 8](image)

**Figure 8:** (a) Geometrical parameterization of the elastic bottom submitted by an hydrostatic pressure of a fluid column of height $h$ with $R_{int} = 0.144$ m and $t = 0.35$ mm; (b) Mesh parameterization, with 20 hexaedral elements, used for the computation of the hydroelastic angular frequencies with $n_r = 10$, $n_t = 10$, $n_\theta = 10$, $n_t = 2$.

In Fig. 9, the evolution of natural angular hydroelastic frequencies are plotted between 0 and 80 Hz in function of the fluid height $h \in [0, 250]$ mm and $dh = 5$.

- 50 hydroelastic reduced eigenvalues problems have been computed by using the projection of prestressed dry modes in 1 hour;
- For each fluid height, the first $N = 25$ dry modes have been selected;
Except for the first modes, the angular natural frequencies decrease, then increase when the fluid height increase in the given fluid height range;

Very good agreements with the experiment is observed, compared to the literature;

One computation of the hydroelastic angular frequencies, for a given fluid height, with the full inversion of the added mass matrix takes more than $3h$ for the same mesh parameterization.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{figure9}
\caption{Evolution of the angular natural hydroelastic frequencies in function of the fluid height with $h \in [0,250]$ mm and $dh = 5$.}
\end{figure}

5 CONCLUSIONS AND OUTLOOKS

In this paper, the computation of the linearized prestressed hydroelastic behaviour of partially filled elastic tanks have been proposed. The numerical estimation, done with the finite element method, of the prestressed effects on the fluid-structure dynamic analysis has been addressed. A methodology based on the projection of the fluid-structure problem on the structural prestressed dry modes is detailed in a discrete framework. It is shown that for a given number of hydroelastic modes, the proposed approach converges to a full
hydroelastic formulation, without computing any full matrix inverse. Consequently, the computational time is reduced. Two numerical examples are treated, one with prestressed effects and one without. Both results shows the effectiveness of the projection on a dry mode basis. Further developments are expected in the future such as the use of the approach on much more complex structures and the selection of a minimum number of dry modes needed to minimize the number of linear system that has to be solved.

REFERENCES


COUPLED RADIATIVE AND CONVECTIVE HEAT LOSSES FROM PRETERM INFANT INSIDE AN INCUBATOR WITH RADIANT HEATERS

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Key words: Preterm neonate, Infant incubator, Convection heat transfer, Radiation heat transfer, Thermal comfort.

Abstract. Preterm infants face difficulties in maintaining their body temperature due to low metabolic rates of heat generation. Therefore, using incubators and radiant warmers is crucial for their comfort and health. The objective of the present work is to analyze the heat transfer processes for a preterm infant nursed in a simplified incubator under two different operating conditions: in the first one a classical simple incubator is considered and in the second case radiant heaters are used. This is achieved by using ANSYS Fluent 19.0 which his based on the finite volume method to discretize the Navier-Stokes, energy and radiation transfer equations. Conduction, convection and radiation heat transfer modes are modelled in the simulations and coupled to empirical correlations for metabolic heat generation and evaporative heat losses. The different incubator scenarios considered here are compared in terms of convection and radiation heat losses and skin temperature to access the thermal comfort of the preterm infant.

1 INTRODUCTION

In 2010, 11.1% of babies were born premature [1]. These babies face difficulties keeping a controlled body temperature without external assistance. Consequently, they can suffer from cold stress and hypothermia. Therefore, it is crucial to maintain an optimal thermal and humidity environment of the neonate by using incubators.

Infant incubators are essential tools to provide thermal comfort for neonates especially
premature and sick infants. The complex heat transfer process in these systems combines convection, conduction, thermal radiation and evaporation. Incubators are used since 1860 in order to maintain an optimal thermal environment for the neonate [2].

Several studies were conducted in the open literature to evaluate the dry and latent heat losses from neonates nursed inside incubators. These studies are classified in three main categories, theoretical bioheat modeling, numerical and experimental.

Bioheat modeling and thermoregulation are based on mathematical models in order to analyze the bioheat transfer in the neonate body and to determine its thermal responses to ambient conditions [3–5].

Numerical simulations of heat losses from neonate use the computational fluid dynamics (CFD) method. The aim of this method is to optimize existing devices and to design new techniques aiming to enhance the thermal comfort of neonates inside the incubators [6–8].

Experimental study are performed on cohort of human neonates or thermal manikins in order to evaluate convection, radiation and evaporation heat transfer coefficients and thermal balance in preterm neonates [9–12].

The aim of the present paper is to perform numerical simulations of the coupled convective and radiative heat transfer in infant incubators under two different conditions. The first case the incubator walls are at mean radiant temperature while in the second case, the incubator walls are assumed to radiate heat at a given heat flux so that to reduce radiation heat losses from the infant skin.

2 COMPUTATIONAL DOMAIN AND BOUNDARY CONDITIONS

An anthropomorphic 3D model representing a preterm neonate is used in the present study. Its dimensions correspond to a preterm with 35 week of gestational age in 50th percentile having a mass of 2.3 kg [13,14]. The neonate is shown in Figure 1 and it has a surface area of 0.133 m² and a body length of 45 cm. The neonate 3D model was built using the SolidWorks CAD software and imported to ANSYS Space Claim in which further modifications are performed. The infant is then inserted in a simplified incubator 25 cm in width, 20 cm in height and 60 cm in length. The incubator has one inlet and one outlet both located at the mattress level as shown in the figure below. The air stream entering the incubator has a speed of 0.2 m/s and a temperature of 38°C. The outlet is assumed at atmospheric pressure. No slip boundary conditions are imposed on all solid surfaces.

To mimic metabolic heat generation, a constant heat flow is imposed on the outer surface of the model according to the empirical equation obtained by Bruck [15] which depends on the infant mass \( m_{inf} \) and age in days \( t_{inf} \) (Eq. (1)). Therefore, for the present simulations the surface heat flow is fixed to 4.23 W.

\[
q_m = m_{inf}(0.0522t_{inf} + 1.64) \tag{1}
\]

The thermal emissivity of the neonate surface is assumed 0.95 [10] and the mean radiant temperature of surrounding surfaces is obtained from empirical correlation obtained by Decima et al. [16] and depending on the air temperature \( T_a \) as given below:

\[
T_r = 0.724(T_a - 31.93) + 29 \tag{2}
\]

Moreover, evaporative heat loss from the skin are obtained from Lyon and Oxley [17] and it depends on the surface area of the neonate and humidity inside the incubator which was
assumed equal 70%. Thus the resulting evaporative cooling is 1.25 W.

Two different cases are studied in this paper. In the first one all surfaces surrounding the baby (mattress and incubator walls) are assumed at standard radiant temperature obtained from Eq. (2). In the second case, radiant heating elements are used and thus the incubator walls are now assumed to radiate heat at an average heat flux of 0.55 W/m².

3 NUMERICAL METHOD

A non-uniform polyhedral mesh is used in the present study with 4 prism layers refined near the neonate skin surface. The total number of elements is around 840,000 cells. A mesh sensitivity analysis was conducted prior to choosing this mesh density in order to verify mesh convergence. The criteria for the mesh convergence are the surface temperature and total surface heat flux. Navier-Stoke and energy equations for laminar flow are using ANSYS Fluent 19.0 which based on the cell centered finite volume method. Second order double precision numerical schemes are used for diffusive and convective terms and Coupled model is adopted for velocity-pressure coupling. The buoyancy effects are included by using the Boussinesq approximation for air density. Radiation heat transfer is computed using the Discrete Ordinates Method which solves the radiative transfer equation for a finite number of discrete solid angles.

The energy equation for heat losses from preterm infants is given below:

\[ q_m - q_{evaporation} = q_{convection} + q_{radiation} + q_{conduction} \]  

The two terms on the left hand side are obtained from empirical equations as discussed previously while the terms on the right hand side are computed. For both cases studied in this paper, conduction heat transfer was very small relative to the other modes of heat losses. Thus we will focus on convective and radiative heat losses and their effects on the neonate skin temperature in the next section.

4 RESULTS

Figure 1 shows the heat rates from the infant nursed inside the incubator for both studied
cases. The metabolic heat generation is lost through latent heat by evaporation which is the same for both cases since it was obtained using empirical correlation.

Meanwhile, radiation heat losses from the neonate are reduced due to the addition of radiant heaters. These radiant heaters will lead also to a slight decrease in conduction heat losses since the mattress temperature will increase. However, convective heat losses have increased since as will be seen next, the skin temperature exceeds the surrounding air leading to higher convective heat loss. However, the overall impact is beneficial since the thermal comfort is enhanced from skin temperature point of view.

![Figure 2: Heat losses from the infant skin for both studied cases](image)

The skin temperature distribution is shown in Figure 3 for both cases. For the case without radiant heaters, the average skin temperature is around 35°C which is smaller than the comfort temperature at 37°C. The temperature is increased by addition of radiant heaters and its average value reaches around 37°C leading to better thermal comfort when compared to the reference case without radiant heaters.
5 CONCLUSION

In this study, convective and radiative heat losses from preterm infant nursed inside an incubator are studied under two different conditions. In the first case, a simplified classical incubator is used, while, in the second case radiant heaters are added. The incubator walls are modeled thus as radiant heaters with imposed heat flux.

The flow and heat transfer are computed using ANSYS Fluent 19.0 which is based on the finite volume method. A polyhedral mesh and second order numerical schemes are adopted for the simulations.

The results show a decrease of radiation heat loss when adding radiant elements with a slight increase in convective heat loss. Moreover, the average skin temperature of the neonate was increased from 35°C to 37°C proving the benefits of these radiant heaters.

In future studies we will use experimental method for a preterm thermal manikin nursed inside a CALEO incubator to validate our numerical simulations.

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REFERENCES


DEVELOPMENT OF A PREDICTION METHOD FOR SOUND CONDUCTION EFFICIENCY OF THE HUMAN MIDDLE EAR – APPLICATION TO TYPE IV OPERATION –

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Key words: Geometric Model, FEM, Vibration Analysis, Human Middle Ear, Auditory Ossicles, Hearing Ability.

Abstract. When the human middle ear is damaged by various ear diseases, the linkage of the auditory ossicles may be reconstructed using the column article called the columella. In a tympanoplasty operation, the sound conduction efficiency changes according to differences in shape, material and the mounting position of the columella. We have proposed a new method for estimating the hearing restoration effect prior to the operation. In this method, a geometric model of the middle ear is constructed using SolidWorks based on CT scanning data. Frequency response characteristics of the stapes displacement in sound conduction are calculated using harmonic vibration analysis. The hearing restoration effect can be estimated by a comparison of differences in the stapes displacement between the reconstruction model and a healthy subject. In the case in which the stapes remains in a normal shape, including the horseshoe portion, the type III operation is performed. In the case in which only the basal plane of the stapes is left, the type IV operation is performed. With the type IV operation, it is more difficult to improve hearing ability than with the type III operation. In the type III model, various verifications have been carried out on the validity of our prediction method. In this study, the validity of our method is verified for the type IV model. On the other hand, the audiogram is made by precise audiometry in the medical field. The audiogram is the record of the value of hearing level at every frequency in the hearing test. Using our proposed calculation formula, the audiogram of the type IV operation model was made. The degree of hearing amelioration can also be evaluated quantitatively in the type IV model prior to an operation. Through this study, the optimization of reconstruction of the middle ear using the columella becomes possible.
1 INTRODUCTION

The human auditory organ is composed of the external, middle and inner ears. The sound collected in the pinna is transmitted to the tympanic membrane through the ear canal. The acoustic wave vibration which the tympanic membrane receives is transmitted to auditory ossicles. The stapes vibration is transmitted to the labyrinthine fluid in the cochlea where electrical signals are generated. Finally, it is recognized in the brain as sound.

When the middle ear is damaged by various ear diseases, the linkage of the auditory ossicles is reconstructed using a medical device called a columella. This is called ‘tympanoplasty’ or auditory ossicles reconstructive surgery. In this operation, the sound conduction efficiency changes due to the difference between shape, material and the mounting position of the columella. Actually, the operation is carried out based on workmanship and experience of the doctor.

In our previous research [1,2,3], a geometric model of the middle ear on the basis of the computerized tomography (CT) scan data was constructed. Several kinds of tympanoplasty models for a middle ear damaged by chronic otitis media have been constructed and analyzed. Frequency response characteristics of the stapes displacement in sound conduction are clarified using three-dimensional finite element harmonic vibration analysis. Based on our previous research, we have proposed that the hearing restoration effect can be estimated by a comparison of the stapes displacement with the result for a healthy subject as a standard, prior to the operation.

In the case in which the stapes remains in a normal shape, including the horseshoe, the type III operation is performed [4]. In the case in which only the basal plane of the stapes is left, the type IV operation is performed [4]. With the type IV operation, it is more difficult to improve hearing ability than with the type III operation. In the type III model, various verifications have been carried out on the validity of our prediction method. In this study, the validity of our method is verified for the type IV model.

In this research, the harmonic vibration analysis result of a healthy subject is shown at first. Next, the case in which a column article of the columella is substituted for the deficient auditory ossicles is analysed. The results for type III and type IV operation models in which mounting positions of the columella are umbilical and intermediate parts of the malleus are shown. Furthermore, the correlation of hearing restoration effect and the columella volume is examined in the type IV operation model.

In the medical field, the audiogram is made by precise audiometry, and the degree of improvement of hearing ability is evaluated in pre- and post-operation. The audiogram is the record of the value of hearing level or minimum audible threshold at every frequency in the hearing test. A calculation formula which is able to obtain hearing level from the stapes displacement using the finite element analysis was devised. The degree of hearing amelioration can be evaluated quantitatively by this formula. In this study, our proposed method is applied to the type IV operation models, and its validity is discussed. Through this study, the optimization of reconstruction of the middle ear using the columella becomes possible. Finally, the efficacy of predicting the hearing restoration effect prior to an operation is clarified.
2 EAR STRUCTURE AND FUNCTIONS

The ear is the organ that controls the sense of hearing and human body balance. The ear is composed of external, middle and inner parts as shown in Figure 1. The external ear is composed of the pinna, ear canal and tympanic membrane. The function of the pinna is to collect sonic reflections, and the function of the ear canal is as a resonance tube.

The middle ear as shown in Figure 2 is composed of auditory ossicles and the auditory tube which connects with the hole of the nose. Auditory ossicles behind the tympanic membrane are in a small space (tympanic cavity) filled with air, and they connect the tympanic membrane with the cochlea of the inner ear. The vibration of the tympanic membrane is amplified by the auditory ossicles and transmitted to the inner ear.

The inner ear is composed of the cochlea and semicircular canal. In the inner ear, the vibration induced by auditory ossicles is transmitted to the labyrinthine fluid which converts it to electric signals. Finally, it is recognized in the brain as sound.

![Figure 1: Ear structure](image1)

![Figure 2: Middle ear structure](image2)
3 HARMONIC VIBRATION ANALYSIS OF THE MIDDLE EAR

3.1 Geometric model of a healthy subject

The geometric model for a healthy subject for finite element harmonic vibration analysis is shown in Figure 3. This model is composed of the tympanic membrane, auditory ossicles, ligaments, joints, stapedial muscle and others. These parts’ names are shown in Table 1. In order to construct a geometric model, the region which contains those ear parts was separated from the CT scanning data of the human head. These CT scanning data were converted to DICOM data, and in addition, converted into STL data which were imported into SolidWorks.

Table 1: Material data

<table>
<thead>
<tr>
<th>Anatomical parts’ name</th>
<th>Young’s Modulus [MPa]</th>
<th>Density [kg/m³]</th>
<th>Poisson's ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>① Tympanic membrane</td>
<td>33.4</td>
<td>1,200</td>
<td></td>
</tr>
<tr>
<td>② Malleus</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>③ Incus</td>
<td>13,436</td>
<td>4,350</td>
<td></td>
</tr>
<tr>
<td>④ Stapes</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>⑤ Lateral malleolar ligament</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>⑥ Superior malleolar ligament</td>
<td>21</td>
<td>2,500</td>
<td>0.3</td>
</tr>
<tr>
<td>⑦ Anterior malleolar ligament</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>⑧ Posterior incudal ligament</td>
<td>0.65</td>
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</tr>
<tr>
<td>⑨ Superior incudal ligament</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>⑩ Stapedial annular ligament</td>
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<td></td>
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</tr>
<tr>
<td>⑪ Incudostapedial joint</td>
<td>6</td>
<td>1,200</td>
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</tr>
<tr>
<td>⑫ Incudomalleolar joint</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>⑬ Stapedial muscle</td>
<td>0.52</td>
<td>2,500</td>
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</tr>
<tr>
<td>⑭ Base plate</td>
<td>$1 \times 10^{10}$</td>
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</tr>
</tbody>
</table>
3.2 Material data

Material data of the analysis model are shown in Table 1 [5,6,7]. The anatomical parts’ number in the table corresponds to the number in Figure 3. The base plate ⑭ is a virtual part for supporting the spring which simulates cochlea labyrinthine fluid. Therefore, its Young’s modulus can be assumed to be that of a rigid body.

3.3 Boundary conditions

The circumference of tympanic membrane, edges of ligament and muscle, and base plate were perfectly fixed in constraint conditions. A sound pressure of 90dB was converted into pressure using the equation (1) as load conditions.

\[ L_p = 20 \log_{10} \left( \frac{p}{P_0} \right) \]  

In equation (1), \( L_p = 90 \) dB is the setting sound pressure (a relative noisy level) and \( P_0 = 20 \times 10^{-6} \) Pa is a standard value (the lowest value of the sound intensity which is audible for humans). As a result, a pressure of \( P = 0.632 \) Pa was obtained. However, in this analysis, \( P = 15.2 \) Pa was given at the contact surface of the tympanic membrane and malleus. The ratio 15.2/0.632 equals the ratio of the total area of the tympanic membrane to the contact surface area of the tympanic membrane and malleus. A spring of 40N/m spring constant was installed between the stapes and the base plate referring to the research of Gan et al [8]. Rayleigh damping was assumed and damping factors of \( \alpha = 0 \) s\(^{-1}\) and \( \beta = 7.5 \times 10^{-5} \) s were adopted.

3.4 Finite element analysis results

In this research, harmonic vibration analysis was performed as a dynamic analysis using the finite element method. Figure 4 shows the harmonic vibration analysis results for a healthy subject. The longitudinal axis shows the average displacement of the stapes bottom in a perpendicular direction to the basal plane, and the lateral axis represents the frequency. The average displacement of the stapes base for the sound pressure of 90dB is \( 5.0 \times 10^{-6} \) mm, which was used as a standard value in this model. In the case where the medical device, called the columella, is substituted for the deficient auditory ossicles, if the stapes displacement is compared with that of a healthy subject, the hearing restoration effect can be estimated.

An example of the type III tympanoplasty model [4] is shown in Figure 5. Figure 5 (a) shows the model in which the columella is attached at the umbilical region, that is, the tip of the malleus. Its analysis result of the frequency response graph of the stapes bottom is shown in Figure 4. The value of the maximum displacement is 4.7 nm at about 1.5 kHz of frequency. This displacement of 4.7 nm is about 94% of the healthy subject. This means that hearing ability recovers to a normal level. For another example, the model in which the columella is attached at the intermediate region, that is, between the tip of the malleus and the short process of the malleus, is shown in Figure 5 (b). Analysis results are shown in Figure 4. In this case, the value of the maximum displacement is 4.4 nm which is about 88% for the healthy subject. This means that hearing ability recovers to an almost normal level.
Figure 4: Frequency response graphs of a healthy subject and the tympanoplasty models

Figure 5: Examples of the type III tympanoplasty model

(a) Umbilical connection model
(b) Intermediate connection model

Figure 6: Example of the type IV tympanoplasty model

(a) Umbilical connection model
(b) Intermediate connection model
An example of the type IV tympanoplasty model [4] is shown in Figure 6. Figure 6 (a) shows the model in which the columella is attached at the umbilical region. The analysis result of the frequency response graph of the stapes bottom is shown in Figure 4. The value of the maximum displacement is 3.01 nm at about 1.5 kHz of frequency. This displacement of 3.01 nm is about 60% of the healthy subject. This means that hearing ability recovers to more than half of a normal level. For another example, the model in which the columella is attached between the intermediate region is shown in Figure 6 (b). Analysis result is shown in Figure 4. In this case, the value of the maximum displacement is 2.79 nm which is about 56% of the healthy subject. This means that hearing ability recovers to about half of the normal level.

By comparing the stapes displacement of the tympanoplasty model with the healthy type, it becomes possible to estimate the restoration ratio, not only in the type III operation but also in the type IV operation. The validity of our proposal has been verified by harmonic vibration analysis.

4 INFLUENCE OF COLUMELLA VOLUME ON SOUND CONDUCTION

4.1 Geometric model

As a part of the optimum design, the correlation of hearing restoration effect and the columella volume has been examined in the type III operation model [10]. In this research, the type IV operation models in which the columella volume is different are examined. The standard model is shown in Figure 7 (a). The additional models are twice and three times the volume of the standard model as shown in Figure 7 (b) and (c). In the analysis of these models, only the size of the columella width was changed.

![Geometric models varying in the volume of columella](image)

Figure 7: Geometric models varying in the volume of columella

4.2 Finite element analysis results

In this research, harmonic vibration analysis was performed as a dynamic analysis using the finite element method. The material data of Figure 7 are the same as Table 1 and the boundary conditions of this model are the same as the conditions described in section 3.3. Figure 8 shows the harmonic vibration analysis results of three models varying in the volume of the columella.

In Figure 8, the longitudinal axis shows the average displacement of the stapes basal plane, and the lateral axis represents the frequency. The solid line is the result for the standard model.
The dashed line is the result for the model where the volume of the columella is 2 times that of the standard model. The dotted line is the result for the model where the volume of the columella is 3 times that of the standard model. Figure 8 shows that the displacement of the stapes base plane increases gradually with an increase in the volume of the columella. By increasing the columella volume, it is possible to more firmly connect the columella on the malleus or stapes. Therefore, it appears to improve the transfer efficiency of sound.

Figure 8: Comparison of frequency response graphs

5 OTOSCLEROSIS MODEL AND EVALUATION OF HEARING ABILITY

5.1 Geometric model for otosclerosis

In otosclerosis, abnormal bone growth occurs around the stapes. For this reason, stapes usually stiffen and conductive hearing loss occurs as one symptom of otosclerosis. In order to reproduce the severe hardening of stapes, a model where the Young’s modulus of a whole annular ligament increased 100 times that of the healthy subject, 0.65 MPa, was made [2]. This model is shown in 9 (a).
In otosclerosis operation, the upper horseshoe part of the stiffened stapes is removed, and a small open window is made in the stapes base plate. Then, a substitute stapes is attached to the hole. As a substitute for the stapes, a Teflon piston was used in this analysis. The operation model using the Teflon piston is shown in Figure 9 (b).

5.2 Materia data

The Teflon piston is composed of the main part and the joint. Teflon (PTFE) was used for the main body, and cartilage for the joint. Material data for Teflon piston is shown in Table 2. Material data for the joint is the same as the value of in Table 1. Other materials are shown in Figure 3 and Table 1.

<table>
<thead>
<tr>
<th>Anatomical parts’ name</th>
<th>Young's Modulus [MPa]</th>
<th>Density [kg/m³]</th>
<th>Poisson's ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stapedial annular ligament</td>
<td>65</td>
<td>2,500</td>
<td>0.3</td>
</tr>
<tr>
<td>Teflon piston (PTFE)</td>
<td>500</td>
<td>2,165</td>
<td>0.46</td>
</tr>
</tbody>
</table>

5.3 Finite element analysis results

In this research, harmonic vibration analysis was performed as a dynamic analysis using the finite element method. Boundary conditions in the analysis models of Figure 9 are the same as the conditions described in section 3.3. Figure 10 shows the harmonic vibration analysis results. The solid line is the result for a healthy subject. The dashed line is the annular ligament hardening model in which the Young’s modulus was increased to 100 times that of the healthy subject due to otosclerosis. The dotted line is the result of the operation model using an artificial Teflon piston as the stapes.

![Figure 10: Comparison of frequency response graphs](image-url)
The operation model is about 2.26 nm in the displacement of the substitute stapes at the resonant frequency. The maximum displacement is lower by about 38% in comparison with the healthy subject (3.66 nanometer, in this model). However, this is greater than the result in which the Young’s modulus of the annular ligament is the strongly hardened model.

5.4 Evaluation of hearing ability

In the medical field, the audiogram is made by precise audiometry, and the degree of improvement of hearing ability is evaluated in pre- and post-operation. The audiogram is the record of the value of hearing level or minimum audible threshold at every frequency in the hearing test. A calculation formula which is able to obtain hearing level from the stapes displacement using the finite element analysis was devised as follows.

\[
L_{HL} = 20 \log_{10} (\delta_0 / \delta)
\]  

In equation (2), \(L_{HL}\) is the hearing level that shows the minimum audible threshold (\(L_{HL} = 0\) [dB], for a healthy subject). \(\delta_0\) is the stapes displacement for a healthy subject and \(\delta\) is the stapes displacement for a patient. The degree of hearing amelioration can be evaluated quantitatively by this formula. In this study, our proposed method is applied to operation models for otosclerosis, and its validity is discussed.

The hearing level which was calculated by equation (2) using the results of Figure 10 is shown in Table 3. Results of Moriyama et al. [9] in Table 3 show the mean value of audiometry results which was carried out in pre- and post-operation for 16 otosclerosis patients. Figure 11 shows the audiogram made by using the result of Table 3. Our pre-operation results correspond to the result of the annular ligament hardening model (dashed line) and our post-operation results correspond to the result of the operation model using an artificial Teflon piston (solid line).

<table>
<thead>
<tr>
<th>Frequency [Hz]</th>
<th>Measured result by Moriyama et al. [dB]</th>
<th>Our analysis result [dB]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Pre-operation</td>
<td>Post-operation</td>
</tr>
<tr>
<td>250</td>
<td>48</td>
<td>15</td>
</tr>
<tr>
<td>500</td>
<td>39</td>
<td>8</td>
</tr>
<tr>
<td>1000</td>
<td>35</td>
<td>6</td>
</tr>
<tr>
<td>2000</td>
<td>25</td>
<td>5</td>
</tr>
<tr>
<td>4000</td>
<td>25</td>
<td>6</td>
</tr>
<tr>
<td>Mean hearing level</td>
<td>33.5</td>
<td>6.25</td>
</tr>
</tbody>
</table>

A decrease in hearing acuity in lower frequencies appears for the result of Moriyama et al. On the other hand, this phenomenon is not seen for the model in which the Young’s modulus
of an annular ligament increased. Therefore, this model has not exactly reproduced the otosclerosis. Though some differences are observed in our analytical results and experimental results of Moriyama et al., both results are quite similar. It seems possible to reproduce the audiogram using our method.

![Comparison of audiogram](image.png)

The mean hearing level of Table 3 is a value calculated according to the following equation used in audiometry:

$$L_{MHL} = \frac{H_{500} + 2H_{1000} + H_{2000}}{4}$$

(3)

In equation (3), $L_{MHL}$ is mean hearing level, $H_{500}$ is minimum audible threshold at 500Hz, $H_{1000}$ is minimum audible threshold at 1000Hz and $H_{2000}$ is minimum audible threshold at 2000Hz. If the difference in mean hearing level between pre- and post-operation is regarded as improvement rate, our result becomes almost 100% of the experimental result.

The hearing restoration effect can be estimated quantitatively prior to the operation using our proposal method. Through this study, the optimization of the reconstruction of the middle ear using the columella becomes possible.

6 CONCLUSIONS

We have proposed that the hearing restoration effect can be estimated by comparison of the displacement of the stapes basal plane quantitatively prior to the operation. In order to verify this proposal, various types of operation models, especially the type IV operation model in addition to the type III operation model, were analyzed using harmonic vibration analysis and compared with a healthy subject. Furthermore, the production method of the audiogram, that is, the record of minimum audible threshold using finite element analytical results was applied to the type IV operation model. As a result, the following knowledge was obtained.

(1) We have analyzed the effect of mounting positions of the columella in type III and type IV operation models. It was shown that the maximum hearing restoration rate in type III and type IV operation models was about 94% and 60% respectively. With the type IV operation, it is more difficult to improve hearing ability than with the type III operation.
(2) In the type IV operation model, the correlation of hearing restoration effect and the columella volume was examined. It was clarified that the hearing restoration effect increased with an increase in the columella volume as shown in the type III operation model too.

(3) The calculation formula which is able to produce an audiogram from stapes displacement was devised and applied to the artificial stapes model for otosclerosis treatment which is considered as a kind of type IV operation. The degree of hearing amelioration can be evaluated quantitatively by this method for not only the type III model but also the type IV model.

(4) Through this study, the optimization of reconstruction of the middle ear using the columella becomes possible. Finally, the efficacy of predicting the hearing restoration effect prior to an operation was verified.

REFERENCES


COMBINING A LEAST-SQUARES APPROXIMATE JACOBIAN WITH AN ANALYTICAL MODEL TO COUPLE A FLOW SOLVER WITH FREE SURFACE POSITION UPDATES

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Key words: Free Surface Flow, Quasi-Newton, Fitting Method, Surrogate Model

Abstract. This paper presents a new quasi-Newton method suitable for systems that can be solved with a black-box solver for which a cheap surrogate model is available. In order to have fast convergence, the approximate Jacobian consists of two different contributions: a full rank surrogate model of the system is combined with a low rank least-squares model based on known input-output pairs of the system. It is then shown how this method can be used to solve 2D steady free surface flows with a black-box flow solver. The inviscid flow over a ramp is calculated for supercritical and subcritical conditions. For both simulations the quasi-Newton iterations converge exponentially and the results match the analytical predictions accurately.

1 INTRODUCTION

Quasi-Newton methods can be used to solve coupled problems in a partitioned way, using existing solvers for each system. A common application is fluid-structure interaction. In this paper, a new approach is presented to construct the approximate Jacobian of a (non-linear) system that can be solved with a black-box for which also a cheap surrogate model is available. To reduce the number of quasi-Newton iterations, two approximations are added: a full rank surrogate model of the system is combined with a low rank model which is constructed with known input-output pairs of the system using a least-squares technique.

The method was developed in [1] for numerically calculating 2D steady free surface flow of water and air as encountered in marine engineering. The free surface is represented...
with a fitting approach, i.e. the computational grid is aligned with it. As the air phase can be neglected for the envisioned flows, the free surface becomes a domain boundary whose position depends on kinematic and dynamic boundary conditions. Both the flow field and the free surface position are unknown, so that this free-boundary problem must be solved iteratively. This is done by reformulating the problem as a root-finding problem and solving it with the new quasi-Newton approach.

In Section 2 the new method to construct the approximate Jacobian is explained for a general system. The method is applied to the steady free surface problem in Section 3: first some details are given about the surrogate model for the flow solver, then the free-boundary problem is given in more detail and a solution method derived based on quasi-Newton iterations. In Section 4 the performance of the method is demonstrated by calculating the inviscid free surface flow over a ramp at different Froude numbers.

2 QUASI-NEWTON METHOD WITH LEAST-SQUARES AND SURROGATE

A general black-box system \( S(x) = y \) is considered, with \( x, y \in \mathbb{R}^{n \times 1} \) respectively the input and output of \( S \). The input vector \( x \) for which \( S(x) = 0 \) (i.e. the root of \( S \)) can be found using quasi-Newton iterations. With superscript \( m \) the iteration index, \( \Delta x^m = x^{m+1} - x^m \) the change in input, and \( J \in \mathbb{R}^{n \times n} \) an approximate Jacobian of \( S \), a new value \( x^{m+1} \) can be calculated using the well-known formula

\[
J \Delta x^m = -y^m = -S(x^m). \tag{1}
\]

The iterations start with a guess \( x^0 \) and continue until \( \|y^m\| \) drops below a small constant \( \varepsilon \). It is assumed that \( S \) is expensive to evaluate, so the number of quasi-Newton iterations must be as low as possible. For this purpose a Jacobian is constructed that consists of two parts which both have advantages and limitations. By combining them, a more robust and effective Jacobian is obtained.

The first approximation is a full rank surrogate model \( J_{\text{sur}} \). It can be based on e.g. analytical considerations or a low fidelity model of the system, depending on the problem at hand. It must be of full rank to ensure that Eq. 1 has a unique solution \( \Delta x^m \). The better \( J_{\text{sur}} \) approximates the behavior of \( S \), the faster the quasi-Newton iterations will converge. However, if the prediction of \( J_{\text{sur}} \) is inaccurate for certain modes, these modes will slow down or even destabilize the iterations.

The second approximation \( J_{\text{IQN}} \) is constructed using the IQN-ILS algorithm by Degroote et al. [2], which was developed originally for doing partitioned fluid-structure interaction with black-box solvers. \( J_{\text{IQN}} \) is a low rank approximation which is built from known input-output pairs of the system. Inputs and outputs of previous iterations are collected in the matrices

\[
V^m = [\Delta x^{m-1} \ldots \Delta x^0], \tag{2}
\]
\[
W^m = [\Delta y^{m-1} \ldots \Delta y^0]. \tag{3}
\]
The Jacobian is then constructed with a least-squares technique:

\[ J^m_{\text{IQN}} = W^m R^{m-1} Q^m T \]  \hspace{1cm} (4)

with

\[ V^m = Q^m R^m \]  \hspace{1cm} (5)

the economy-size QR-decomposition. With each iteration \( J^m_{\text{IQN}} \) grows in rank and improves. The modes which are picked up by \( J_{\text{IQN}} \) are those that hinder convergence of the quasi-Newton iterations, which are precisely those modes for which \( J_{\text{sur}} \) is inaccurate.

\( J^m_{\text{IQN}} \) only affects the part of \( x \) which is in range(\( V^m \)) = range(\( Q^m \)). As these modes can be extracted using \( Q^m Q^m T \), the combined Jacobian can be written as

\[ J^m = J^m_{\text{IQN}} + J_{\text{sur}} (I_n - Q^m Q^m T) \]  \hspace{1cm} (6)

with \( I_n \) the identity matrix. In a nutshell: most of the work is done by the full rank surrogate model \( J_{\text{sur}} \), but the low rank least-squares based \( J_{\text{IQN}} \) is crucial to stabilize and accelerate convergence of the iterations when \( J_{\text{sur}} \) is inaccurate for some modes. The method is accordingly called Quasi-Newton method with Least-Squares and Surrogate and an overview of it is given in Algorithm 1.

**Algorithm 1** Quasi-Newton method with Least-Squares and Surrogate.

1: \( m = 0 \)
2: \( y^0 = S(x^0) \)
3: while \( \|y^m\| > \varepsilon \) do
4: \quad if \( m > 0 \) then
5: \quad \quad update \( V^m, W^m \) \hspace{1cm} \( \triangleright \) Eqs. (2) and (3)
6: \quad \quad QR-decomposition \( V^m = Q^m R^m \)
7: \quad \quad end if
8: \quad construct \( J^m \) \hspace{1cm} \( \triangleright \) Eq. (6)
9: \quad solve \( J^m \Delta x^m = -y^m \)
10: \quad \( x^{m+1} = x^m + \Delta x^m \)
11: \quad \( m = m + 1 \)
12: \quad \( y^m = S(x^m) \)
13: end while

Note that if a surrogate model is available for the system’s inverse \( S^{-1} \), the quasi-Newton iteration of Eq. (1) can be rewritten as \( \Delta x^m = -J^{-1} y^m \), avoiding the need to solve a linear system. In addition the least-squares Jacobian \( J_{\text{IQN}}^{-1} \) does not have to be constructed explicitly, avoiding matrix-matrix products.
3 APPLICATION TO STEADY FREE SURFACE FLOW

Before the free-boundary problem is solved with the new quasi-Newton technique, a free surface perturbation analysis is discussed in Section 3.1. Not only does this analysis provide the basis for constructing the flow solver’s surrogate model, it also shows that additional conditions are needed to obtain a unique free surface solution for subcritical flows. In Section 3.2 the 2D steady free surface problem is discussed in more detail, then it is expressed as a free-boundary problem and finally a solution algorithm based on quasi-Newton iterations is outlined.

3.1 Surrogate model from perturbation analysis

In [3] the 2D inviscid free surface flow over a flat bottom is investigated in detail. This flow is characterized by its Froude number $\text{Fr} = \frac{U}{\sqrt{gh}}$ which is based on the average flow velocity $U$ and flow depth $h$. The steady flow solution of this case is a horizontal free surface and a uniform velocity $U$. It is shown in [3] that when the free surface height $\eta(x)$ is perturbed with a sine wave, the free surface pressure $p(x)$ changes proportionally. This analysis leads to a relation between free surface height perturbations $H(k)$ and pressure perturbations $P(k)$ in the wavenumber domain:

$$P(k) = L(k)H(k)$$  \hspace{1cm} (7)

with

$$L(k) = \rho g \left( \text{Fr}^2 \frac{kh}{\tanh kh} - 1 \right).$$  \hspace{1cm} (8)

Here $\rho$ is the density, $g$ the gravitational acceleration and $k = \frac{2\pi}{\lambda}$ the wavenumber. This relation between perturbations can be used to approximate the Jacobian of a general 2D free surface flow. An expression for $J_{\text{sur}}$ for uniform free surface grids is derived in [1] using the discrete Fourier transform. For stretched free surface grids $J_{\text{sur}}$ can be calculated using the convolution Fourier theorem as explained in [4].

The behavior of free surface flow changes at $\text{Fr} = 1$. For supercritical flow ($\text{Fr} > 1$), the wave speed of surface gravity waves is smaller than the flow speed $U$ for all wavenumbers so that disturbances can only travel downstream. For subcritical flow ($\text{Fr} < 1$) this is not the case: waves below a certain wavenumber travel faster than the flow, so disturbances can travel upstream. This change in behavior corresponds to a zero in $L(k)$, Eq. (8): the wave with this wavenumber travels at the same speed as the flow and thus appears stationary. This so-called steady gravity wave is a solution of the flow and therefore gives no change in pressure ($L = 0$). This is problematic: it means that for subcritical flow, this wave can be present with arbitrary phase and amplitude without influencing the free surface pressure. As a consequence, two additional conditions will need to be added to find a unique solution for the free-boundary problem.
3.2 Solving the free-boundary problem with quasi-Newton

The 2D immiscible steady flow of water and air as encountered in marine engineering is considered as application. The free surface is represented with a fitting approach, which means that the computational grid is aligned with it. Due to the large density difference with water, the air phase can be neglected for these flows. The free surface then becomes a domain boundary whose position depends on kinematic and dynamic boundary conditions. For steady flow, the kinematic boundary condition (KBC) requires that the flow is tangential to the free surface. The dynamic boundary condition (DBC) requires continuity of the stresses at the free surface. This condition can be split into tangential and normal components which can be simplified. To fulfill the tangential DBC the shear stresses at the free surface must be zero. For the normal DBC the pressure must be constant along the free surface.

The flow field and free surface position cannot be determined simultaneously by a standard CFD solver, so the free-boundary problem needs to be solved iteratively: in one step the flow field is solved with a given free surface position, in the other step a new free surface position is calculated. The distribution of the free surface boundary conditions over these two steps varies between different methods found in literature [5, 6, 7]. In this paper the conditions are distributed in such a way that the free-boundary problem becomes a root-finding problem. The black-box system of this problem is the flow solver $F$ which uses a free-slip wall at the free surface boundary—this way the KBC and tangential DBC are satisfied in the flow solver step. The input and output of $F$ are respectively the free surface height $\eta \in \mathbb{R}^{n \times 1}$ and the free surface pressure $p \in \mathbb{R}^{n \times 1}$, so that $p = F(\eta)$. The normal DBC requires that $p = p_{\text{cst}} \mathbf{1}$ with $\mathbf{1}$ the all-ones vector. This cannot yet be formulated as a root-finding problem as $p_{\text{cst}}$ is unknown. It follows from the perturbation analysis in Section 3.1 that changing the value of $p_{\text{cst}}$ corresponds to a change of the average free surface height. Instead of specifying $p_{\text{cst}}$ it is more convenient to impose e.g. the free surface inlet height $\eta(0) = h$ to fix the average free surface height. $p_{\text{cst}}$ is removed from the normal DBC by subtracting the average value (or constant mode) from the pressure. The flow solver $F$ and pressure $p$ after removing the average value are denoted as $F_\emptyset$ and $p_\emptyset$, so that the normal DBC becomes

\[ F_\emptyset(\eta) = p_\emptyset = 0. \]  

(9)

This is a root-finding problem for a black-box system $F_\emptyset$ with input $\eta$ and output $p_\emptyset$, which can be solved with quasi-Newton iterations. The inlet height condition must be added to the system for a unique solution. With $J^m$ the approximate Jacobian of $F_\emptyset$, the iterative scheme becomes:

\[
\begin{cases}
J^m \Delta \eta^m = -p_\emptyset^m \\
\Delta \eta^m(0) = h - \eta^m(0)
\end{cases}
\]  

(10)

This system has $n + 1$ equations for $n$ unknowns and must therefore be solved with least-squares. The system is still well-determined though, because the rank of $J$ is $n - 1$ due
to subtraction of the average value from \( p \).

In Section 3.1 it is explained that for subcritical flow two additional conditions need to be added to ensure that the free surface solution is unique. A physically relevant option is to require that the free surface is flat upstream. This is enforced by the conditions

\[ \eta(i) = h \quad \text{with} \quad i = i_1, i_2 \]  

(11)

where \( x(i_1) \) and \( x(i_2) \) are points close to the domain inlet \( x(0) \). Adding these conditions, the system that has to be solved in the quasi-Newton iterations becomes:

\[
\begin{aligned}
J^m \Delta \eta^m &= -p_0^m \\
\Delta \eta^m(i) &= h - \eta^m(i) \quad \text{with} \quad i = 0, i_1, i_2
\end{aligned}
\]  

(12)

The Free Surface Quasi-Newton method with Least-Squares and Surrogate (FreQ-LeSS) is summarized in Algorithm 2.

**Algorithm 2** Free Surface Quasi-Newton method with Least-Squares and Surrogate.

1: \( m = 0 \)
2: \( p_0^0 = \mathcal{F}_\emptyset(\eta^0) \)
3: while \( \| p_0^m \| > \varepsilon \) do
4: \quad if \( m > 0 \) then
5: \quad \quad update \( V^m, W^m \) \hspace{1cm} \triangleright \text{Eqs. (2) and (3)}
6: \quad \quad QR-decomposition \( V^m = Q^m R^m \)
7: \quad \quad end if
8: \quad construct \( J^m \) \hspace{1cm} \triangleright \text{Eq. (6)}
9: \quad solve system for \( \Delta \eta^m \) \hspace{1cm} \triangleright \text{Fr > 1: Eq. (10) | Fr < 1: Eq. (12)}
10: \quad \eta^{m+1} = \eta^m + \Delta \eta^m
11: \quad m = m + 1
12: \quad p_0^m = \mathcal{F}_\emptyset(\eta^m)
13: end while

4 INVISCID FREE SURFACE FLOW OVER A RAMP

The free surface method is demonstrated by calculating the inviscid free surface flow over a ramp as shown in Fig. 1, using the same geometry and flow parameters as Muzaferija and Perić [5]. The total mechanical energy \( E \) (in J/kg) is conserved between inlet and outlet of the domain. Assuming a uniform flow velocity in each section, it can be shown that

\[ E_i = \frac{U_i^2}{2} + gh_i + gy_{b,i} = \text{cst} \]  

(13)

with \( U_i \) the flow velocity, \( h_i \) the depth of the flow and \( y_{b,i} \) the vertical position of the bottom. Combining Eq. (13) with the continuity equation gives analytical expressions
for the outlet water depth $h_2$ and outlet velocity $U_2$ for known inlet conditions and ramp geometry.

Two cases are simulated: a supercritical and a subcritical flow. For both cases the ramp is 0.2 m high, $h_1 = 1$ m, density $\rho = 1$ kg/m$^3$ and gravity $g = 9.81$ m/s$^2$. The supercritical flow has $U_1 = 1$ m/s (Fr = 1.92), the subcritical flow $U_1 = 6$ m/s (Fr = 0.32). In the flow solver the bottom and free surface are modeled as free-slip walls. At the outlet a hydrostatic pressure is imposed, at the inlet a uniform velocity $U_1$. For both simulations, the initial free surface is horizontal and corresponds to the inlet height. Structured quadrilateral grids are used, with 100 cells in the y-direction and 50 cells per meter in the x-direction. As the free surface grid is uniform, $J_{\text{surf}}$ is constructed based on Eq. (8) and the discrete Fourier transform, as described in [1].

The free surface for both cases is shown in Fig 2. The supercritical free surface is a smooth curve, while the subcritical free surface has the characteristic wave train downstream of the obstacle. To avoid wave reflections at the outlet, a wave damping zone is
Table 1: Analytical result for outlet depth $h_2$ and error in numerical result.

<table>
<thead>
<tr>
<th>Fr</th>
<th>$h_2$ (analytical)</th>
<th>$h_2$ (numerical)</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.92</td>
<td>1.089730 m</td>
<td>-0.008%</td>
<td></td>
</tr>
<tr>
<td>0.32</td>
<td>0.763544 m</td>
<td>+0.127%</td>
<td></td>
</tr>
</tbody>
</table>

Figure 3: Normalized pressure residuals of the quasi-Newton iterations.

implemented near the outlet using momentum source terms [8]. In Table 1 the outlet depth of the flow $h_2$ is given: the analytical result based on Eq. (13) is compared to the result of the simulations, giving excellent results. The subcritical result is a bit less accurate, most likely because of the wave train and the damping zone.

Fig. 3 shows the residuals for both cases: they converge exponentially and in a low number of iterations. The subcritical case takes longer: this is due to the presence of the steady gravity wave, which makes the steady free surface problem –and the root-finding problem– much harder to solve.

5 CONCLUSIONS

This paper presents a new quasi-Newton method suitable for systems that can be solved with a black-box solver for which a cheap surrogate model is available. In order to have fast convergence, the approximate Jacobian consists of two different contribution: a full rank surrogate model of the system is combined with a low rank least-squares model based on known input-output pairs of the system. It is then shown how this method can be used to solve 2D steady free surface flows with a black-box flow solver. The inviscid flow over a ramp is calculated for supercritical and subcritical conditions. For both simulations the quasi-Newton iterations converge exponentially and the results match the analytical predictions accurately.
REFERENCES


MBS/FEM CO-SIMULATION FOR HYBRID MODELING OF RAILWAY DYNAMICS

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Key words: Coupled Problems, Railway, Dynamics, Vibrations, Co-Simulation

Abstract. Nowadays in railway traffic, specific speed limitations exist depending on the train charge, due to a fragile subsoil or even an old building that has to be preserved. Depending on the type of vehicle, the type of soil or even the vehicle speed, the ground-borne vibration characteristics can significantly vary. It becomes thus important to predict the vibrations generated by a train passing on a track in the surrounding soil. In order to achieve this prediction, a hybrid modeling approach, consisting in a vehicle modeled using the minimal coordinates approach in multibody systems theory and a soil modeled using a finite element method, is developed. The recoupling of this hybrid system is performed using co-simulation between two different software packages with their own solvers. The first software is EasyDyn, an in-house C++ library package dedicated to multibody dynamics and the second software is ABAQUS that is dedicated to finite element analysis. The aim of this paper is to illustrate the results given by this hybrid model. Then two different co-simulation schemes (the sequential Gauss-Seidel scheme and the parallel Jacobi scheme) will be used and compared in terms of accuracy for this specific railway application.

1 INTRODUCTION

Whether for a commercial or a personal purpose, railway transportation is currently a popular mean of transportation. Moreover, due to the permanently growing population, railway could follow an important development in the next decades. Simultaneously, homes and buildings are built close to stations and railway tracks. Depending on the type of tracks, the speed of the vehicle and a large range of different parameters, the passing of a train on a track usually generate significant ground-borne vibrations.
The effect of soil dynamics on the train dynamics and on the ground-borne vibrations was already studied in the literature. Yang recently depicted the effect of a train passing under an hotel in order to determine if the level of vibrations during day and night shifts do not exceed the levels imposed in China [1]. Like many models [2, 3, 4] in this field, Yang used a two-step model to determine the ground-borne vibrations generated by a running train on specific tracks.

The first step of two-step models is usually the estimation of the force applied by the vehicle or the track on the soil depending in which part the track is modeled. The second step is the computation of the vibrations generated on the soil due to the application of the estimated forces. In order to produce the best estimation of forces applied on the soil, a reduction of the soil can be included in the first step (containing the vehicle dynamics). There exist different models of soil reduction such as the Winkler or the coupled lumped mass (CLM) model [5].

Through two-step models, it is possible to decouple substantial monolithic modelings to integrate the two different parts (vehicle dynamics and soil dynamics) separately. However, even if the efficiency of this kind of model was proven many times in the literature, the step-decoupling is limited for soft soil cases since the coupling between the track and the soil is weaker when the soil is stiffer than the ballast [6]. Therefore this work will focus on the simulation of a coupled vehicle/track/soil model using co-simulation techniques between two-different software packages. The vehicle/track subsystem will be time-integrated in EasyDyn [7], an in-house C++ library package dedicated to multibody modeling using the minimal coordinates approach. The soil subsystem will be modeled and simulated in a commercial finite element software called ABAQUS. Through different comparisons between the vibrations predicted by co-simulated models and a two-step model, it will be demonstrated that both types of simulations are efficient in their specific domain.

2 MODEL CONSTRUCTION

The vehicle/track/soil model used to investigate the possibilities offered by co-simulation techniques is illustrated in Figure 1. It is based directly on the two-step model proposed by Kouroussis [8] that consists in the following steps:

- The vehicle and the track are modeled with a reduced CLM model of the soil in order to compute the forces acting on the ground applied by the sleepers through the ballast. The CLM model of the soil includes five different parameters that are tuned so that the frequency response of the reduced model overlaps sufficiently with the response of the 3D finite element modeling of the soil.

- The forces computed in the first step are applied on the soil that is modeled as a finite element meshed hemisphere. The contact surface between the ballast and the soil is reduced at the surface generated by the orthogonal projection of the sleeper on the ground as depicted in Figure 1.
The co-simulated model is cut following the same logic as the one used in the two-step model. Therefore, the first subsystem will contain the vehicle and the track and the second subsystem will contain the soil only. The following sections will describe both subsystems and the method used to couple them during the time-integration process.

2.1 Subsystem 1: Vehicle and track subdomains

The vehicle/track subsystem is modeled in an in-house C++ software dedicated to multibody dynamics. It contains three different parts:

1. A multibody modeling of the vehicle. From a simple wheel to a complete car, the vehicle is composed of bodies that are defined by their mass and inertial properties and the position of their center of mass depending on the different degrees of freedom. These degrees of freedom are included in homogeneous transformation matrices that express the position and orientation of the frame of a body with respect to the main frame. The choice of a unique wheel for the vehicle definition was made in order to test the co-simulation effect on a simple case.

2. A finite element representation of the rail. The rail is split into Euler-Bernoulli beam elements so that the whole rail system is represented by its global mass and stiffness matrices.
3. A discrete representation of the sleepers. Each sleeper only has one degree of freedom (vertically oriented) and is considered as a moving mass.

The coupling between the different elements is performed through a non-linear Hertz contact between the wheel and the rail while the railpads (rail/sleepers coupling) and the ballast (sleepers/soil coupling) are represented by linear spring and dashpot elements.

2.2 Subsystem 2: Soil subdomain

The soil subsystem is modeled in a commercial finite element software called ABAQUS. It is mainly composed of two different parts:

1. A meshed soil kernel. The soil on which the track lays is defined as an hemisphere meshed with tetrahedral elements including a variable mesh seed. This soil can be divided into different layers to model as well as possible the soil composition but in the simulations performed, the hypothesis of an homogeneous soil composition is made for the sake of simplicity.

2. A semi-infinite shell. The soil kernel is surrounded by an hemispherical shell composed of semi-infinite elements. The internal surface of the semi-infinite shell and the external surface of the soil are tied together. The purpose of the semi-infinite elements is to prevent undesirable wave reflections on the external surface of the soil kernel if fixed boundary conditions were specified.

2.3 Coupling technique

The coupling technique is here divided into two different aspects:

- The coupling approach that defines the data exchange management as well as the time-integration management of each subsystem.
- The coupling type that defines the type of the input and output variables of each subsystem used to re-couple them during the integration process.

As depicted in Figure 2, the coupling approaches can be either completely sequential or parallel. This Figure illustrates the two co-simulation approaches used in this work over a macrotimestep $h$ that is defined as the common timestep at which both subsystems exchange data. The sequential approach (called Gauß-Seidel) consists in a first integration of the vehicle/track subsystem then the integration of the second subsystem whose input variables $u_{GS}$ directly comes from the first subsystem integration. The parallel approach (called Jacobi), performs both subsystems integration over a macrotimestep simultaneously. This means that no communication exists between both subsystems during a macrotimestep and that the input variables of each subsystem are taken from the results of the previous timestep performed.
For each step

\[ z_{t+h} = \begin{bmatrix} z_{1t+h} \\ z_{2t+h} \end{bmatrix} \]

Figure 2: Gauß-Seidel scheme (plain) - Jacobi scheme (dashed). The symbols \( u \) and \( z \) define the input and state variables respectively.

Figure 3 illustrates the type of input and output variables of each subsystem to complete the coupling. The input variables of the vehicle/track subsystem (also the output variables of the soil subsystem) are defined as the displacement and velocities of the coupling surfaces (sleeper print on the soil). Using the vertical displacement and velocities of all the coupling surfaces, the vehicle/track subsystem can be integrated over a macro-timestep and the force developed by the sleepers to the soil through the ballast are computed. Therefore, those forces that are the output variables of the vehicle/track subsystem (also the input of the soil subsystem) are applied on the coupling surfaces after being transformed into pressures. This way, the soil can be time-integrated and the coupling surface positions and velocities can be updated for the next vehicle/track subsystem integration.

3 RESULTS

Using typical values of the track parameters [9], simulations were undertook using three different type of soil: a stiff (E=750 MPa), a medium (E=155 MPa) and a soft (E=10 MPa) soils. Moreover, both Gauß-Seidel (denoted GS) and Jacobi (denoted J) coupling approaches were tested. The reference model, to which the co-simulated ones will be compared, is the two-step model (denoted TS) detailed in the previous sections.

Figure 4 compares the Peak Particle Velocity (PPV) in the vertical direction of the vibration signals generated by the running wheel with respect to the distance from the track. The PPV is defined as the maximum absolute value of a signal over a given period of time. This indicator is often employed to compare vibratory signals and evaluate the vibrations effect on people’s comfort and structures [10]. It can be seen in the Figures that the stiffer the soil is, the closer the co-simulated and the two-step models results
are. Moreover, in the soft soil case, even if the divergence is clearly noticeable, the PPV obtained using the Gauß-Seidel co-simulated scheme remains close to the PPV obtained using the two-step model already validated by Kouroussis in his research [11]. However, the PPV obtained using the Jacobi coupling approach diverges completely from the regular shape because the simulation becomes unstable due to the loss of information implied by the data exchange management [12].

![-figure 3](image)

**Figure 3:** Coupling type used to exchange data between subsystems

The loss of information due to the Jacobi co-simulation approach can be diminished if the data are exchanged more often. This can be possible if the macrotimestep decreases. Figure 5 illustrates the PPV with respect to the distance from the track for the soft soil only. However, two different macrotimesteps are compared: 1 ms in Figure 5a and 0.1 ms in Figure 5b. Those two Figures clearly shows that using a smaller macrotimestep...
increases the convergence of the solutions obtained using the different models.

![Figure 5: Vertical Peak Particle Velocity with respect to the distance from track for the soft (E=10 MPa) soil type. Comparison of 1 ms (left) and 0.1 ms (right) macrotimesteps.](image)

The results obtained can also be compared in terms of frequency content. The frequency content with respect to time is computed using the wavelet transform of the vertical velocity of specific points at 2.5 and 5 meters from the track. The Continuous Wavelet Transform (CWT) [13] is a time-frequency analysis method which does not present the drawback of the time-frequency limitation, unlike the Fourier Transform, allowing for a fine-scale analysis. It is therefore well adapted to transient phenomenon such as railway-induced ground vibrations [14].

The results comparison between the two-step model and the two different co-simulation approaches for the three types of soil are depicted in Figures 6 and 7 respectively. The macrotimestep for those simulations is 1 ms. Generally speaking, the wheel rolling on the track can clearly be noticed by the increase of the frequency content from a certain time. As for the PPV comparison in the soft soil case (Figure 5a), it can be seen that the Jacobi coupling leads to unstable results while the Gauss-Seidel coupling stays stable. Moreover, it seems that the tendency of the wavelet coefficients are more similar if the stiffness of the soil increases.

4 CONCLUSIONS

After the definition of a reference two-step model that was experimentally validated, a vehicle/track/soil model using co-simulation techniques was detailed. The co-simulation link was performed using two different software packages: a multibody software in which the vehicle/track subsystem was modeled and a finite element software for the soil. Three different types of soil were considered and two co-simulation techniques were compared to the two-step reference: a parallel and a sequential approaches.

In order to efficiently compare the results obtained using the different modelings, the
peak particle velocity depending on the distance from the track were compared as well as the frequency content of the vibratory signals at two different distances from the track through their wavelet transform.

Finally it was noticed that a soft soil with a Jacobi coupling approach can lead to unstable results if the macrotimestep becomes too large. Meanwhile, changing the coupling approach to the Gauß-Seidel one or even changing the soil stiffness while keeping the
same macrotimestep (that lead to instabilities) can provide stable results. Moreover, it was also noticed that the convergence of the results given by the co-simulated approaches and the two-step reference are closer if the soil becomes stiffer.
REFERENCES


PREDICTION OF EACH ROAD DETERIORATION CONSIDERING TRAFFIC AND THE INTERACTION WITH OTHER SURFACE DETERIORATIONS, USING AUTOMATED LEARNING MACHINE TECHNICS

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Key words: Road Deterioration Model Prediction, Learning Machine Technics

Abstract: For road user, the pavement is a surface that must allow the circulation of mixed traffic, in conditions of safety and comfort, under any climatic condition, for a long time. Once the pavement is in service, it begins to have deteriorations that can cause that the user modifies their behavior and start driving at a slower speed in order to maintain traffic safety conditions; this circumstance causes travel times increasing and therefore circulation costs increase.

There are different deteriorations to consider, roughness, road surface adherence, rutting, cracking and potholes. Periodic deterioration evaluation and prediction modelling allows that corrective actions can be anticipated, so that road quality does not fall below acceptability limits. To prioritize improvements and routine maintenance, it is necessary to develop adequate tools to predict the deterioration evolution, which can be incorporated into the pavement management systems used to prepare multi-year works and maintenance plans.

Periodic observations of surface deteriorations of sections in service located on routes of Littoral region of Argentina were used in the paper. It was possible to develop predictive models using Support Vector Machine Regression SVR and Random Forest Regression RFR; these are learning machine tools, which can be used to solve estimation problems of multidimensional functions. First a model to predict cracking was developed. When it was optimized, the model to predict rutting was realized. And at the end, the model to predict roughness was adjusted, using cracking and rutting models developed previously. Results indicate that SVR and RFR regression models have the capacity to perform training and prediction that help to develop road surface deterioration models.

1 INTRODUCTION

In this paper, "automated learning" techniques are presented to predict pavement surface deteriorations evolution; where analysed models for roughness, rutting and cracking.

Machine Learning is the subfield of computer science and a branch of artificial intelligence that aims to develop techniques that allow computers to learn.

The current analysis of the problem was focused on supervised learning, whose objective is to create a function capable of predicting the value corresponding to any valid input object, after having seen a series of examples. This makes predictions of unknown variables based on
behaviors or characteristics that have been seen in the data already stored.

What machine learning algorithm is the appropriate to use? The algorithm to be used depends on the size, quality and nature of the data. The fundamental idea of automated learning is to find patterns that can be generalized, in order to apply this generalization about cases that have not yet been observed, and make predictions. The objective of the regression is to minimize the error between the approximate function and the value of parameter. Many variables can lock some learning algorithms and cause the training time to be too long. To develop good regression models, is very important the selection of independent variables as an input of models.

Python was used as language for the development of test techniques, and Scikit-learn was used as software packages. These libraries also facilitate the evaluation, diagnosis and validation tasks since they provide several factory methods included to perform these tasks in a very simple way. [1]

It is expected that this tool can be implemented in road management systems, and as a transfer function in structural design programs.

2 REGRESSION MODELS USED

Two regression models were analyzed and compared: Support Vector Machine Regression and Random Forest Regression. [2,3,4,5]

2.1 Support Vector Machine Regression (SVR)

SVR objective is to make the prediction from a problem of geometric optimization, which can be written as a problem of quadratic convex optimization with linear constraints, in principle solvable by any non-linear optimization procedure.

The technique of support vectors is a universal tool for solving estimation problems of multidimensional functions. The aim is to select the hyperplane regressor that best fits the training data set, based on considering a distance margin $\varepsilon$, so that all the examples are in a band or tube around said hyperplane. The function is intended to be as close as possible to the points, that is, the formation of the band or tube around the true regression function.

To define the hyperplane, only data points that are more far than $\varepsilon$ of the hyperplane are considered. These data points are the considered support vectors; they are identified with the strict possibility of the associated artificial variables, which quantify the error between the approximation and the real value of each data point of the training set. In Figure 1 the reduction in support vectors is shown when $\varepsilon$ increase.

![Figure 1](image-url)

Figure 1. Left to right: regression (solid line), data points (small dots) and SVs (big dots) for an approximation with $\varepsilon = 0.1, 0.2$ and $0.5$. Note the decrease in the number of SVs. [6]
2.2 Random Forest Regression (RFR)

They are a combination of predictive trees in such a way that each tree depends on the values of a random vector sampled independently and with the same distribution for all trees in the forest. The generalization error for forests converges to a limit as the number of trees in the forest becomes large.

RFR are a set of different regression trees and are used for multiple non-linear regressions, where each sheet contains a distribution for the continuous output variable(s). The objective of these methods is to inject the algorithm with just randomness to maximize the independence of the trees while maintaining a reasonable precision. The results turn out to be insensitive to the number of features selected to divide each node. In general, when selecting one or two characteristics, optimal results are obtained.

Random forests are effective in eliminating noise in the input data of the model. Given a long list of input variables and a reduce data set, it is very likely that any predictive model will discover false relationships between those inputs and the target variable chosen.

Because RFR constructs many trees using a subset of input variables and their values, it contains underlying decision trees that omit the noise-generating variable. In the end, when it is time to generate a prediction, there is a vote among all the underlying trees and the majority prediction value wins.

3 PAVEMENT SURFACE DETERIORATIONS

Since a road is built deterioration process begins, and evolves causing reduction in road quality, and increase maintenance and user costs.

Once put in service and influenced by the climate and traffic, the pavement will have a loss of quality and deterioration will appear. To reduce these deteriorations, certain periodic maintenance and rehabilitation activities must be carried out on time, in order to reduce the impact that different failures may have on the structure, in order to optimize the available resources and to avoid reconstruction.

For this, pavement management techniques and pavement road evaluation methodologies are required, which consist in the evaluation of superficial and structural deteriorations level that affect the quality of the service provided to the users, using defined analysis methodologies and appropriate equipment.

There are different deterioration parameters to evaluate road surface quality provided to users: roughness, rutting, cracks, potholes, raveling, bleeding, etc. [7,8]

3.1 Roughness

Roughness evaluates the deviations of road longitudinal profile with respect to a flat surface, that affect in a very important way vehicle dynamics, quality of circulation, dynamic effect of the loads and the drainage. Users perceive roughness as vibratory movements that affect the comfort of circulation.

Roughness value is expressed in IRI (International Roughness Index, defined in 1982 by the World Bank), which is an index obtained by a mathematical simulation of the passage of a virtual vehicle, circulating on road profile at a speed of 80 km/h.
IRI is a continuous type variable, where the range goes from zero for ideally flat surfaces (runways of airports can provide values lower than unity), with values between 1 and 2 m/km for new pavements, and values higher than 6 m/km for deteriorated surfaces.

Data used in the present work are measurements made with dynamic response equipment, according to class 3 World Bank.

3.2 Rutting

Rutting is the loss of the road transversal profile, with depressions located in correspondence with the wheel path; this is the area where most of heavy vehicles circulate.

In Argentina, rutting is measured as the depression under a 1.20 m straight edge. Data used in this work have been obtained from manual measurement made by trained people, at 1 km intervals.

3.3 Cracking

The presence of cracking in asphalt surface layer is an indicator that the material has consumed its fatigue capacity. This indicator is only visualized by the user when the surface presents a high degree of deterioration, when there is loss of material. When cracks are in early stages of development, it is an indicator that layer material is failing, but the user does not perceive them, because it does not affect circulation comfort.

In Argentina, this parameter is measured assigning deterioration degrees according to evolution pattern, because of fatigue, increasing from 0 to 10. Grade 0, no cracks. Grade 2, are fine and isolated cracks located in correspondence with wheel path. Grade 4, are branched cracks with tendency to form meshes. Grade 6, are interconnected cracks forming blocks. Grade 8, are high severity level cracks, alligator cracking. Grade 10 are generalized cracks, pieces may move and can be lost.

Data used in the present work have been obtained from visual survey performed by trained personnel walking along the road, analyzing 20 meters at 1 km intervals. After that, measurements have been expressed as total cracking, using correlations between methodologies.

4 ROAD NETWORK DETERIORATION MODELING

4.1 Independent variables selection

Independent variables, predictors in the future, are independent in the sense that they are external and measurable variables.

The choice of these variables is as important as the choice of the target variable, since it determines modeling success. Most of the time invested in the development of models is used precisely in the analysis and selection of independent variables set.

In the present analysis, data used are: year of measurement, deflection, annual ESAL, rutting, percent of total cracking, and roughness. The objective parameter is roughness, and intermediate models were developed for rutting and cracking.
4.1.1 Traffic

It is an important variable in road design, because truck loads are responsible of deterioration. It is necessary to know the number and type of vehicles that will pass, as well as load intensity and axle configurations. In the present study, traffic intensity and loads are expressed in annual equivalent single axle of 80 KN (ESAL), for each year of service.

4.1.2 Rutting

Rutting is the changes in road transversal profile, with respect to the original profile. These variations of the transversal profile are found in the tracks and appear because of permanent deformation caused by heavy traffic. This deformation has a fundamental impact on the functional conditions (for the user) and structural conditions (for the engineer) of the existing pavement. This causes water accumulation in wheel tracks, loss of control of the vehicle, driving insecurity, lack of comfort, and increasing accidents risk.

4.1.3 Cracking

Cracking is the discontinuity in surface layer material. This deterioration reduces layer resistance, and after them more deteriorations appears, like raveling, potholes and roughness. They also provide a potential water access to the lower layers, which accelerates the deterioration evolution.

These variables are known to have significant impact on roughness. The prediction of rutting and cracking as intermediate models, improve roughness prediction.

4.2 Data used

Data were obtained from different sections located on in service roads. Measurements were made by Road Administration staff and shared with the University.

Data are from homogeneous sections, with same structure and traffic. Sections are located in different geographic location from Argentina Littoral Region. From each section the following information were known: traffic, structure, layer materials, maintenance applied, and periodic measurements results: rutting, cracking and roughness.

For the sections analyzed in this study 325 data points were collected from 59 homogeneous sections. Benkelman beam deflection was not measured every year, and was assumed constant during years without data. Roughness was measures annually. Table 1 shows and example of section data for sections 51 and 55.

4.3 Experimental models analysis

In this point progressive analysis tested with SVR and RFR are described, using data for model training and validation as described previously.

First a model to predict cracking was developed. When it was optimized, the model to predict rutting was done. And at the end, the model to predict roughness was adjusted, using cracking and rutting models developed previously. Standard deviation of prediction error was used to compare both techniques.

To minimize errors, data were filtered using following criteria:

- When roughness increased more than 0.6 m/Km IRI from one year to the other, it was assumed that surface maintenance was conducted and it was not documented. Then this section
data was divided into two sections. One section up to roughness increment, and another section after that.

- In roughness data, when difference between results of two consecutive years was more than 0.3 m/km and less than 0.6 m/Km, a filter was applied. The strange data was removed and a new data was obtained using a grade 3 polynomial regression between data from previous an after year. This situation was noted in roads with high deterioration level.

- For years without deterioration data, like year 2012 of section 51, data were created as extrapolation of previous data using a grade 3 polynomial regression between data from previous an after year. In this period, traffic was increased using 2% increment rate.

- Deterioration data were forced to have an increment between years. Then, if cracking, rutting or roughness from one year to the other were decreasing, they were force to increase.

- To train with Support Vector Machine Regression, the input vector was normalized over all data (less roughness), that is, the characteristics were readjusted so that they have the properties of a standard normal distribution with $\mu = 0$ and $\sigma = 1$. In Python, we used the preprocessing library that provides a quick and easy way to perform this operation in a single data set.

### Table 1: Example of section data available

<table>
<thead>
<tr>
<th>Sec.</th>
<th>Year</th>
<th>Benk Beam Deflection (0.001 mm)</th>
<th>ESAL Annual (10$^6$)</th>
<th>All Crack (%)</th>
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<th>IRI (m/Km)</th>
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<td>33</td>
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<td>1.85</td>
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</tr>
</tbody>
</table>

### 4.4 Training models with n-1 year’s data

Training was done for three parameters: first cracking, after that rutting containing cracking, and at last roughness containing rutting and cracking; in the same way that is recommended in Highway Development and Management software (HDM). Results indicate that SVR and RFR regression models have the capacity of perform training and prediction. [9]
4.4.1 Cracking prediction

First, the model was trained with n-1 year’s data to adjust both regression models. Cracking percentage of previous year was taken as input data, and cracking percentage of the present year was the prediction objective. Year, deflection, ESAL annual were data entry too.

In Figure 2 actual cracking percentage versus SVR and RFR prediction is shown. Prediction errors, expressed in percentage, are 4.41 for SRV model and 4.19 for RFR.

![Figure 2: Actual cracking percentage versus SVR and RFR prediction](image)

4.4.2 Rutting prediction

As second step, rutting prediction model was adjusted. It was done by training the models with n-1 year’s data. Cracking of previous year was obtained using cracking prediction model data. Rutting of previous year was taken as data, and rutting of present year was the objective.

In Figure 3 measured rutting versus SVR and RFR prediction is shown. Prediction errors, expressed in mm, are 1.13 for SRV model and 1.60 for RFR.

4.4.3 Roughness prediction

In a similar way than for cracking and rutting, roughness prediction was done. Roughness measurement of previous year, cracking and rutting predicted were used as data, and roughness of the present year was the objective.

In Figure 4 roughness measured versus SVR and RFR prediction is shown. Prediction errors, expressed IRI (m/Km), are 0.20 for SRV model and 0.10 for RFR.
Figure 3: Rutting measured versus SVR and RFR prediction

Figure 4: Roughness measured versus SVR and RFR prediction
4.4.4 Prediction analysis using developed models

Up to now, data from n-1 year were used for models training, and the ability of models to predict each deterioration for the last year was analyzed. The errors obtained using SVR and RFR were similar. Roughness prediction errors expressed in IRI (m/Km), were 0.20 for SRV model and 0.10 for RFR.

Now is time to use data and models to validate prediction for many years. Beginning with the first data, models were used to predict year by year roughness evolution, using the three models of SVR and RFR.

For this analysis, data were taken as follows: year was incremented in one year, deflection was considered as a constant, traffic increment rate was 2%, and cracking and rutting were obtained from adjusted models.

Figure 5 shows roughness evolution for one section, as an example.

Results show that both methodologies are capable to be trained and predict deteriorations. The present study was our first intention to use SVR and RFR regression models to training and prediction deteriorations. Results look good and we are going to continue our researches using another group of sections data, for other regions of Argentina.

5 CONCLUSIONS

For road routine maintenance planning, it is necessary to have adequate tools/models to predict the evolution of deterioration. These models can be incorporated into pavement management systems to prepare the multi-year works and maintenance plans.
Other use of models is to use as transfer functions in mechanistic pavement design software as, to predict deterioration like cracking, rutting and roughness, as MEPDG guide. [10]

The present study was our first intention to use SVR and RFR regression models to training and prediction deteriorations. Results look good and we are going to continue our researches using another group of sections data, for other regions of Argentina.

REFERENCES


Semi-Analytical Hybrid Approach for Modelling Wave Motion Excited by a Piezoelectric Transducer in a Laminate with Multiple Cracks

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Key words: Coupled Problems, Wave Propagation, Piezoelectric Transducer, Delamination, Hybrid Method, Computational Mechanics

Abstract. A semi-analytical hybrid approach is presented here to simulate the dynamic behaviour of a multi-layered elastic waveguide with a system of delaminations and a piezoelectric transducer mounted on the surface of the waveguide. The proposed hybrid approach combines the advantages of the frequency domain spectral element method, which is applied to discretize a complex-shaped piezoelectric structure, and the boundary integral equation method employed to simulate wave propagation in multi-layered waveguide with multiple delaminations. The proposed method is applicable to the multi-parameter analysis of the phenomena related to elastic wave scattering and excitation. The advantages of the presented extended semi-analytical hybrid approach method along with the results of the parametric analysis of wave propagation in the considered structures are discussed.

1 INTRODUCTION

A considerable number of methods employed in non-destructive evaluation and structural health monitoring (SHM) for damage identification are related to elastic waves. Any structural defect reflects the guided waves and the response signal is used to obtain the position and the size of the defect. Among the latter, cracks and interface disbonds are main goals of inspection, due to their potential role in possible breaks of integrity and catastrophic failures of the structures employed, for instance, in aircraft and spacecraft, and the rotor blades of wind turbines. For this reason, the scattering of elastic waves by cracks has been extensively studied applying various methods ranging from purely...
numerical ones to more analytically oriented approaches. A number of built-in or on-
board piezoelectric transducers and sensors are used to excite wave motion and record
structural responses afterwards. Refinement of the corresponding SHM systems demands
understanding and simulation of the interaction between transducers and multi-layered
structures with defects. Development of practical techniques for damage detection is im-
possible without efficient tools for simulation and numerical analysis. In order to simulate
piezo-induced guided waves propagation and scattering from the internal delaminations
accurate and reliable mathematical models should be developed.

This paper presents a semi-analytical hybrid approach (SAHA) for dynamic behaviour
simulation of a multi-layered elastic waveguide with system of delaminations and piezo-
electric actuators mounted on the surface. The presented method extends the hybrid
approach proposed in [1] for modelling of the dynamic interaction of perfectly bonded or
partially debonded piezoelectric structures with a layered elastic waveguide. The SAHA
combines the advantages of the frequency domain spectral element method (FDSEM) [2]
to discretize complex-shaped piezoelectric structures and the boundary integral equation
method (BIEM) [3, 4] to simulate wave propagation in multi-layered waveguides with
a set of horizontal delaminations. The coupling of these two methods is performed in
the contact area between waveguide and transducer via the introduction of an unknown
traction vector-function. To the authors’ knowledge, only the hybrid method [6] is rather
similar to the SAHA in this sense. However, a solution in a perfectly bonded rectangu-
lar transducer was approximated in [6] via Chebyshev polynomials without discretization
into finite elements, and it is not applicable to simulate debonded transducers and inter-
nal delaminations. The proposed method is applicable to the multi-parameter analysis
of the phenomena related to elastic wave scattering and excitation. The advantages of
the presented extended SAHA along with the results of the parametric analysis of wave
propagation in the considered structures are discussed.

2 STATEMENT OF THE PROBLEM

The piezoelectric wafer active sensor (PWAS) exciting wave motion occupies domain
\( V^{(a)} = \{ 0 \leq x_1 \leq w_a, 0 \leq x_2 \leq h_a \} \), while the laminate structure occupies the domain
\( V^{(0)} = \{ |x_1| < \infty, -H \leq x_2 \leq 0 \} \). Accordingly, \( w_a \) and \( h_a \) denotes width and height of the
PWAS. The composite consists of \( N \) elastic layers \( V^{(n)} = \{ |x_1| < \infty, -h_n \leq x_2 \leq -h_{n-1} \}
with Lame constants \( \mu^{(m)}, \lambda^{(m)} \) and mass density \( \rho^{(m)} \). \( M \) strip-like cracks with stress-free
surfaces occupy domains \( \Omega^{(m)} = \{ |x_1 - c_m| \leq l_m, x_2 = -d_m \} \), see Figure 1.

Constitutive equations for the PWAS are given as follows
\[
\sigma_{ij} = C_{ijkl}s_{kl} - e_{kij}E_k,
\]
\[
D_i = e_{ikl}s_{kl} + \varepsilon_{ij}E_j.
\]
Here \( \sigma_{ij} \) is stress tensor, \( s_{ij} \) is strain tensor, \( D_i \) is electric displacements vector and
\( E_i \) is electric field vector, while \( C_{ijkl} \), \( e_{kij} \) and \( \varepsilon_{ij} \) are matrices of the elastic constants,
piezoelectric constants and dielectric constants measured with zero strain respectively ($i, j, k, l = 1, 3$). Laminate $V^{(0)}$ with the boundaries ($S^{(0)} = \{|x_1| < \infty, x_2 = \{-H, 0\}\}$) is assumed elastic, so electric components are absent. The dependence between strain $s_{kl}$ and mechanical displacements $u_k$ is expressed with relation

$$s_{kl} = \frac{1}{2} (u_{k,l} + u_{l,k}),$$

where $u_{k,l}$ denotes derivatives of $u_k$ with respect to $x_l$. The components of electric field vector are expressed in terms of electric potential $\phi$ as follows:

$$E_i = -\phi_i.$$

The two-dimensional time-harmonic vibrations with the circular frequency $\omega$ are considered with plane strain assumption. Accordingly, governing equations for the piezoelectric media $V^{(a)}$ have the following form:

$$C_{ijkl}u_{k,lj} + e_{kij}\phi_{kj} + \rho \omega^2 u_i = 0, \quad (1)$$

$$e_{ikl}u_{k,li} - \varepsilon_{ik}\phi_{ki} = 0. \quad (2)$$

Electric potentials $V^\pm$ are applied at the lower ($S^- = \{0 \leq x_1 \leq w_a, x_2 = 0\}$) and the upper ($S^+ = \{0 \leq x_1 \leq w_a, x_2 = h_a\}$) surfaces of the PWAS:

$$\phi = V^\pm, \quad x \in S^\pm. \quad (3)$$

At the side boundaries of the PWAS $S^{(a)} = \{x_1 = \{0, w_a\}, 0 \leq x_2 \leq h_a\}$, zero electric displacements are given:

$$D_i = 0, \quad x \in S^{(a)}. \quad (4)$$

The lower boundary $S^- = V^{(0)} \cap V^{(a)}$ is common for the PWAS and the waveguide. Therefore, the continuity of the displacement and the traction vector composed of normal and tangential stresses $\tau = \{\sigma_{12}, \sigma_{22}\}$ is assumed at $S^-$:

$$\begin{bmatrix} \tau \end{bmatrix} = \begin{bmatrix} u \end{bmatrix} = 0, \quad x \in S^-. \quad (5)$$
Here square brackets denote a jump. All the other surfaces of the PWAS and the waveguide with normal $\eta_j$ are assumed stress-free:

$$\sigma_{ij}\eta_j = 0, \quad x \in S^{(a)} \cup S^+ \cup (S^{(0)} \setminus S^-).$$  \hspace{1cm} (6)

At the surfaces of cracks the stress free boundary conditions are assumed:

$$\tau = 0, \quad x \in \Omega^{(m)}.$$

$$\tau = q, \quad x \in S^-, \hspace{1cm} (8)$$

where the traction vector $q$ is assumed to be given.

It is convenient to introduce the decision vector $y = \{u_1, u_2, \phi\} \in Y$ being assumed from the Sobolev space $H^2$ of square-integrable functions and their derivatives of orders $k < 2$:

$$Y = \left\{ y(x) | y_i \in H^2(V^{(a)}), y_3(x) = V^+(x), \quad x \in S^+; \quad y_3(x) = V^-(x), \quad x \in S^- \right\}$$

The variational formulation of the equations (1) and (2) can be written using test functions $v = \{v_1, v_2, v_3\}$ from the space

$$W = \left\{ v(x) | v_i(x) \in L^2(V^{(a)}), v_3(x) = 0, \quad x \in S_1 \cup S_3 \right\}$$

as follows

$$\iint_{V^{(a)}} \sigma_{ij} v_i dS + \rho \omega^2 \iint_{V^{(a)}} u_i v_i dS = 0, \hspace{1cm} (9)$$

$$\iint_{V^{(a)}} D_{ij} v_i dS = 0. \hspace{1cm} (10)$$

After integration by parts, equations (9)–(10) are rewritten:

$$\int_{\partial V^{(a)}} q_i v_i ds - \iint_{V^{(a)}} \sigma_{ij} v_{ij} dS + \rho \omega^2 \iint_{V^{(a)}} u_i v_i dS = 0, \hspace{1cm} (11)$$
\[ \int_{\partial V^{(\alpha)}} D_4 v_3 \eta_t \, dS - \int_{V^{(\alpha)}} D_4 v_3 \, dS = 0. \]  \hfill (12)

According to the FDSEM, the solution of the auxiliary problem can be approximated using Lagrange interpolation polynomials \( C^I(x_1, x_2) \) at Gauss–Lobatto–Legendre points

\[ y_k = \sum_I y_k^I C^I(x_1, x_2), \]  \hfill (13)

here special index \( I \) used to identify each node in the PWAS (for more details see [1]). Test functions \( v \in W \) are chosen the same \( v_k(x) = C^I(x_1, x_2) \) as basis functions except another index is used below to distinguish from \( I \).

### 4 THE BOUNDARY INTEGRAL EQUATION METHOD

Let us consider second auxiliary problem, where a surface load function \( q(x_1) \) is assumed known at the part \( S^{(0)} \) of the upper surface of the waveguide \( V^{(0)} \), while \( M \) cracks \( \Omega^m \) are situated in the waveguide itself. The corresponding boundary value problem is stated as the governing equation (1), given for pure elastic material, and the boundary conditions (6), (8) and (7). The total wave-field is then a sum of the wave-field \( u^{(in)} \) incident by the load and wave-fields \( u^m \) scattered by each of \( M \) cracks.

\[ u = u^{(in)} + \sum_{m=1}^M u^m. \]

The BIEM can be applied to obtain the integral representation [4]:

\[ u^{(in)}(x) = \frac{1}{2\pi} \int_{\Gamma} K^{(0)}(\alpha, x_2) Q(\alpha) e^{-i\alpha x_1} \, d\alpha. \]  \hfill (14)

Here \( K^{(0)}(\alpha, x_2) \) is the Fourier transform of Green’s matrix of the waveguide, \( Q(\alpha) \) is the Fourier transform of the surface load function \( q(x_1) \) with respect to \( x_1 \) coordinate, while \( \Gamma \) is a contour along real axis surrounding poles of the integrand. For the scattered wave-fields the following integral representation is valid:

\[ u^m(x) = \frac{1}{2\pi} \int_{\Gamma} K^{(m)}(\alpha, x_2) W^{(m)}(\alpha) e^{-i\alpha x_1} \, d\alpha, \]  \hfill (15)

where \( K^{(m)}(\alpha, x_2) \) is the Fourier transform of Green’s matrix and \( W^{(m)}(\alpha) \) is the Fourier transform of the unknown crack opening displacement (COD) \( w^m(x_1) \) for \( m \)-th crack. Similar integral representations can be written for traction vectors:

\[ \tau^{(in)}(x) = \frac{1}{2\pi} \int_{\Gamma} T^{(0)}(\alpha, x_2) Q(\alpha) e^{-i\alpha x_1} \, d\alpha, \]  \hfill (16)
\[ \tau^{(m)}(x) = \frac{1}{2\pi} \int T^{(m)}(\alpha, x_2) W^{(m)}(\alpha) e^{-i\alpha x_1} d\alpha, \] (17)

Here \( T^{(0)} \) and \( T^{(m)} \) are matrices obtained after differential stress operator has been applied to representations (14)-(15).

The COD for \( m \)-th crack is expanded via Chebyshev polynomials of the second kind with square-root weight \( p_n^{(m)}(x_1) \):

\[ w_k^{(m)}(x_1) = \sum_{n=0}^{N_m} \gamma_{kn}^{(m)} p_n^{(m)}(x_1). \] (18)

Following [4], the unknown COD can be determined using Galerkin method if the surface load is known.

5 HYBRID METHOD

The solution of the coupled problem (1)–(7) is constructed below in the assumption that the traction vector \( q(x_1) \) as well as CODs \( w^{(m)}(x_1) \) and values of \( y(x_1, x_2) \) at the nodal points within the PWAS domain \( V^{(a)} \), i.e. \( y^T(x_1, x_2) \), are unknown. The traction vectors \( \mathbf{q} \) introduced at the intersection \( S^- \) of domains \( V^{(a)} \) and \( V^{(0)} \) are assumed equal for both domains and expressed in terms of splines

\[ s^+(x) = \begin{cases} 1 - x, & 0 \leq x \leq 1 \\ 0, & \text{otherwise} \end{cases} \quad s^-(x) = \begin{cases} 1 + x, & -1 \leq x \leq 0 \\ 0, & \text{otherwise} \end{cases} \] (19)

Based at the nodal points belonging to the contact area \( S^- \). Employing the special index \( J \) to number nodes \( \chi_J \) lying at \( S^- \), \( q(x_1) \) is expanded as follows

\[ q(x_1) = \sum_J q^J s_J(x_1), \] (20)

Here \( s_J(x_1) \) are the combinations of splines (19) with basis at nodal point \( \chi_J \). The Fourier transform of \( q(x_1) \) is obtained via the application of the Fourier transform to (20):

\[ Q(\alpha) = \sum_J q^J S_J(\alpha), \] (21)

where \( S_J \) are Fourier transforms of the splines (19).

Thus, a system of the linear algebraic equations with respect to the vector of unknowns

\[ \mathbf{g} = \{ y_1^I, y_2^I, y_3^I, q_1^I, q_2^I, \gamma_{11}^{(1)}, \gamma_{12}^{(1)}, \cdots, \gamma_{11}^{(M)}, \gamma_{12}^{(M)} \} \]
composed of expansion coefficients can be written:

\[
\begin{pmatrix}
A_{ij} & B_{jk} & 0 & \cdots & 0 \\
C_{ij} & D_{jk} & F^{(1)}_{jk} & \cdots & F^{(M)}_{jk} \\
0 & C^{(1)}_{jk} & H^{(11)}_{jk} & \cdots & H^{(1M)}_{jk} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & C^{(M)}_{jk} & H^{(M1)}_{jk} & \cdots & H^{(MM)}_{jk}
\end{pmatrix}
\begin{pmatrix}
y \\
q \\
\gamma^{(1)} \\
\vdots \\
\gamma^{(M)}
\end{pmatrix}
= \begin{pmatrix}
V \\
0 \\
0 \\
\vdots \\
0
\end{pmatrix}
\] (22)

The first set of equations in the system is obtained via the substitution of (13) and (20) into (11) and (12). The formulae for \(A_{ij}\) and \(B_{jk}\) are the same as given in [1]. The second set arises from the condition of the continuity of the displacement vector \(u_{i}^{(in)} + \sum_{m=0}^{M} u_{i}^{(m)} = y_{i}, \quad x \in S^{-}\). (23)

In order to satisfy (23), two methods have been applied: collocation method with points \(\chi_{J}\) and Bubnov-Galerkin. Matrices forming the system have different values. In the case of the collocation method, substitution of (14) and (15) into equality (23) gives

\[
C\cdot^{J;IJn}_{nJ} = \delta_{JJ}\delta_{nj},
\]

\[
D\cdot^{J;JK}_{JK} = -\frac{1}{2\pi} \int_{\Gamma} K_{jk}^{(0)}(\alpha,0)S_{j}\gamma(\alpha)e^{-in\chi_{J'}}d\alpha,
\]

\[
F^{(m)}_{J'n;lk} = -\frac{1}{2\pi} \int_{\Gamma} K_{jk}^{(m)}(\alpha,0)P_{n}(\alpha)e^{-in\chi_{J'}}d\alpha,
\]

while employment of Bubnov-Galerkin method leads to the following relations:

\[
C\cdot^{J;n}_{J;nj} = B_{IJ}\delta_{nj},
\]

\[
D\cdot^{J;JK}_{JK} = -\frac{1}{2\pi} \int_{\Gamma} K_{jk}^{(0)}(\alpha,0)S_{j}\gamma(\alpha^{*})d\alpha,
\]

\[
F^{(m)}_{J'n;lk} = -\frac{1}{2\pi} \int_{\Gamma} K_{jk}^{(m)}(\alpha,0)P_{n}(\alpha)S_{j'}^{*}(\alpha^{*})d\alpha.
\]

The representations (16)–(17) are substituted into boundary conditions (7) and Bubnov-Galerkin method only is applied. The resulting equations are components of the system (22):

\[
C\cdot^{m}_{J';ij} = -\frac{1}{2\pi} \int_{\Gamma} T_{jk}^{(0)}(\alpha,-d_{m'})S_{j}\gamma(\alpha^{*})d\alpha,
\]

\[
H\cdot^{mm'}_{n'n;jk} = -\frac{1}{2\pi} \int_{\Gamma} T_{jk}^{(m)}(\alpha,-d_{m'})P_{n}(\alpha)P_{n'}^{*}(\alpha^{*})d\alpha.
\]
6 NUMERICAL ANALYSIS

In this section, some examples of computations provided by the SAHA are given for the piezoelectric transducer of width \( w_a = 10 \) mm and height \( h_a = 1 \) mm made of PIC155 material and the aluminum elastic structure (material properties can be found in [1]). The input voltage signal is applied at the lower boundary of the PWAS \( V^- = 30 \) V, while the upper one is grounded \( (V^+ = 0 \) V).

\[
|u_2|, \text{ nm}
\]

![Figure 2: Amplitudes of out-of-plane displacements \( |u_2(x_1,0)| \) at the surface of the waveguide with \( M = 1 \) crack at frequency \( f = 100 \) kHz](image)

In [1], the semi-empirical formulae for the number of elements for the SAHA employed for one transducer depending on frequency was derived. According to the estimation, the number of nodal points should be more than 12 nodes per wavelength. The results presented here are obtained using this estimation, when the PWAS has been discretized via the FDSEM. The main focus here is on the number of Chebyshev polynomials necessary to compute solution with good accuracy. Figures 2 and 3 demonstrate amplitudes of out-of-plane displacements at the upper surface \( x_2 = 0 \) of the waveguide with \( M = 1 \) crack at frequencies \( f = 100 \) kHz and \( f = 500 \) kHz respectively \((\omega = 2\pi f)\). The dimensions of the crack are \( l_1 = 5 \) mm, \( d_1 = 0.5 \) mm, \( c_1 = 30 \) mm, the thickness of the host structure is \( h_1 = 2 \) mm. The results presented at these plots are computed via the SAHA using the collocation method and Galerkin scheme. The results calculated by the standard FEM software (COMSOL Multiphysics) [7], where PML layers [8] were used at the edges of the finite plate, are exhibited in the figures as well. One can observe a good agreement between the FEM solution and the developed hybrid method. Number of Chebyshev
polynomials necessary for the accurate solution calculation has been determined as $N_1 = 10$ for frequency $f = 100$ kHz and $N_1 = 16$ for frequency $f = 500$ kHz.

Figure 3: Amplitudes of out-of-plane displacements $|u_2(x_1, 0)|$ at the surface of the waveguide with $M = 1$ crack at frequency $f = 500$ kHz

Figure 4: Amplitudes of out-of-plane displacements $|u_2(x_1, 0)|$ at the surface of the waveguide with $M = 3$ cracks at frequency $f = 100$ kHz
Figure 5: Amplitudes of out-of-plane displacements $|u_2(x_1, -H)|$ at the surface of the waveguide with $M = 3$ cracks at frequency $f = 100$ kHz

The out-of-plane displacements on the upper ($x_2 = 0$) and lower ($x_2 = -h_1$) boundaries of an elastic layer at frequency $f = 100$ kHz in the case of impact-induced damage modelled as a stack of three cracks are shown in Figures 4 and 5. The distances between the centres of delaminations and the origin of coordinates have been chosen the same ($c_1 = c_2 = c_3 = 30$ mm), while their depth and sizes were different: $l_1 = 6$ mm, $l_2 = 5$ mm, $l_3 = 4$ mm; $d_1 = 0.25$ mm, $d_2 = 0.5$ mm, $d_3 = 0.75$ mm. Collocation and Galerkin methods have been again used to perform coupling of the two methods in the contact area. Good agreement with the FEM is clearly seen outside the damaged zone. A certain discrepancy in the solutions is observed right under and above the cracks. This disagreement can be explained by a certain difference in eigenfrequencies calculated by the BIEM and the FEM [9].

7 CONCLUSIONS

The coupled hybrid mathematical model based on the FDSEM and the BIEM has been developed. The model can be applied to simulate guided waves excitation by piezoelectric transducer as well as wave propagation and scattering by multiple horizontal delaminations. Two different approaches for coupling two methods in the contact area have been used. The obtained solution has been compared for two variation of the hybrid method with the results calculated with the standard FEM software (COMSOL Multiphysics). Good agreement has been demonstrated, though Galerkin method provides less discrepancy with the FEM.
8 ACKNOWLEDGEMENTS

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REFERENCES


A METHOD FOR MULTI-OBJECTIVE TOPOLOGY OPTIMIZATION OF ACOUSTIC AND FLUID FLOW PROPERTIES

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Key words: Coupled Problems, Brinkman Penalization, Impedance Mismatch, NURBS

Abstract. A framework for multi-objective topology optimization is presented with the purpose to simultaneously optimize both fluid flow and acoustic quantities. The proposed method uses a coupled approach on fixed grids with immersed solid boundaries. For the fluid flow part the incompressible Navier-Stokes equations are solved and the immersed boundaries are modeled with a Brinkman penalization method. The acoustic field is computed by an acoustic/viscous splitting technique and the solution of the resulting linearized Euler equations. The reflecting boundaries are modeled by a mismatch in the acoustic impedance between solid and fluid. To describe the geometry of the boundaries a NURBS-based approach is introduced. Two test cases are investigated to validate the immersed boundary method for the fluid flow problem and the acoustics, respectively. Finally, the capability for topological changes of the proposed method is shown with a multi-objective optimization test case, which is solved with the gradient-free evolutionary algorithm NSGA-II.

1 INTRODUCTION

Topology optimization is a commonly used method in various fields of engineering for improving the design of a product or individual components of it in an early stage of development. Used in the past mainly for structural optimization, it has recently gained increasing attention in other disciplines such as fluid flow or acoustic optimization. However, not much research has been done in simultaneously optimizing the acoustic as well as the fluid flow properties of a coupled problem in a multi-objective manner. This paper therefore deals with the topology optimization of such problems and presents a framework that can be used for this purpose.

Usually, non-body-fitted fixed grids are used for topology optimization to avoid the difficulties that can arise when regenerating a body-fitted grid due to large deformations
or topological changes of the computational domain. For fluid flow problems, one possible approach to realize this, which is also used in the present work, is the Brinkman penalization method [1]. Here arbitrarily complex solid bodies can be introduced into the flow domain, which are modeled as a porous medium with a permeability approaching zero. In order to also consider acoustics in terms of a sound reflection of these bodies, an impedance mismatch between fluid and solid is introduced. This approach is also used by the Impedance Mismatch Method, which was originally proposed by Chung and Morris [2] for steady mean flows and later applied for unsteady non-uniform flows by Cohen et al. [3]. For the numerical description of the interface between solid and fluid an approach proposed by Munz and Schäfer [4] is used, which utilizes non-uniform rational basis splines (NURBS) and uses the coordinates of the control points as design variables. The NURBS allow complex geometries to be described with a small number of design variables compared to other approaches, making it possible to use gradient-free global optimization techniques, such as genetic algorithms. For the numerical solution of the fluid flow as well as the acoustic problem the block-structured in-house solver FASTEST [5] is used. The incompressible Navier-Stokes equations are solved with a finite volume discretization. For the acoustic field an acoustic/viscous splitting technique [6, 7, 8] is used and the acoustic quantities are computed with the linearized Euler equations.

The objective of this work is to investigate the proposed framework with respect to numerical accuracy of the immersed boundary method and its suitability for topology optimization. Two test cases are examined to validate the presented method. For the first problem, a steady flow around a cylinder in a channel is investigated without considering the acoustics and the results are compared with results from the literature. In the second test case, the acoustic scattering of a Gaussian pulse from a cylinder is simulated and the results are compared with an analytical solution. Finally, the capability for topological changes of the proposed method is shown with a multi-objective optimization test case. Here the pressure drop of a channel flow and the acoustic permeability of the channel are minimized simultaneously. The gradient-free Non-dominated Sorting Genetic Algorithm II (NSGA-II) [9] is used to optimize these two competing objective functions.

2 NUMERICAL FRAMEWORK

In the following, the framework for topology optimization of multi-objective problems is presented. First the numerical description of the interface is discussed. Then the governing equations are introduced and a short overview of the optimization is given. Finally, the process of the complete framework is summarized.

2.1 Numerical description of the interface

The basis of the presented framework is a NURBS-based approach to describe the interface between solid and fluid, which was proposed by Munz and Schäfer [4]. Here the control point coordinates of the NURBS are coupled to the design variables of the
optimization algorithm, which allows the optimizer to change the geometry of the interface. The NURBS are, in the two-dimensional case, transformed into polygons, which are then used to calculate the volume fraction $\varphi$ of the solid in each control volume. This leads to the three possible cases

$$\quad x_i \in \begin{cases} 
\Omega_f & \text{if } \varphi(x_i) = 0, \\
\Omega_s & \text{if } \varphi(x_i) = 1, \\
\partial\Omega_s & \text{if } 0 < \varphi(x_i) < 1,
\end{cases}$$  

(1)

where $\Omega_f$ is the fluid part of the computational domain, $\Omega_s$ is the solid part and $\partial\Omega_s$ is the interface between the two. Here, a smooth transition at the interface is necessary to obtain a continuous objective function. The volume fraction is calculated using the Sutherland-Hodgman algorithm [10]. In this algorithm the polygons derived from the NURBS curves are clipped against each control volume. The area of the resulting clipped polygon is then set in ratio to the total area of the control volume to determine the volume fraction of the solid. By introducing multiple NURBS, which may overlap each other or disappear, it is also possible to realize topological changes in the domain during the optimization process. The disappearance is achieved by the fact that the algorithm for calculating the volume fraction is designed to return a negative value if a polygon or parts of a polygon “twist”. This means that these parts of the polygon change their counting direction, for example from clockwise to counterclockwise. A negative volume fraction is then assumed to be equal to a volume fraction of zero.

2.2 Governing equations

For the derivation of the aeroacoustic equations an acoustic/viscous splitting technique is used, which was originally proposed by Hardin and Pope [6], then slightly modified by Shen and Sørensen [7] and later further developed by Kornhaas [8]. Here the fluid flow quantities are decomposed into an incompressible part and an acoustic perturbation, which reads

$$\quad \rho = \rho^{\text{inc}} + \rho^{\text{ac}}, \quad u_i = u_i^{\text{inc}} + u_i^{\text{ac}}, \quad p = p^{\text{inc}} + p^{\text{ac}},$$  

(2)

with the density $\rho$, the flow velocity $u_i$ and the pressure $p$. The superscript $(\cdot)^{\text{inc}}$ indicates the incompressible part and the superscript $(\cdot)^{\text{ac}}$ the acoustic perturbation.

Fluid flow equations To compute the fluid flow, the incompressible Navier-Stokes equations are solved. In order to take the immersed boundaries into account, the momentum equation is extended by a penalization term. The equations then read

$$\quad \frac{\partial u_i^{\text{inc}}}{\partial x_i} = 0, \quad \rho^{\text{inc}} \frac{\partial u_i^{\text{inc}}}{\partial t} + \rho^{\text{inc}} \frac{\partial \left( u_i^{\text{inc}} u_j^{\text{inc}} \right)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial u_i^{\text{inc}}}{\partial x_j} + \frac{\partial u_j^{\text{inc}}}{\partial x_i} \right) \right] - \frac{\partial p^{\text{inc}}}{\partial x_i} + \rho^{\text{inc}} f_i - \alpha u_i^{\text{inc}},$$  

(3)
with the time $t$, the dynamic viscosity $\mu$, the external body forces $f_i$ and the Brinkman penalization parameter
\[ \alpha (\varphi) = \alpha_f + (\alpha_s - \alpha_f) \varphi, \] (5)
where $\alpha_f$ refers to the fluid region and $\alpha_s$ to the solid region. The value for $\alpha_f$ is set to zero for the present work, which, together with the volume fraction $\varphi$, causes the penalization term to disappear in the fluid area, leading to the original Navier-Stokes equations. To realize the no-slip boundary condition at the interface of the solid, a high value for $\alpha_s$ has to be chosen, which causes the flow velocity in the solid to approach zero. According to [11], where a value of $\alpha > 10^4$ is suggested as sufficiently large, the value inside the solid parts is set to $\alpha_s = 10^5$ for the present work.

**Acoustic equations** For the computation of the acoustics the linearized Euler equations
\[
\frac{\partial \rho^{\text{ac}}}{\partial t} + \rho^{\text{inc}} \frac{\partial u_{i}^{\text{ac}}}{\partial x_i} + u_{i}^{\text{inc}} \frac{\partial \rho^{\text{ac}}}{\partial x_i} = 0, \]
\[ \rho^{\text{inc}} \frac{\partial u_{i}^{\text{ac}}}{\partial t} + \rho^{\text{inc}} u_{j}^{\text{inc}} \frac{\partial u_{i}^{\text{ac}}}{\partial x_j} + \frac{\partial p^{\text{ac}}}{\partial x_i} = 0, \]
\[ \frac{\partial p^{\text{ac}}}{\partial t} + c^2 \rho^{\text{inc}} \frac{\partial u_{i}^{\text{ac}}}{\partial x_i} + u_{i}^{\text{inc}} \frac{\partial p^{\text{ac}}}{\partial x_i} = - \frac{\partial p^{\text{inc}}}{\partial t} \] (8)
are solved with the speed of sound $c$. To obtain the reflection of the acoustic waves at the immersed boundaries, the density $\rho^{\text{inc}}$ is increased. This causes a mismatch in the acoustic impedance
\[ Z = \rho^{\text{inc}} c \] (9)
between fluid and solid. According to the reflection coefficient
\[ C_r = \frac{p_{\text{ref}}}{p_{\text{in}}} = \frac{Z_2 - Z_1}{Z_2 + Z_1} \] (10)
this leads to a reflection of the sound wave. Here $p_{\text{in}}$ is the incident and $p_{\text{ref}}$ is the reflected acoustic pressure. The impedance of the fluid is $Z_1$ and the impedance of the solid is $Z_2$. For $Z_2 = Z_1$ the reflection coefficient equals zero and therefore no reflection occurs. For $Z_2 > Z_1$ the value of $C_r$ becomes positive, so there is reflection without a phase change, which is the desired behaviour. On the other hand, for $Z_2 < Z_1$ the value of $C_r$ becomes negative and thus the acoustic wave experiences a phase reversal. Therefore, the density is defined as
\[ \rho^{\text{inc}} (\varphi) = \rho_{\text{f}}^{\text{inc}} + (\rho_{\text{s}}^{\text{inc}} - \rho_{\text{f}}^{\text{inc}}) \varphi, \] (11)
where $\rho_{\text{f}}^{\text{inc}}$ refers to the density in the fluid and $\rho_{\text{s}}^{\text{inc}}$ to density in the solid. In the present work the solid density is increased by a factor of 1000 compared to the fluid density. This leads to a theoretical amplitude error of the reflected wave of 0.2% according to equation (10). It should be noted that the increased density is only used to compute the acoustics.
2.3 Optimization

The last part of the framework is the optimizer. There are a variety of optimization methods to perform a multi-objective optimization, which can be roughly divided into gradient-free and gradient-based methods. A gradient-based optimization can be advantageous in terms of computational speed, especially with a large number of design variables, if an adjoint method is used. However, one major problem with these methods is that they tend to get stuck in local minima, which can occur especially during topology optimizations, since the value of the objective function can change abruptly due to a change in the topology of the computational domain. To overcome this problem, the present work uses the comparatively small number of design variables resulting from the NURBS-based approach to make it feasible to use the gradient-free evolutionary algorithm NSGA-II.

2.4 Procedure of the framework

The complete process of a multi-objective topology optimization with the presented framework is shown schematically in Figure 1 and can be summarized as follows:

1. Generation of NURBS depending on design variables
2. Derivation of polygons $P$ and transfer to the fluid flow as well as to the acoustic solver
3. Calculation of volume fractions using the Sutherland-Hodgman algorithm within the solver
4. Solving flow equations and transfer of fluid objective function $J^f$ to the optimizer as well as transfer of resulting fluid flow quantities to the acoustic solver
5. Solving acoustic equations and transfer of acoustic objective function $J^a$ to the optimizer
6. Checking convergence criteria and repeating the process if criteria are not reached

3 VALIDATION

To validate the proposed method, two different test cases are investigated. First a steady channel flow around a cylinder at Re = 20 is simulated. The cylinder is modeled with the Brinkman penalization method and the results are compared to results from literature. For the second test case, the acoustic scattering of a Gaussian pulse from a cylinder is simulated. To model the reflecting solid boundaries, a mismatch in the acoustic impedance between fluid and solid is introduced. The acoustic pressure is measured over time at three monitoring points and the results are compared with an analytical solution.
3.1 Steady channel flow around a cylinder

The first test case is intended to investigate the suitability of the Brinkman penalization method for modeling solid boundaries. For this purpose, a two-dimensional steady flow around a circular cylinder in a channel is considered. The benchmark problem is taken from [12], where it is referred to as test case 2D-1 and where several results for different solution approaches can be found. The geometry of this test case is shown in Figure 2. The kinematic viscosity is set to $\nu = 0.001 \text{ m}^2\text{s}^{-1}$ and the fluid density to $\rho = 1.0 \text{ kg m}^{-3}$.

![Figure 2: Geometry and boundary conditions of the channel flow test case](image)

At the inlet, a parabolic flow velocity profile

$$u(0, y) = 4u_m y \left( \frac{h - y}{h^2} \right), \quad v = 0$$

(12)

is applied with the channel height $h = 0.41 \text{ m}$ and the maximum flow velocity $u_m = 0.3 \text{ m s}^{-1}$, which leads to a Reynolds number of $\text{Re} = \bar{u} d/\nu = 20$. Here the mean velocity is defined as $\bar{u} = 2u_m/3$. The Brinkman penalization parameter is set to $\alpha = 10^5$. The results of the simulations are compared with two of the criteria that can be found in [12]. These are the length of the recirculation zone $L_a$, as well as the pressure difference between the front and the back of the cylinder $\Delta P$. The computations are carried out on three successively refined grids with a maximum of $800 \times 400$ control volumes. The values of the volume fraction in the vicinity of the cylinder are shown exemplary for the coarsest grid in Figure 3 and the results of the simulations are shown in Table 1. For both criteria, the results are

![Figure 3: Volume fraction](image)

<table>
<thead>
<tr>
<th>Grid</th>
<th>$L_a$</th>
<th>$\Delta P$</th>
</tr>
</thead>
<tbody>
<tr>
<td>200 $\times$ 100</td>
<td>0.0847</td>
<td>0.1185</td>
</tr>
<tr>
<td>400 $\times$ 200</td>
<td>0.0844</td>
<td>0.1167</td>
</tr>
<tr>
<td>800 $\times$ 400</td>
<td>0.0849</td>
<td>0.1175</td>
</tr>
<tr>
<td>2D-1 [12]</td>
<td>[0.0842, 0.0852]</td>
<td>[0.1172, 0.1176]</td>
</tr>
</tbody>
</table>

![Table 1: Benchmark results](image)
in the range of the results of [12]. Therefore, it is assumed that the Brinkman penalization method is suitable to model solid boundary conditions.

3.2 Scattering of acoustic waves from a cylinder

The second benchmark test case is an acoustic two-dimensional initial value problem without background flow. It is particularly well suited to investigate the scattering of acoustic waves at curved solid boundaries as they can usually occur during topology optimization. The test case corresponds to problem 2 of category 2 in [13], where an analytical solution to this problem can also be found. All variables are non-dimensionalized using the diameter $d$ of the cylinder as length scale, $c$ as velocity scale, $d/c$ as time scale, $\rho_{\text{inc}}$ as density scale and $\rho_{\text{inc}}c^2$ as pressure scale. The basic configuration of the test case is shown in Figure 4. Here, the circular cylinder is located in the center of a square computational domain with $x, y \in [-10, 10]$. Next to this cylinder a Gaussian pressure wave is initiated. This pressure wave then propagates over time, is reflected from the cylinder and finally leaves the computational domain. The acoustic pressure is measured over time at the three monitoring points A ($r = 5, \theta = 90^\circ$), B ($r = 5, \theta = 135^\circ$) and C ($r = 5, \theta = 180^\circ$). Since there is only an interest to investigate whether the introduced impedance mismatch is suitable to model solid boundaries, the half-width of the Gaussian pulse is increased compared to the original test case in order to reduce the influence of numerical diffusion. The density of the solid is set to $\rho_{\text{inc}} = 1000$ and the center of the Gaussian pulse is located at $x_s = 4$ and $y_s = 0$ with the half-width $w = 0.5$. The initial conditions for this test case are $t = 0$, $u^{\text{ac}} = v^{\text{ac}} = 0$ and

$$p^{\text{inc}} = \exp \left[ - \ln 2 \left( \frac{(x - x_s)^2 + (y - y_s)^2}{w^2} \right) \right]. \quad (13)$$

The problem is solved on three successively refined Cartesian grids with $512 \times 512$, $1024 \times 1024$ and $2048 \times 2048$ control volumes. To avoid spurious oscillations the Osher
flux limiter [14] with $\beta = 1$ is used according to [8]. The time step size is $\Delta t = 0.0125$ for the coarsest, $\Delta t = 0.00625$ for the medium and $\Delta t = 0.003125$ for the finest grid, yielding a constant acoustic CFL number of 0.32. Figure 5 shows the contour plots of the acoustic pressure for the time steps $t = 2, 4, 6$ on the finest grid. As can be seen,

![Figure 5: Scattering of the initial Gaussian pulse from the cylinder at different time steps](image)

the acoustic wave propagates smoothly in the computational domain and is scattered at the cylinder. Figure 6 compares the results of the simulations with an analytical solution for the three monitoring points in the time interval from $t = 5$ to $t = 11$. For

![Figure 6: Acoustic pressure over time for the scattering of the Gaussian pulse at the three monitoring points](image)

the undisturbed acoustic wave, which first reaches point A ($\theta = 90^\circ$) and then point B ($\theta = 135^\circ$), the amplitude approaches the analytical solution as the grid size increases. At point C ($\theta = 180^\circ$), however, the wave diffracted by the cylinder shows a time-shift
of about $\Delta t = 0.01$ compared to the analytical solution. In the further course, the wave scattered from the cylinder reaches the monitoring points where it shows an amplitude error which is almost independent of the grid size. Nevertheless, the main characteristics of the wave propagation are correctly represented and the simulation is generally in good agreement with the analytical solution. In addition, topology optimization is essentially about creating a first draft rather than a detailed design, so the accuracy achieved is sufficient to use the proposed approach for topology optimization.

4 APPLICATION TO MULTI-OBJECTIVE OPTIMIZATION

In the following, a multi-objective topology optimization of a two-dimensional channel is investigated. Two competing objective functions are considered, which are the pressure drop between inlet and outlet as well as the acoustic permeability of the channel, both of which should be minimized. The geometry of the test case is shown in Figure 7. In order to quantify the acoustic permeability, an acoustic wave is initiated at the position $x_s = 1.0 \text{ m}$ with the initial conditions

$$p^{ac} = 1.5 \exp \left[ - \ln 2 \left( \frac{(x - x_s)^2}{w^2} \right) \right] \text{ N m}^{-2}, \quad (14)$$

$$u^{ac} = 0.001 \exp \left[ - \ln 2 \left( \frac{(x - x_s)^2}{w^2} \right) \right] \text{ m s}^{-1}, \quad v^{ac} = 0 \text{ m s}^{-1}, \quad (15)$$

and a half-width of $w = 0.05 \text{ m}$. The speed of sound is set to $c = 1000 \text{ m s}^{-1}$. Two closed NURBS curves, whose shapes are varied by the optimization, are introduced into the channel. Both of these curves are defined by six control points, whereby the first two points are repeated according to the degree of the curves. The positions of the control points are defined relative to the centers of the curves, which are $(2.0, 0.3)$ and $(2.0, 0.7)$. An unclamped, uniform node vector $U = \{0, \ldots, 8\}$ is used and all weights are set to one. Each of the control point coordinates is determined by a separate design variable, resulting in a total of 16 design variables. The upper and lower bounds of the design variables are defined.
in such a way that there will always be a gap at the top and bottom of the channel, but the curves can overlap in the middle. The acoustic pressure is measured at the monitoring point $P = (3.5, 0.5)$ and the maximum value within a time interval of $\Delta t = 0.004 \text{s}$ is determined and used as objective function. For the inlet boundary condition, a parabolic flow velocity profile according to equation (12) is used with a channel height $h = 1 \text{m}$ and a mean flow velocity $\bar{u} = 20 \text{m/s}^{-1}$. The kinematic viscosity is set to $\nu = 1.0 \text{m}^2\text{s}^{-1}$ and the fluid density to $\rho_{\text{inc}} = 1.0 \text{kg/m}^3$, which leads to a Reynolds number of $\text{Re} = 20$, based on the channel height. In order to obtain the sound reflection by the impedance mismatch, the solid density is set to $\rho_{\text{inc}} = 1000 \text{kg/m}^3$. Since two competing objective functions are to be optimized, the gradient-free NSGA-II is used. The two objective functions should then come into conflict, since it is expected that minimizing the pressure drop leads to a channel without obstacles, while the optimum for minimum acoustic permeability should correspond to the opposite, i.e. a channel with the largest possible reflective obstacles. The results of the topology optimization are shown in Figure 8 and as expected a set of Pareto optimal solutions can be seen. On the right side of Figure 8, the optimized geometries for the extreme points as well as for two other characteristic points from the Pareto front are shown as examples. In case of a minimal pressure drop (point a), the impermeable areas disappear as predicted because the polygons have twisted, as explained in section 2.1. On the way to a minimum of the acoustic permeability (point b and c), the two NURBS curves increasingly close the channel. At the optimum of the acoustic permeability (point d), the upper curve reaches the maximum height and the lower curve its minimum height. In the middle, however, the expected overlap does not occur, leaving a small gap between the two curves. At this point, the two curves approach each other until they both intersect the same control volume but do not cover it completely, resulting

![Figure 8: Pareto set of the multi-objective optimization and the geometry of four selected points (a-d) with the resulting flow velocity fields](image)

Figure 8: Pareto set of the multi-objective optimization and the geometry of four selected points (a-d) with the resulting flow velocity fields
in an intermediate value for the Brinkman penalization parameter and the impedance mismatch, respectively. This value is just large enough to reflect most of the incident acoustic wave, but not large enough to completely prevent the fluid flow between the two curves. This can also be seen in Figure 8 in the plot for point d, where the light blue area between the two curves indicates a slow but non-zero flow. The acoustic permeability has thus reached an optimum which additionally allows to reduce the pressure drop slightly compared to two overlapping curves. This state is actually not desired, since it is based on the unphysical assumption that there may be areas which are partially permeable. However, these intermediate values in the control volumes serve only to ensure smooth objective functions and should not to be exploited by the optimizer to improve an objective function. Further research is therefore needed at this point to prevent this behaviour.

5 CONCLUSIONS

A framework for multi-objective topology optimization of fluid flows and acoustics has been presented, which uses a coupled aeroacoustic solver for all computations. It is based on the solution of the incompressible Navier-Stokes equations for the fluid flow problem and an acoustic/viscous splitting technique together with the linearized Euler equations for the acoustic problem. For the fluid flow computations it uses the Brinkman penalization method to account for solid areas in the flow domain, while for the acoustics an impedance mismatch between solid and fluid is introduced. In both cases the geometry of the solid boundaries is mathematically described by NURBS curves. The control point coordinates of these NURBS are used as design variables, which has the advantage that complex geometries can be described with a relatively small number of parameters. Thus, the number of design variables can be reduced to such an extent that it is possible to use gradient-free optimization methods, like the Non-dominated Sorting Genetic Algorithm (NSGA-II).

The proposed method has been validated with two test cases taken from literature and has shown a good agreement. Finally, a multi-objective optimization problem has been investigated, which has basically shown the expected results, but also revealed a problem. The optimizer exploits the possible intermediate values in the control volumes to improve the objective functions. Although this is a logical result for the optimization, it was not expected and further research is needed to prevent such loopholes for the optimizer. The next step will be to use this coupled framework for the topology optimization of aeroacoustic problems, where the acoustic sources are generated by the fluid flow.

REFERENCES


ANALYSIS OF FUNCTIONALLY GRADED MATERIAL ACTUATOR USING NEW FINITE ELEMENTS

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Key words: Instructions, Coupled Problems, Multiphysics Problems, Applications, Computing Methods.

Abstract. Actuator is a mechatronic system that transforms one type of energy (e.g. electric energy) into the mechanical displacement and mechanical force (mechanical energy). Nowadays, these actuators can be made of Functionally Graded Materials (FGM) to ensure simple shape of the actuator and to improve its effectiveness, particularly for micro systems. FGM is built as a mixture of two or more constituents which have almost the same geometry and dimensions. The variation of macroscopic material properties can be induced by variation of both the volume fractions and material properties (e.g. by a non-homogeneous temperature field) of the FGM constituents.

The paper deals with a new approach in analysing of the systems made of FGM using our new beam finite elements. Multiphysical analysis (weak coupled electro-thermo-mechanical analysis) and spatial continuous variation of material properties are supported. The analysis of the micro actuator with constant cross section made of FGM is presented in the paper. This simple-shaped actuator is supplied by electric current and the efficiency of the actuator is optimised. The solution results will be compared with those obtained by using solid elements of a FEM commercial program.

1 INTRODUCTION

Nowadays, the scientific and technological progress are already at such level that for the development of new systems in classical way (such as mechanical and heating systems, systems in construction industry, etc.) it is not enough to propose new shapes of components and their optimization, but it requires use of new materials with the desired properties that lie outside the parameters of materials commonly used for that purpose. New materials like Functionally Graded Material (FGM) are necessary for sophisticated structures like Micro-Electro-Mechanical Systems (MEMS), advanced electronic devices, etc. In all these applications, using new materials like FGM can greatly improve efficiency of a system e.g. classic shape of
actuator (Figure 1a) can be replaced by new type – simply-shaped actuator (Figure 1b) where functionality is caused by varying material properties.

![Images of actuator shapes](image)

**Figure 1:** a) Classic shape of MEMS actuator, b) New shape of FGM actuator

FGM is built as a mixture of two or more constituents which have almost the same geometry and dimensions. From macroscopic point of view, FGM is isotropic in each material point but the material properties can vary continuously or discontinuously in one, two or three directions. The variation of macroscopic material properties can be caused by varying the volume fraction of the constituents or with varying of the constituents’ material properties (e.g. by non-homogeneous temperature field). The methods based on the homogenization theory have been designed and successfully applied to determine the effective material properties of heterogeneous materials from the corresponding material behaviour of the constituents (and of the interfaces between them) and from the geometrical arrangement of the phases. Coupled electro-thermo-mechanical analysis of actuator made of FGM using our new beam finite elements will be presented.

2 FEM EQUATIONS FOR COUPLED ELECTRO - THERMO - MECHANICAL ANALYSIS

Derivation process of the new FEM equations for coupled electro-thermo-mechanical element is based on differential equations for electric thermal and structural fields for 1D type of analysis, respectively. All quantities in following equations are the polynomial functions of $x$. Homogenization process of the varying material properties and the calculation of other effective finite element parameters have been done by extended mixture rule [1] and multilayer method is fully described in [2, 3].

2.1 Differential equations

Homogeneous 1D static differential equation for FGM (with non-constant coefficients on the left-hand side) for electric field with boundary conditions has a form:

$$-\sigma(x) \frac{d^2 \varphi(x)}{dx^2} - \frac{d \sigma(x)}{dx} \frac{d \varphi(x)}{dx} = 0$$

$$\varphi(0) = \varphi_0 \quad J(L) = J_L$$

where $x$ [m] is the longitudinal coordinate, $\varphi(x)$ [V] is the electric potential, $\sigma(x)$ [S/m] is the specific electric conductivity and $J(x)$ [A/m$^2$] is the current density.

Static differential equation for heat transfer with non-constant auxiliary thermal source $Q(x)$ [W/m$^3$] in the volume, with non-constant convective heat transfer coefficient $a(x)$ [W/m$^2$K$^{-1}$] and with coupled to the electric field has a form (2). One-way coupling between the electric and thermal field is provided by Joule heat $P_{jou}(x)$ [W/m$^3$], that can be calculated as one of the outputs from electric analysis and it enters the thermal analysis as volume heat (beside or instead of $Q(x)$).
\[-\lambda(x) \frac{dT(x)}{dx} - \frac{d\lambda(x)}{dx} T(x) + \alpha(x) T(x)^{\circ} = P_{J_1}(x) + Q(x) + \alpha(x) T_{amb}^{\circ}\]

with boundary conditions, e.g.:

\[T(0) = 0 \quad q(L) = q_L\]

where \(\lambda(x)\) [Wm\(^{-1}\)K\(^{-1}\)] is the thermal conductivity, \(T(x)\) [K] is the temperature, \(\alpha\) [m] is the perimeter, \(A\) [m\(^2\)] is the cross section area, \(T_{amb}\) [K] is the ambient temperature and \(q(x)\) [Wm\(^{-2}\)] is the heat flux.

Homogeneous differential equation for structural analysis with effect of thermal expansion (coupling with the electro-thermal analysis) for pure tensile and compressive stress has a form:

\[E_{L}^{NH}(x) \frac{du(x)}{dx} + dE_{L}^{NH}(x) \frac{du(x)}{dx} = -\frac{n(x)}{A} + \alpha_t(x) \Delta t(x) \frac{dE_{L}^{NH}(x)}{dx} + \Delta T(x) E_{L}^{NH}(x) \frac{d\alpha_t(x)}{dx} + E_{L}^{NH}(x) \alpha_t(x) \frac{d\Delta t(x)}{dx}\]

with boundary conditions, e.g.:

\[u(0) = u_0 \quad \sigma_N^*(L) = \sigma_{N,L}^*\]

where \(E_{L}^{NH}(x)\) [Pa] is the Young modulus for tension/compression, \(u(x)\) [m] is the displacement, \(n(x)\) [Nm\(^{-1}\)] are the distributed axial forces, \(N(x)\) [N] is the normal force and \(\alpha_t\) [K\(^{-1}\)] is the coefficient of thermal expansion.

Homogeneous differential equation for structural analysis for bending has a form:

\[\frac{d^2 w(x)}{dx^2} = \frac{M(x)}{E_{L}^{MH}(x) I_y}\]

with boundary conditions, e.g.:

\[w(0) = w_0 \quad \sigma_y(L) = \sigma_{y,L}\]

where \(w(x)\) [m] is the transversal displacement, \(M(x)\) [Nm] is the bending moment, \(E_{L}^{MH}(x)\) is the Young modulus for bending, \(\varphi_0(x)\) [rad] is the angle of the cross section rotation, \(I_y\) [m\(^4\)] is the quadratic moment of the cross section.

The solution of these differential equations is based on numerical method for solving 1D differential equation with non-constant coefficients and with right-hand side described in [4] in detail.

### 2.2 New beam/link FGM finite element equations

The finite element equations for electric analysis in FGM link have a form:

\[
\begin{bmatrix}
\begin{array}{cc}
\frac{c_0(L)}{c_1(L)}
\end{array}
\end{bmatrix}
- \left( \begin{array}{cc}
c_0(L) - \frac{c_1(L) c_0'(L)}{c_1'(L)}
\end{array} \right)^{-1}
\begin{bmatrix}
\varphi_0
\end{bmatrix}
\cdot
\begin{bmatrix}
\varphi_L
\end{bmatrix}
= \begin{bmatrix}
\frac{c_1(L)}{\sigma_0} J_0
\end{bmatrix}
\begin{bmatrix}
\frac{c_1(L)}{c_1'(L)} J_L
\end{bmatrix}
\]

(8)
FEM equations for thermal analysis considering the convective effect, generated heat and Joule heat (coupling between the electric and thermal field) have a form:

$$
\begin{align*}
&\begin{bmatrix}
    c_0(L) \\
    -\left(c_0(L) - \frac{c_1(L)c_0'(L)}{c_1'(L)}\right)
\end{bmatrix}^{-1} \begin{bmatrix}
    T_0 \\
    T_L
\end{bmatrix} = \\
&= \begin{bmatrix}
    \frac{c_1(L)}{\lambda_0} q_0 - \sum_{j=0}^{g} \varepsilon_j b_{j+2}(L) \\
    \frac{c_1(L)}{c_1'(L)\lambda_L} q_L - \frac{c_1(L)}{c_1'(L)} \sum_{j=0}^{g} \varepsilon_j b'_{j+2}(L) + \sum_{j=0}^{g} \varepsilon_j b_{j+2}(x)
\end{bmatrix}
\end{align*}
$$

(0)

Derived FEM equations for the structural analysis for pure tensile and compressive stress with coupling to the electro-thermal analysis (thermal expansion coefficient) have a form:

$$
\begin{align*}
&\begin{bmatrix}
    c_0(L) \\
    -\left(c_0(L) - \frac{c_1(L)c_0'(L)}{c_1'(L)}\right)
\end{bmatrix}^{-1} \begin{bmatrix}
    u_0 \\
    u_L
\end{bmatrix} = \\
&= \begin{bmatrix}
    \frac{c_1(L)}{E_L^NH_A} N_0 - c_1(L)\alpha_{t0}\Delta T_0 - \sum_{j=0}^{g} \varepsilon_j b_{j+2}(L) \\
    \frac{c_1(L)}{E_L^NH_A} \left(\frac{N_L}{E_L^NH_A} + \alpha_{tL}\Delta T_L - \sum_{j=0}^{g} \varepsilon_j b'_{j+2}(L) \right) + \sum_{j=0}^{g} \varepsilon_j b_{j+2}(L)
\end{bmatrix}
\end{align*}
$$

(10)

and FEM equations for bending of the beam have general form:

$$
\begin{align*}
&\begin{bmatrix}
    K_{11} & K_{12} & K_{13} & K_{14} \\
    K_{21} & K_{22} & K_{23} & K_{24} \\
    K_{31} & K_{32} & K_{33} & K_{34} \\
    K_{41} & K_{42} & K_{43} & K_{44}
\end{bmatrix} \begin{bmatrix}
    w_0 \\
    \varphi_{y,0} \\
    w_L \\
    \varphi_{y,L}
\end{bmatrix} = \begin{bmatrix}
    T_{z,0} \\
    M_0 \\
    T_{z,L} \\
    M_L
\end{bmatrix}
\end{align*}
$$

(11)

where $T_z(x)$ [N] is the transversal force. The terms $c_i(x), c_i'(x), b_i(x), b_i'(x), i \in <0, 1>$ are the transfer functions (for particular solution and for uniform solution) of the differential equations (1) - (6) which can be calculated by simple numerical algorithm [4].

### 3 NUMERICAL EXPERIMENT

Let us consider actuator with constant cross section made of FGM according to Figure 2. It consists of 3 parts (beams) that lengths are: $L_1 = 5$ mm, $L_2 = 0.3$ mm and $L_3 = 5$ mm. Their constant rectangular cross-section is $b = 0.2$ mm and $h = 0.1$ mm.
Actuator is made of FGM that consist of two components: matrix denoted with index $m$ and fibre denoted with index $f$. Material properties of the components are constant (not temperature dependent), Matrix: Young modulus $E_m = 211$ GPa, thermal conductivity $\lambda_m = 80.4$ Wm$^{-1}$K$^{-1}$, electric conductivity $\sigma_m = 1 \times 10^7$ Sm$^{-1}$, thermal expansion coefficient $\alpha_m = 2.18 \times 10^{-5}$ K$^{-1}$; Fibre: Young modulus $E_f = 119$ GPa, thermal conductivity $\lambda_f = 401$ Wm$^{-1}$K$^{-1}$, electric conductivity $\sigma_f = 5.96 \times 10^7$ Sm$^{-1}$, thermal expansion coefficient $\alpha_f = 1.65 \times 10^{-5}$ K$^{-1}$. The variation of material properties is caused by varying volume fraction. Variation of the fibre’s volume fraction has been chosen as the polynomial function of longitudinal ($L$) and lateral ($h$) directions of individual beams. Coordinates for these directions are denoted $x$ and $y$ for the variation of material properties. Through the depth $b$ of the beams the material properties are constant and they are derived from the variation in longitudinal and lateral directions.

Variation of the fibres volume fraction $v_f (x, y)$ for the first (from point A to B) and third beam (from point C to D) are shown in Figure 3. The constant fibres volume fraction $v_f (x, y) = 0.143$ for the second beam (from point B to C) is considered.

The effective material properties (Young modulus for tension/compression $E_{L}^{NH}(x)$ [Pa], Young modulus for bending $E_{L}^{MH}(x)$ [Pa], thermal conductivity $\lambda_{L}^{H}(x)$ [Wm$^{-1}$K$^{-1}$], electric conductivity $\sigma_{L}^{H}(x)$ [Sm$^{-1}$], thermal expansion coefficient $\alpha_{L}^{H}$ [K$^{-1}$]) of the homogenized beam have been calculated by multilayered method [2, 3]. An example of the results for the first beam are:
\[
\sigma_L^H(x) = 4.61 \times 10^7 - 2.67 \times 10^{13} x^2 + 1.53 \times 10^{16} x^3 - 3.16 \times 10^{18} x^4 + 2.23 \times 10^{20} x^5
\]
\[
\lambda_L^H(x) = 313.8 - 1.73 \times 10^6 x^2 + 9.9 \times 10^{10} x^3 - 2.04 \times 10^{13} x^4 + 1.44 \times 10^{15} x^5
\]
\[
E_L^{NH}(x) = 1.44 \times 10^{11} + 4.95 \times 10^{16} x^2 - 2.84 \times 10^{19} x^3 + 5.86 \times 10^{21} x^4 - 4.13 \times 10^{23} x^5
\]
\[
E_L^{MH}(x) = 1.57 \times 10^{11} + 3.7 \times 10^{16} x^2 - 2.12 \times 10^{19} x^3 + 4.37 \times 10^{21} x^4 - 3.08 \times 10^{23} x^5
\]
\[
\alpha_L^H(x) = 1.86 \times 10^{-5} + 9.01 \times 10^{-4} x + 1.45 x^2 - 989.6 x^3 + 2.15 \times 10^5 x^4 - 1.56 \times 10^7 x^5
\]

The homogenized thermal conductivity \( \lambda_L^H(x) \) for the first and third beam is shown in Figure 4.

![Figure 4: Homogenized thermal conductivity, red - beam 1, purple - beam 3](image)

The applied constrains and loads are:
- electric potential and current: \( V_A = 0 \text{ V}, \ I_D = 5 \text{ A} \);
- temperatures: \( T_A = 25 \text{ °C}, \ T_D = 25 \text{ °C} \);
- fixed support: \( u_A = 0 \text{ m}, \ u_D = 0 \text{ m}, \ w_A = 0 \text{ m}, \ w_D = 0 \text{ m}, \)
  \( \varphi_A = 0 \text{ rad}, \ \varphi_D = 0 \text{ rad} \)

The coupled electro-thermo-mechanical analysis of FGM actuator has been done using our new FGM beam/link finite elements. The calculation has been done using software MATHEMATICA. Only three our new finite elements have been used (one for each part). The same problem has been solved using a fine mesh – 29 000 of PLANE223 elements of the FEM program ANSYS (see Figure 5). The average relative difference \( \Delta [\%] \) between quantities calculated by our method and the ANSYS solution has been evaluated.
Electric analysis was performed as the first solution and the nodal electric variables have been obtained (see Table 1).

**Table 1:** The results of electric analysis

<table>
<thead>
<tr>
<th>electric potential [V] new element</th>
<th>ANSYS</th>
<th>Δ [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>φₐ</td>
<td>0.0581</td>
<td>0.0576</td>
</tr>
<tr>
<td>φₖ</td>
<td>0.0656</td>
<td>0.0614</td>
</tr>
<tr>
<td>φₖ</td>
<td>0.0982</td>
<td>0.0937</td>
</tr>
</tbody>
</table>

Thermal analysis was performed as the second one. Distributed thermal load – Joule heat caused by electric current was included into the analysis. The results of thermal analysis are presented in Table 2.

**Table 2:** The results of thermal analysis

<table>
<thead>
<tr>
<th>temperature [°C] new element</th>
<th>ANSYS</th>
<th>Δ [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tₐ</td>
<td>188.70</td>
<td>174.01</td>
</tr>
<tr>
<td>Tₖ</td>
<td>177.08</td>
<td>167.82</td>
</tr>
</tbody>
</table>

Structural analysis is performed as the last analysis, where thermal forces caused by thermal expansion were included into the model. The results of structural analysis are the displacements $u$ for longitudinal direction and $w$ for transversal direction (see Table 3).

**Table 3:** The results of structural analysis

<table>
<thead>
<tr>
<th>displacement [mm] new element</th>
<th>ANSYS</th>
<th>Δ [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u_B$</td>
<td>0.0114</td>
<td>0.0095</td>
</tr>
<tr>
<td>$w_B$</td>
<td>−0.0286</td>
<td>−0.0237</td>
</tr>
<tr>
<td>$u_C$</td>
<td>0.0080</td>
<td>0.0067</td>
</tr>
<tr>
<td>$w_C$</td>
<td>−0.0292</td>
<td>−0.0245</td>
</tr>
</tbody>
</table>
As it can be seen in Tables 1 - 3, there are considerable differences between results obtained by our new element and FEM program ANSYS especially for the analyses (e.g. structural) that are based on the results from preliminary analyses (e.g. thermal and electric analyses). This is caused by the fact that junctions B and C (see Figure 2) are not spot junctions (considered in the beam theory) but they are spatial junctions (see Figure 5), so the current and heat flow in these junctions are not strictly 1D flows as it is considered in the beam theory. This fact also explains lower electric potentials, temperatures and finally displacements in longitudinal and transversal directions in ANSYS results compared to the results from the system based on our new element.

The comparison of total deformation, temperature distribution and electric potential distribution of the FGM actuator calculated by our new approach and commercial FEM program ANSYS is shown in Figure 6.

![Figure 6: Results of electro-thermo-mechanical analysis, top left – electric potential, top right – temperature, bottom – displacement (displacement scaling 5:1)](image)

4 CONCLUSIONS

New FEM equations for weak coupled static electro-thermo-mechanical analysis of the FGM beam structures have been presented in this contribution. The numerical experiment – multiphysical analysis of micro actuator made of FGM has been done using our new approach and obtained results have been compared with ones obtained by solution with software
ACKNOWLEDGEMENT
This work was supported by the Slovak Grant Agency: VEGA No. 1/0102/18, VEGA No. 1/0081/18, APVV-14-0613 and APVV-0246-12. Authors are also grateful to the HPC Centre at the STU - SIVVP project, ITMS code 26230120002.

REFERENCES
FLOW TOPOLOGY OPTIMIZATION IN PERIODIC DOMAINS WITH APPLICATION TO MICRO HEAT EXCHANGER OPTIMIZATION

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Key words: Topology optimization, Density–based, External flow, Micro heat–exchangers, Pseudo–spectral scheme

Abstract. The focus of this paper is topology optimization of fluid flow systems, particularly 2D laminar flows, widely found in microfluidic devices. The flow equations are solved numerically using a pseudo–spectral scheme and accurate derivatives are directly derived to facilitate gradient–based optimization. The proposed tool is utilized to enhance the performance of micro heat exchangers, in terms of minimizing the total pressure drop required to be supplied by micro pumps. It is well known that the geometry and arrangement of pinned fins play a pivotal role in total pressure drop of the system. Hence, in this work we aim to find the optimum topologies for various test cases by minimization of drag force on pinned fins with a constraint on volume.

1 Introduction

Optimal design of flow systems is an important concern meanwhile a complex task, aiming performance enhancements. The accurate analysis of flow behavior is widely done using computational fluid dynamics (CFD) tools. Topology optimization (TO) [1] is a powerful approach towards finding the optimal systems. In contrast to shape optimization techniques, TO is free to modify topological features of a system to find the optimum design and ideally does not rely on initial designs. TO was initially developed for design of solid structures, and has been widely studied in the past decades (see [2]). A common TO approach is the so-called density-based method. In this approach material distribution is stated by design variables in space, ranging from 0 (empty) to 1 (full solid). Topology optimization in flow systems can be treated in a similar way: a continuous material function, ranging from 0 to 1, is used to define whether at a specific location the material

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is fluid, solid, or a porous material (solid with permeability) for the case of values between 0 and 1 [3].

TO of flow systems are widely studied, particularly for internal flow problems. For example, [4] studied steady channel flow case, [5] using the lattice Boltzmann method for TO of unsteady flow problems. More recently [6] developed a TO tool for turbulent flows. External flow TO studies are very limited in literature, possibly due to the deficiency of the conventional density-based approach, in which the pressure field is propagated through solid bodies [7]. External flow TO using density based methods are mainly developed in the basis of fluid–structure interaction (FSI) problems [8, 9] and [10].

In this work we present a TO tool developed to find the optimal topologies of pin fin type micro heat exchangers [11]. A common configuration of such devices is an array of cylindrical pins uniformly spread between two plates (see figure 1), in which fluid is pumped inside plates in order to increase the cooling performance.

The performance of micro heat sinks is evaluated by first, maximum heat transfer rate and second, by the pressure drop [13] required to be supplied by micro pumps, which the latter is our prior concern in this paper. In this paper, we aim to find the optimal topologies of micro pin-fins with a volume constraint (cross section area) to minimize the pressure drop.

2 Governing equations

2.1 Fluid equation

Let us consider an incompressible and viscous fluid flow across a two dimensional and doubly periodic square domain, Ω, with neglected external forces. The flow is mathematically modeled using the time–dependent Navier–Stokes equations:

\[
\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + \frac{1}{\rho} \nabla P - \nu \Delta \mathbf{u} = 0
\]

(1)

and

\[
\nabla \cdot \mathbf{u} = 0,
\]

(2)

Figure 1: Schematic of a cylindrical micro pin fin heat exchanger (from [12]).
where \( \mathbf{u} \) is the velocity vector, \( P \) is the hydrodynamic pressure, \( \nu \) is the kinematic viscosity and \( \rho \) is the density of the fluid. Using the method of Brinkman penalization [14, 15], in order to define a material (solid or fluid) distribution, the equation 1 is modified such that the flow velocity in solid zones \( (\Omega_s) \) is forced to become 0, i.e. no permeability into the solid material. Therefore, similar to what developed in [16], the penalized Navier–Stokes is formed as

\[
\frac{\partial \mathbf{u}_\epsilon}{\partial t} + \mathbf{u}_\epsilon \cdot \nabla \mathbf{u}_\epsilon + \frac{1}{\rho} \nabla P - \nu \Delta \mathbf{u}_\epsilon - \frac{1}{\epsilon} \chi(\mathbf{x})\mathbf{u}_\epsilon = 0 
\]

(3)

\[
\nabla \cdot \mathbf{u}_\epsilon = 0
\]

(4)

where \( \mathbf{u}_\epsilon \) is the approximated solution of equations (1) and (2) for fluid velocity, \( \epsilon \) the penalization parameter which controls the flow permeability within solid zones and the dimensionless function \( \chi(\mathbf{x}) \) defines solid and fluid zones of the domain. \( \chi(\mathbf{x}) \) is set to 1 if \( \mathbf{x} \in \Omega_s \) (solid bodies, \( \Omega_s \)) and 0 otherwise (fluids). In [17] it is shown that the solution of penalized equations 3 and 4 converges to the solution of 1 and 2 wherein the error norm is bounded by

\[
||\mathbf{u} - \mathbf{u}_\epsilon|| \leq C\epsilon^{1/4}
\]

(5)

meaning smaller the \( \epsilon \), smaller the penalization error. However [17] reported \( \epsilon^{1/2} \) as the upper bound on error norm based on numerical experiments. Penalization technique is suitable for topology optimization (density-based approach), because solid bodies are defined easily by modifying equations instead of modifying computational meshes. The corresponding boundary conditions in our case are defined as

\[
\begin{cases}
\mathbf{u} = 0 & \text{on } \partial\Omega_s \\
\mathbf{u} \text{ is double periodic on } \Omega,
\end{cases}
\]

(6)

and the mean flow velocity is \( \mathbf{u}_\infty \) at upstream. The pressure term in equation 3 is eliminated by utilizing an orthogonal projector \( \mathbb{P} \) onto the divergence–free space [18] for a space–periodic domain, which is based on Helmholtz decomposition providing a unique solution [19]. Equations 3 and 4 after projection become

\[
\frac{\partial \mathbf{u}_\epsilon}{\partial t} + \mathbb{P}(\mathbf{u}_\epsilon \cdot \nabla \mathbf{u}_\epsilon) - \nu \Delta \mathbf{u}_\epsilon - \frac{1}{\epsilon} \chi(\mathbf{x})\mathbf{u}_\epsilon = 0,
\]

(7)

where \( \mathbb{P} \) is an orthogonal projector. In what follows, the \( \epsilon \) subscription is removed for brevity.

### 2.2 Numerical method

In this work, the pseudo–spectral method presented by [16], is used to numerically approximate the solution of equation 7 by Fourier series; therefore, the 2–D flow velocity is approximated at point \( \mathbf{x} \) and time \( t \) by

\[
\mathbf{u}(x_1, x_2, t) = \sum_{k \in \mathbb{Z}^2} \mathbf{u}_k(t) \exp \left[ 2\pi i \left( \frac{k_1 x_1}{L} + \frac{k_2 x_2}{L} \right) \right]
\]

(8)
where \( x_1, x_2 \in [0, L] \), in which \( L \) is the width or height of the physical domain, and \( k_1 \) and \( k_2 \) the wave numbers. The 2-d Fourier transform of equation 8 in the matrix form is simply performed by

\[
U = DU_kD^T
\]

(9)

where \( U \) and \( U_k \) are \( N \)-by-\( N \) matrices of the flow velocity \( u \) and \( u_k \) discretized in the physical and Fourier domain, respectively, and \( D \) the 2-D discrete Fourier transform matrix. In addition to the high spectral accuracy of the method, and the convenience of the spatial differentiations to be calculated in the Fourier space [20], the highly simple and well-structured form of the method allows a more convenient way of sensitivity analysis required for gradient based optimizations, in contrary to common flow numerical solving approaches, e.g. SIMPLE [21] in which the complexity and iterative nature of the solvers, discrete sensitivity analyses are rather much complex and error-prone. Discrete Fourier transform of 9 can be either easily parallelized for direct computations or computed using fast Fourier transform packages, e.g. FFTW [22]. The equation 7 after using a divergence-free projector \( P \), becomes

\[
\frac{\partial u}{\partial t} = u \times \omega + \nu \Delta u + \frac{1}{\epsilon} \chi(x)u = \Gamma(u, \chi(x)),
\]

(10)

where \( \omega \) is the flow vorticity. The projection is performed in the Fourier space and \( P \) is

\[
P = (k_1^2 + k_2^2)^{-1} \left[ \begin{array}{cc} k_2^2 & -k_1k_2 \\ -k_1k_2 & k_1^2 \end{array} \right].
\]

(11)

### 3 Topology optimization

The general optimization problem we study in this paper is as follows:

\[
\begin{align*}
\text{minimize} \quad & C(\chi(\gamma), u(\chi(\gamma))) \\
\text{subject to} \quad & V^* \leq V(\chi(\gamma)) \\
& 0 \leq \gamma_i \leq 1 \quad \forall \gamma_i \in \Omega_D.
\end{align*}
\]

(12)

where \( C \) is the objective function, which is particularly the drag force in this work, \( V \) is the volume (cross-section area) and \( \gamma \) is the vector of design variables. \( V^* \) is the minimum required volume, and the topology function \( \chi \) is defined as a function of design variables, \( \gamma \), using a continuous projection function as suggested in [23]:

\[
\chi(\gamma) = \frac{\tanh(\beta \eta) + \tanh(\beta(\gamma - \eta))}{\tanh(\beta \eta) + \tanh(\beta(1 - \eta))},
\]

(13)

where, \( \eta \) and \( \beta \) are projection parameters which control sharpness of transition from solid to fluid by changing \( \gamma \). In this paper, \( \eta = 0.5 \) and \( \beta = \{1, 2, 4, 8, 16\} \), depending on the problem. It should be also noted that the gradients are updated using chain-rule since the derivatives are required to be with respect to the design variables \( \gamma \).
As the optimization algorithm, the globally convergent method of moving asymptotes (GCMMA) [24] is used. This optimization algorithm is specially suited for problems with large number of design variables which is up to \( \sim 3000 \) in our case. The optimizer is adjusted with the standard settings, but the step move parameter and the maximum number of sub-cycles limits are limited to 0.1 and 10, respectively.

3.1 Drag force

The drag force is the measure of the design to be minimized in this work and is simply calculated by integrating the Brinkman penalization term over the solid zones [14] as

\[
F_D = \frac{1}{\epsilon} \int \chi u \, dx.
\]

(14)

It is noticeable that the drag force is accurately calculated at low cost [25] without the need for the knowledge of solid–fluid boundary, which is difficult to be tracked within the topology optimization process.

3.2 Sensitivity analysis

It is essential to provide an accurate sensitivity analysis of the flow system in order to take the gradient based optimization techniques. \( C \) (the drag force) using the equation 14 is as follows

\[
C = C(u, v, \chi).
\]

(15)

Therefore, the total derivative of \( C \) with respect to design variables, \( \gamma \), using the chain rule is calculated by

\[
\frac{DC}{D\gamma} = \frac{\partial C}{\partial \chi} \frac{\partial \chi}{\partial \gamma} + \frac{\partial C}{\partial u} \frac{Du}{D\chi} \frac{D\chi}{D\gamma} + \frac{\partial C}{\partial v} \frac{Dv}{D\chi} \frac{D\chi}{D\gamma},
\]

(16)

in which, the simplicity of equation 14 allows calculation of \( \frac{\partial C}{\partial \chi} \), \( \frac{\partial C}{\partial u} \) and \( \frac{\partial C}{\partial v} \), at low cost and \( \frac{D\chi}{D\gamma} = \frac{\partial \chi}{\partial \gamma} \) is simply derived from equation 13. The total derivatives \( \frac{Du}{D\chi} \) and \( \frac{Dv}{D\chi} \) are derived by taking the derivative of the discrete solution of equation 10. The solution of 10 at time step \( n + 1 \), using Euler time integration scheme is

\[
\begin{align*}
  u^{n+1} &= u^n + \Delta t \Gamma_u(u^n, v^n, \chi) \quad \text{and} \quad u^0 = u_{init} \\
  v^{n+1} &= v^n + \Delta t \Gamma_v(u^n, v^n, \chi) \quad \text{and} \quad v^0 = v_{init},
\end{align*}
\]

(17)

where \( \Delta t \) is the time step size, chosen based on CFL condition for numerical stability. By taking the derivative of equations 17 with respect to \( \chi \), we derive

\[
\begin{align*}
  \frac{Du}{D\chi}^{n+1} &= \frac{Du}{D\chi} + \Delta t \left[ \frac{\partial \Gamma_u}{\partial \chi} + \frac{\partial \Gamma_u}{\partial u} \frac{Du}{D\chi} + \frac{\partial \Gamma_u}{\partial v} \frac{Dv}{D\chi} \right]^{n} \quad \text{and} \quad \frac{Du}{D\chi}^0 = 0 \\
  \frac{Dv}{D\chi}^{n+1} &= \frac{Dv}{D\chi} + \Delta t \left[ \frac{\partial \Gamma_v}{\partial \chi} + \frac{\partial \Gamma_u}{\partial u} \frac{Du}{D\chi} + \frac{\partial \Gamma_v}{\partial v} \frac{Dv}{D\chi} \right]^{n} \quad \text{and} \quad \frac{Dv}{D\chi}^0 = 0,
\end{align*}
\]

(18)
where the partial derivatives for \( \Gamma_u \) and \( \Gamma_v \) could be assembled once for each geometry using the converged solution of equations 17. Since the flow is laminar and steady-state (for relatively low Reynolds numbers), after sufficiently large number of steps, \( \frac{Du^n}{DX} \) and \( \frac{Dv^n}{DX} \) are converged; hence, the total derivative of equation 16 is calculated. Deriving sensitivities are iterative in this approach but rather fast since the information from previous optimization steps are used as the initial values of the derivatives. This method is simply parallelization and accurate, and no specific strategy, e.g. automatic differentiation (AD) [26] is used. The sensitivities accuracies are controlled by convergence tolerance and are validated using finite differencing method.

### 4 Topology optimization of micro heat exchangers

In this section we focus on three optimization cases for the design and configuration of pin–fin micro heat exchangers, aiming to minimize the drag. In the first case, we start the optimization process with an initial design which is commonly used for such micro–fluidic devices: an array of cylinders. In the second case, in contrary to the first case, we initiate the optimization from nothing, i.e. no initial solid zones are set initially. This test case examines the capability our numerical approach in terms of providing a flexible and robust design tool for external flow topology optimization problems. And lastly, similar to the first case, we attempt finding an optimized topology and initially start from a cylinder array; however, we fix the initial design during the optimization. The first two cases are constrained optimizations problems by defining a minimum volume to be shaped in the final design and the last case is unconstrained, i.e. the optimizer is free to add solid parts throughout the design domain.

Figure (2) shows the simulation setup. The Reynolds number is fixed to 25, common value for micro scale fluidic devises with steady laminar flows, based on the unit length scale \( L_{ref} = 1 \) of the reference domain \( (\Omega_{ref}) \). Flow simulation domain \( (\Omega) \) has a fixed size of \( L = 2 \), based on pitch-to-diameter ratio \( L/L_{ref} = 2 \) configuration, however the design domain \( (\Omega_D \subseteq \Omega) \) is defined for each case, separately. The mean upstream flow velocity is considered \( u_{up} = 2 \) with two angles: 0 (in–line) and \( \pi/4 \) (staggered). Penalization parameter is \( \epsilon = 0.005 \) which demonstrates nearly impermeable solid. The physical domain is discretized by \( 64 \times 64 \) points and simulations are computed on the
Phoenix cluster of TU Braunschweig in parallel. The volume (cross section area) is defined by summation of \( \chi_i' \)'s over \( \Omega_s \) and the drag coefficient \( C_D \) for a better comparison, similar to Reynolds number, is calculated based on fixed upstream flow velocity and the unit length of the reference domain (\( \Omega_{\text{ref}} \), for all cases.

### 4.1 Case 1: minimum drag from an initial design

Any topology optimization tool essentially is required to be able to optimize shapes as well. In this setting, we aim to examine the present optimization framework. In this example we investigate the optimal heat exchanger topologies, in terms of minimum pressure drop, starting from an initial configuration: a cylinder array. We seek for a design which satisfies the minimum volume constraint equivalent to the initial cylinder. Figure (3) illustrates the initial and final topologies within the fluid flow. In (3a) and (3c), we observe larger wake areas where the flow velocity is close to zero, and consequently larger flow acceleration in gaps between cylinders. However, in (3b) and (3d) the final optimum topologies feature reduced cross-flow area, and hence, reduced the wake areas with the same volume. As listed in table (1), we see the new geometries have successfully reduced the drag force considerably, both for in-line and staggered configurations. In (3b), due to the jet-like format of flow structure, the optimum topology has nearly maximum aspect ratio while preserving a topology with aerodynamically shaped geometry. Therefore we observe the final optimum is spanned throughout \( \Omega_D \). In staggered case, the flow velocity direction and magnitude is changed frequently. In (3d), we observe the new topology has eliminated most of the wake region in (3c) and flow is well directed with less maximum flow velocity due to the larger gap space in between. It should be noted that the final topologies and the drag reductions listed in table 1 are well in agreement with the numerical experiments performed by [12].

### 4.2 Case 2: minimum drag from zero initial solid volume

In this example, we try to find the optimum topologies initially from zero sold volume. It is an ideal feature of a topology optimization tool that is capable of creating topologies from nothing and here we aim to investigate this item. We restart examples in (4.1) with the same constraints on volume; hence, the optimizer begins with an infeasible starting inputs. As shown in (4), we observe topologies successfully similar to the case 1. This observation is approved also by comparing the drag values in table (2), where the drag

<table>
<thead>
<tr>
<th>Test case</th>
<th>Initial ( C_D )</th>
<th>Final ( C_D )</th>
<th>Change (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>#1: In-line</td>
<td>2.2093</td>
<td>1.3675</td>
<td>−38.1%</td>
</tr>
<tr>
<td>#1: Staggered</td>
<td>3.6466</td>
<td>2.2324</td>
<td>−38.8%</td>
</tr>
</tbody>
</table>

Table 1: Drag and drag reduction for case 1.
forces are close to the case 1. This is a considerable achievement and brings insight to develop a more generalized flow topology optimization framework.

4.3 Case 3: drag minimization for a fixed design

Based on the promising performance of the present topology optimization approach, we aim to improve the initial design by performing an unconstrained optimization. In this case, we consider in-line and staggered cylinder arrays similar to part 4.1, but increased the initial volume. We choose a rather large design domain in order to give sufficient freedom to the optimizer to seek the best design. For this case, GCMMA parameters require adjustments, otherwise no meaningful results are achieved, and we used $\eta = 0.5$.
A. Ghasemi and A. Elham

0.5 1 1.5 2
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2
0.5
1
1.5
2
2.5
3

(a) In-line (optimized)

(b) Staggered (optimized)

Figure 4: Illustration of solid topologies designed from zero solid volume and contours of flow velocity magnitude.

Test case | Initial $C_D$ | Final $C_D$ | Compared to case 1
---|---|---|---
#2: In-line | 0.0 | 1.3689 | +1.543% 
#2: Staggered | 0.0 | 2.2434 | +0.098% 

Table 2: Drag force for case 2 compared to case 1.

and $\beta = 16$ for projection. The design domain is split into two parts: first, passive nodes inside the initial design to be unchanged within the optimization process and second, the active nodes to be either solid or fluid at the end.

The test cases are shown in figure 5. The enhanced topologies are noticeable in the sense that the optimization tool is well aware of the flow structure supported by accurate sensitivity analysis throughout the design domain. Both stream–wise fore-end and back-end of the cylinders are touched by the optimizer, in order to better guide the flow. In (5a), the wake is more intensive because the flow at up-stream is the wake region of the front cylinder. Hence, the added solid zones are wisely placed such that this area is filled and the aspect ratio is increased as we expect for a better aerodynamic performance. In (5b), a sharp element is added in the tip of the cylinder which improves the flow guidance and removes stagnation of fluid. At the tip, we observe a meaningful solid structure is merged to the cylinder which tends to minimize wake effect by elimination of flow circulations. Overall, as reported in table (3), the drag reductions are $\sim 1\%$ which are expectable because the flow is laminar without unsteady flow separation, in which the flow behavior at wake region and the boundary layer are more important. However, in the present test case, our topology optimization approach again demonstrated a great performance in terms of robustness, flexibility and accuracy. It is worth noting that the present optimization process requires considerably low iterations since in some cases we
Table 3: Drag reduction for case 3.

<table>
<thead>
<tr>
<th>Test case</th>
<th>Initial $C_D$</th>
<th>Final $C_D$</th>
<th>Change (%)</th>
<th>Initial $V/V_{ref}$</th>
<th>Final $V/V_{ref}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>#3: In-line</td>
<td>4.2274</td>
<td>4.1979</td>
<td>$-0.697%$</td>
<td>0.793</td>
<td>0.859</td>
</tr>
<tr>
<td>#3: Staggered</td>
<td>6.7451</td>
<td>6.7058</td>
<td>$-0.581%$</td>
<td>0.793</td>
<td>1.051</td>
</tr>
</tbody>
</table>

reached to the optimum topology with less than $\sim 50$ iterations.

Figure 5: Contours of flow magnitude and optimized topologies for in-line and staggered configurations. Black dots are passive nodes and white dots active nodes. The red-line represents again the solid-fluid boundary.

5 Conclusion

A new topology optimization tool has been developed for flow systems with incompressible laminar 2D flows in a doubly periodic domain. Using pseudo–spectral scheme and accurate sensitivity calculation, we attempted to minimize the drag force on each fin by optimizing the topology of pin–fin micro heat–exchanger. The total drag forces were successfully reduced by $\sim 38\%$ in both in–line and rotated configurations with the optimum topologies in agreement with the literature. In addition, we found that a noticeable feature of the present tool is the ability to find optimal topologies without providing an initial design for the optimization process, with final topologies well consistent with the initial case. Finally, we optimized topology of the cylindrical pin–fin geometries by limiting the optimizer to only adding material to the initial design. We observed that our topology optimization approach were able to successfully create meaningful topologies although due to the flow physics the drag reduction was limited to $\sim 1\%$. 
REFERENCES


OPTIMUM DESIGN OF HYDRODYNAMIC THRUST BEARINGS WITH RAYLEIGH'S POCKET PROFILES

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Key words: Thrust bearing, Optimum design, Rayleigh’s pocket, Load Capacity.

Abstract. Optimum design problem for hydrodynamic self-aligning acting thrust bearings was considered. Based on results for rectangular region the problem for sector region was solved. As an objective function, the maximum of pressure integral over the lubricant layer surface was used and five geometrical parameters described Rayleigh's pocket shape were used as optimization variables during optimization procedure. The bearing pressure distribution was determined on the basis of the Navier-Stokes equations using the ANSYS / CFX software. Numerically the optimization problem was solved using three different methods: IOSO, SIMPLEX and piOPT+AFilter SQP realized in two commercial optimization software IOSO and modeFRONTIER.

The aim of this investigation was designing the technologically advanced profiles of thrust bearing sector microgeometry ensuring the maximum load capacity.

1 INTRODUCTION

In face of growing demand of effective thrust bearings with optimal performance characteristics, has prompted engineers to apply advanced numerical procedures and optimization methods in bearing design. In this field one of the important problems is the load capacity maximization, which generally determines the efficiency of the bearings. Otherwise, load capacity maximization problem is equivalent to the problem of profiling the microgeometry of the lubricating layer on the basis of the maximum lift force.

In this investigation, the problem of optimal design is considered in relation to the design of a thrust bearing with self-aligning segments. Typical thrust bearings with self-aligning segments are shown in Figure 1. Mostly, for this type of bearings, the shape of the profile is determined by the segment geometry (lining of the segment) and the segment installation angles in the lubricant flow. In work [1], for thrust bearing with self-aligning segments
hydrodynamic characteristics were considered in detail.

![Figure 1: Typical thrust bearings [2,3]](image)

Here we consider the problem of designing an optimal thrust bearing sector profile based on Rayleigh's pockets. Notable that the first formulations of the considered problem goes back to the work by J.W. Rayleigh published in 1918 [4] and the work by S. Y. Maday published in 1967 [5]. In 1918, Rayleigh established that the optimal profile in one-dimensional case problem is piecewise-step, and indicated that in the spatial case it has the shape of a pocket.

In later works [6, 7] the Rayleigh’s results were confirmed already for two-dimensional case in framework of variational problem solution.

In our study, the previous results are enlarged in relation to the sector thrust bearings with profiles based on Rayleigh’s pocket shape using advanced computing technologies.

2 THEORETICAL BACKGROUND

In our current investigation we formulate the optimization problem in such a way: find among continuous in \( \Omega \) functions \( p \) that satisfy the boundary value problem for Reynolds equation (1, 2) and among piecewise continuous functions \( h \) satisfying the condition (3) those that provide minimum to functional (4).

\[
div(h^3 \nabla p - hV) = 0 \text{ in } \Omega
\]

Here the dimensionless pressure \( p \) and the equation (1) is an equation for the excess pressure in the lubricant layer in region \( \Omega \).

The boundary conditions for equation (1) correspond to zero pressure on the boundary \( \partial \Omega \) of region \( \Omega \):

\[
p|_{\partial \Omega} = 0
\]

Restriction for the lubricant layer profile function \( h \):

\[
h \geq l
\]

And (4) is the lifting force of the lubricant layer. Note that the negative sign is chosen only
according to traditional rules of the variational calculus for searching a functional minimum.

$$W = - \int_{\Omega} pd\Omega$$

(4)

This problem statement was described in details in author’s previous work [8]

3 OPTIMIZATION PROBLEM STATEMENT AND RESULTS FOR SECTOR REGION

It is quite obvious that solving a full-scale variational problem it is a very time-consuming task. Therefore, for industrial engineering it is important to apply advanced computational technologies based on widely available software resources such different software for optimization [8,] and solving computational fluid dynamics problems. It makes possible to reduce the laboriousness in solving an optimal problem, but requires its specific reformulation.

In our case, this new formulation assumes, firstly, the replacement of the boundary value problem (1, 2) by the boundary value problem for the Navier–Stokes equation in order to determine the pressure distribution, secondly, the parametric specification of the flow region (bearing profile). Note that the functional of our problem remains the same.

Based on results for rectangular region [9, 10] the problem for sector region was solved. In this case profile was approximated by curve consisted of two parts: straight line and generalized ellipse. Figure 2 shows sector region received by transformation from rectangular region and four geometrical parameters defined the generalized ellipse.(5)

$$\left(\frac{x}{a}\right)^n + \left(\frac{y - c}{b - c}\right)^n = 1$$

(5)

These four parameters a, b, c and n together with Rayleigh’s pocket depth h were used as optimization variables during optimization procedure (n is generalized ellipse exponent).
The optimization problem was solved using three different numerical methods: IOSO, SIMPLEX and pilOPT+AFilter SQP. First one is realized in commercial optimization code IOSO and two others are integrated in code modeFRONTIER.

pilOPT is a multi-strategy self-adapting algorithm that combines the advantages of local and global search, and balances in an intelligent way the real and RSM-based [11] optimization in the search for the Pareto front. pilOPT gives remarkable performance even when handling complex output functions and highly-constrained problems. It can be used for both single and multi-objective optimization problems, even though it performs better with the latter.

Adaptive Filter SQP (AFSQP) [12] is a Sequential Quadratic Programming algorithm which obtains global convergence through an adaptive filter technique. AFSQP is developed by Esteco scientific team [13] with the purpose of reducing the number of evaluations required and of handling constraints characterized by possibly different numerical scales.

Finally, SIMPLEX is the «Nelder & Mead Simplex» [14] updated to take into account discrete variables and constraints. SIMPLEX is an algorithm for non-linear optimization problems, not the simplex method for linear programming. It does not require derivatives evaluations, so it is more robust than algorithm based on local gradients.

The IOSO software uses an algorithm whose key step is to divide each iteration of the Pareto frontier search into two stages: the construction of functions approximating the objective functions in a certain area and the extremes search of these approximation functions. Below are the results obtained using the IOSO and modeFRONTIER software.

Let's proceed directly to the optimization procedure. To solve the optimization problem, the CFD mesh for investigated domain was generated and the hydrodynamics problem, using Navier–Stokes equations, was solved. As an objective function, the maximum of pressure integral over the lubricant layer surface was used.
Initially dependences of pressure are received separately for each of the optimization variables. Figure 3 shows the typical dependence for generalized ellipse exponent and also demonstrates the greatest impact on the load capacity value. Based on these preliminary results variables ranges were defined. Figure 4 illustrates selected ranges.

![Figure 4: Dependence of lifting force on generalized ellipse exponent](image)

The numerical simulation of the problem was carried out using St. Petersburg Polytechnic Supercomputer Center. As a result, using three different methods, the optimal parameters were found.

Table 1 presents four of them. In Figure 5 the pressure distribution for the optimum profile is shown and in Figure 6 the dependence of the maximum pressure on a coordinate for section y=0 is demonstrated.

<table>
<thead>
<tr>
<th>Method/parameter</th>
<th>a,m</th>
<th>b,m</th>
<th>c,m</th>
<th>n</th>
</tr>
</thead>
<tbody>
<tr>
<td>IOSO</td>
<td>0.089</td>
<td>0.090</td>
<td>0.035</td>
<td>3.7</td>
</tr>
<tr>
<td>SIMPLEX</td>
<td>0.090</td>
<td>0.089</td>
<td>0.030</td>
<td>3.5</td>
</tr>
<tr>
<td>pilOPT+AFilter SQP</td>
<td>0.090</td>
<td>0.089</td>
<td>0.030</td>
<td>4.5</td>
</tr>
</tbody>
</table>
4 CONCLUSION

The results obtained are well correlated with results obtained earlier in the framework of full scale variational problem and can be used in design process of wide range of thrust bearings.

ACKNOWLEDGEMENT

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REFERENCES


SURROGATE MODELS FOR THE ITERATIVE OPTIMUM-OPTIMORUM THEORY AND THEIR APPLICATIONS

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Key words: Surrogate Models, Coupled Viscous-Inviscid Flow, Iterative Global Shape Optimization, Aerospace Applications, Exploration of Supersonic Flow.

Abstract. The author has developed non-classical three-dimensional hyperbolic analytic solutions (HASs) for the axial disturbance velocities over several flying configurations (FCs) in supersonic flow. The lift, pitching moment, inviscid drag coefficients and the distributions of pressure coefficients on FCs, at moderate angles of attack, can be rapid computed. The HASs are also used as start solutions for the design of inviscid, global optimized (GO) shapes of FCs, by using the own optimum-optimumorum strategy. These inviscid GO shapes are proposed as surrogate models and are used in the first step of an iterative optimum-optimumorum theory. Up the second step of iterations the HASs are replaced by hybrid analytic-numeric solutions for the Navier-Stokes layer and the friction drag coefficient is computed.

1 INTRODUCTION

The author uses the principle of minimal singularities of M. van Dyke, the compatibility conditions of P. Germain and the hydrodynamic analogy of E. Carafoli, for the development of non-classical three-dimensional HASs for the boundary value problems of hyperbolic PDEs of the axial disturbance velocities, over several FCs, in supersonic flow. These solutions are written in integrated forms and use minimal singularities, which are located only along the singular lines (like subsonic leading edges, junction lines wing-fuselage, junction lines wing-leading edge flaps etc.) and fulfill the local jumps. These non-classical HASs are used in the first step of her iterative optimum-optimumorum (IOO) strategy, as start solutions for the design of inviscid GO shapes of FCs. New performant FCs models with GO shapes are designed and tested in the trisonic wind tunnel of DLR Cologne. A new optimized variant of Saenger project for the touristic flight in space is proposed. The inviscid GO shapes of FCs are also used as surrogate models of IOO, in its first step of iteration. Up the second step of IOO, the use of hybrid analytic-numeric solutions for the PDEs of the three-dimensional Navier-Stokes layer (NSL) are proposed. These hybrid NSL’s solutions use the HASs two time namely, as boundary values at the NSL’s edge and to reinforce the NSL’s solutions. These hybrid NSL’s solutions which are products between the HASs and polynomials with free coefficients, have important analytic properties like: correct last behaviors, correct jumps over the singular lines. the singularities are balanced, the condition on the characteristic surfaces, which occurs in supersonic flow and the non-slip condition are automatically fulfilled. A
logarithmic density function is introduced instead of the density, in order to split the NSL’s PDEs, as in [1] - [3]. The total drag of a FC, including friction, is computed.

2 THREE-DIMENSIONAL HYPERBOLIC POTENTIAL START SOLUTIONS FOR THE INVISCED, GLOBAL OPTIMIZATION

The author supposes that the downwashes of an FC are picewise given or approximate in form of superpositions of homogeneous polynomes in two variables and proposes some corresponding non-classical three-dimensional HASs for the axial disturbance velocities over the FCs, which are expressed in integrated forms and can be easy and rapid used: for the computation of the lift, pitching moment, inviscid drag coefficients and of the distributions of pressure coefficients over the FCs, as start solutions for the design of performant inviscid GO shapes of FCs, as outer flow for the Navier-Stokes layer (NSL) and for the generation of hybrid solutions for the NSL, as in [1]-[4]. The HASs are presented here for three-dimensional FCs with arbitrary camber, twist and thickness distributions like delta wing alone and, delta wing fitted with central fuselage. Let us firstly introduce dimensionless coordinates

\[
\begin{align*}
\tilde{x}_1 &= \frac{x_1}{h_1}, \\
\tilde{x}_2 &= \frac{x_2}{\ell_1}, \\
\tilde{x}_3 &= \frac{x_3}{h_1}, \\
\end{align*}
\]

\[
\begin{pmatrix}
\tilde{y} = \frac{y}{\ell}, \\
\ell = \frac{\ell_1}{h_1}, \\
\nu = B\ell, \\
B = \sqrt{M_{\infty}^2 - 1}
\end{pmatrix},
\]

\[
w = \tilde{w}, \quad w^* = \tilde{w}^*, \quad u = \ell \tilde{u}, \quad u^* = \ell \tilde{u}^*
\]

Hereby \(u\) and \(u^*\) and \(w\) and \(w^*\) are the axial disturbance velocities and the downwashes on the thin and thick-symmetrical wing components \(\ell_1, h_1\) and \(\ell\) are the half-span, maximal depth and the dimensionless span and \(\nu\) is the similarity parameter of the planform.

Let us consider firstly the delta wing alone. The distributions of the downwashes \(w\) and \(w^*\) on the thin and thick-symmetrical components of the thick, lifting delta wing are the following:

\[
w \equiv \tilde{w} = \sum_{m=1}^{N} \tilde{x}_1^{n-1} \sum_{k=0}^{n-1} \tilde{w}_{m-k-1,k} |\tilde{y}|^k, \quad w^* \equiv \tilde{w}^* = \sum_{m=1}^{N} \tilde{x}_1^{n-1} \sum_{k=0}^{n-1} \tilde{w}_{m-k-1,k}^* |\tilde{y}|^k
\]

(2a, b)

The corresponding axial disturbance velocities on the thin and on the thick components fitted with a central ridge, are:

\[
u \equiv \ell \tilde{u} = \ell \sum_{n=1}^{N} \tilde{x}_1^{n-1} \left\{ \frac{\delta (n)}{2} \sum_{q=0}^{n-1} \tilde{A}_{n,2q} \tilde{y}^{2q} + \frac{\delta (n-1)}{2} \sum_{q=1}^{n-1} \tilde{C}_{n,2q} \tilde{y}^{2q} \cosh^{-1} \sqrt{\frac{1}{\tilde{y}^2}} \right\}
\]
\[ u^* = \ell \, \bar{u}^* = \ell \sum_{n=1}^{N} \tilde{x}_1^{n-1} \left\{ \sum_{q=0}^{n-1} \tilde{H}_{nq} \tilde{y}^q \left( \cosh^{-1} M_1 + (-1)^q \cosh^{-1} M_2 \right) \right\} + \sum_{q=1}^{\lfloor \frac{n-1}{2} \rfloor} \tilde{C}_{n,2q} \tilde{y}^{2q} \cosh^{-1} \frac{1}{\sqrt{\nu^2 \tilde{y}^2}} + \sum_{q=0}^{\lfloor \frac{n-2}{2} \rfloor} \tilde{D}_{n,2q} \tilde{y}^{2q} \sqrt{1 - \nu^2 \tilde{y}^2} \right\}, \quad (3a, b) \]

\[ M_1 = \sqrt{\frac{(1 + \nu)(1 - \nu \tilde{y})}{2\nu(1 - \tilde{y})}} \] \[ M_2 = \sqrt{\frac{(1 + \nu)(1 + \nu \tilde{y})}{2\nu(1 + \tilde{y})}} \]

The coefficients of the axial disturbance velocity are linear and homogeneous functions of the coefficients of the downwash, it is:

\[ \tilde{A}_{n,2q} = \sum_{j=0}^{n-1} \tilde{a}_{n,2q,j} \tilde{w}_{n-j-1,j} \] \[ \tilde{C}_{n,2q} = \sum_{j=0}^{n-1} \tilde{c}_{n,2q,j} \tilde{w}_{n-j-1,j} \]

\[ \tilde{H}_{nq} = \sum_{j=0}^{n-1} \tilde{h}_{n,2q,j} \tilde{w}_{n-j-1,j} \] \[ \tilde{C}_{n,2q} = \sum_{j=0}^{n-1} \tilde{c}_{n,2q,j} \tilde{w}_{n-j-1,j} \]

\[ \tilde{D}_{n,2q} = \sum_{j=0}^{n-1} \tilde{d}_{n,2q,j} \tilde{w}_{n-j-1,j} \] \quad (4a-e)

If the delta wing fitted with a central fuselage is now treated, this FC is considered as a discontinuous wing fitted with two artificial ridges along the junction lines wing-fuselage.

The downwashes on the thin and thick-symmetrical wing components of FC are given, as in (1a, b) and, of the non-integrated central fuselage zone, are given or approximate in the following forms:

\[ w^* = \bar{w} = \sum_{m=1}^{N} \tilde{x}_1^{m-1} \sum_{k=0}^{m-1} \tilde{w}_{m-k-1,k} |\tilde{y}|^k \] \[ w^* = \bar{w}^* = \sum_{m=1}^{N} \tilde{x}_1^{m-1} \sum_{k=0}^{m-1} \tilde{w}_{m-k-1,k}^* |\tilde{y}|^k \] \quad (5a, b)

The corresponding axial disturbance velocities on the components of the non-integrated wing-fuselage FC are, as in [1], it is:

\[ u = \ell \, \bar{u} = \ell \sum_{n=1}^{N} \tilde{x}_1^{n-1} \left\{ \sum_{q=0}^{n-1} \tilde{G}_{nq} \tilde{y}^q \left( \cosh^{-1} S'_1 + (-1)^q \cosh^{-1} S'_2 \right) \right\} \]

443
\[
\begin{aligned}
&+ \sum_{q=0}^{\ell(n-2)} \tilde{A}_{n,2q} \tilde{\gamma}^{2q} \sqrt{1 - \tilde{v}^2} + \sum_{q=0}^{\ell(n-2)} \tilde{C}_{n,2q} \tilde{\gamma}^{2q} \cosh^{-1} \frac{1}{\sqrt{\tilde{y}^2}} \\
S_i &= \sqrt{\frac{(1 + \tilde{v}) (1 - \tilde{v})}{2 (\tilde{v} - \tilde{v} \tilde{y})}}, \quad S_2 = \sqrt{\frac{(1 + \tilde{v}) (1 + \tilde{v})}{2 (\tilde{v} \tilde{v} - \tilde{v})}}, \\
& u^{**} = \ell \sum_{n=1}^{N} \tilde{b}_n \tilde{y}^{n-l} \left\{ \sum_{q=0}^{\ell(n-2)} \tilde{H}_{nq} \tilde{y}^q \left( \cosh^{-1} M_1 + (-1)^q \cosh^{-1} M_2 \right) \\
&+ \sum_{q=0}^{\ell(n-2)} \tilde{D}_{n,2q} \tilde{y}^{2q} \sqrt{1 - \tilde{v}^2 \tilde{y}^2} + \sum_{q=0}^{\ell(n-2)} \tilde{C}_{n,2q} \tilde{y}^{2q} \cosh^{-1} \frac{1}{\sqrt{\tilde{y}^2}} \\
&+ \sum_{q=0}^{\ell(n-2)} \tilde{G}_{nq} \tilde{y}^q \left( \cosh^{-1} S_1 + (-1)^q \cosh^{-1} S_2 \right) \right\}, \quad (6a, b) \\
S_i &= \sqrt{\frac{(1 + \tilde{v}) (1 - \tilde{v} \tilde{y})}{2 (\tilde{v} - \tilde{v} \tilde{y})}}, \quad S_2 = \sqrt{\frac{(1 + \tilde{v}) (1 + \tilde{v} \tilde{y})}{2 (\tilde{v} \tilde{v} + \tilde{y})}}, \quad c = \frac{c}{h}, \quad \tilde{v} = Bc 
\end{aligned}
\]

Hereby \( c_i \) and \( c \) are the half-span, and the dimensionless span and \( \tilde{v} \) is the similarity parameter of the planform of the fuselage. The coefficients of axial disturbance velocity are linear and homogeneous functions of the coefficients of the downwash, it is:

\[
\tilde{A}_{n,2q} = \sum_{j=0}^{n-1} \left( \tilde{a}_{n,2q,j} \tilde{w}_{n-j-1,j} + \tilde{a}_{n,2q,j} \tilde{w}_{n-j-1,j} \right), \quad \tilde{C}_{n,2q} = \sum_{j=0}^{n-1} \tilde{c}_{n,2q,j} \tilde{w}_{n-j-1,j},
\]

\[
\tilde{G}_{nq} = \sum_{j=0}^{n-1} \left( \tilde{g}_{n,q,j} \tilde{w}_{n-j-1,j} + \tilde{g}_{n,q,j} \tilde{w}_{n-j-1,j} \right)
\]

\[
\tilde{H}_{nq} = \sum_{j=0}^{n-1} \tilde{h}_{n,q,j} \tilde{w}_{n-j-1,j}, \quad \tilde{C}_{n,2q} = \sum_{j=0}^{n-1} \tilde{c}_{n,2q,j} \tilde{w}_{n-j-1,j},
\]

\[
\tilde{D}_{n,2q} = \sum_{j=0}^{n-1} \left( \tilde{d}_{n,2q,j} \tilde{w}_{n-j-1,j} + \tilde{d}_{n,2q,j} \tilde{w}_{n-j-1,j} \right),
\]
\[ \tilde{G}_{nq} = \sum_{j=0}^{n-1} \left( \tilde{g}_{n,q,j}^* \tilde{w}_{n-j+1,j}^* + \tilde{g}_{n,q,j}^* \tilde{w}_{n-j+1,j}^* \right) \] (7a-g)

The integrated wing-fuselage FC, considered for the design of GO FC’s shape, has continuous mean surface and the same tangent planes along the junction lines wing-fuselage, in order to avoid the corners. The corresponding axial disturbance velocity of its thin component has the form (3a). Now the HAS are further used as start solutions for the design of GO shape of integrated wing-fuselage FCs.

3 INVISCID, GLOBAL OPTIMIZED SHAPES OF FLYING CONFIGURATIONS

The free parameters of the design of the inviscid GO shape of the integrated wing-fuselage FC are the coefficients of the downwashes \( w, w^*, w^{**} \).

The constraints for the thin component of FC are the following: given lift and pitching moment coefficients and the Kutta condition along the subsonic leading edges, in order to avoid the conturmentation of the flow, at cruise. The constraints for the thick-symmetrical component of FC are: given relative volumes of the wing and of the fuselage zone and the integration conditions along the junction lines wing-fuselage in order to avoid the corners on the FC’s surface. The design of the GO shape of an integrated wing-fuselage FC leads to an enlarged variational problem with free boundaries. The author has developed an enlarged variational strategy called optimum-optimorum strategy, as in [1]-[4], in order to solve this enlarged variational problem. The separate treatment of the variational problems of the thin and thick-symmetrical components lead to the solving of two linear algebraic systems for the determination of the best values of the coefficients of the downwashes. But these systems are coupled, due to their common similarity parameters, which enter in the coefficients of these systems and which must be also, simultaneously be optimized. Due to the fact that the quotient of the similarity parameters of the planforms of the wing and of the fuselage are determined for the purpose of the FC, this quotient is taken constant during the optimization process and the similarity parameter of the wing with subsonic leading edges is sequentially varied between 0 and 1. A lower limit line of the drag coefficients of elitary FCs, as function of the similarity parameter of the planform of the wing is obtained and the position of the minimum of this limit line is the optimal value of the similarity parameter of the planform of the wing and the corresponding elitary wing is in the same time the GO shape of the FC. Three GO models, namely ADELA, a wing alone and two GO shapes of the fully-integrated wing-fuselage FCs, namely FADET I and FADET II were designed by the author, for the cruising Mach numbers 2, 2.2 and, respectively, 3.

A theoretical and experimental exploration of supersonic flow over FCs was performed by using eight models designed by the author, namely: a wedged delta wing, a double wedged delta wing, a wedged delta wing fitted with a central conical fuselage, a GO delta wing alone ADELA, global optimized at cruising Mach number \( M_c = 2 \), a wedged rectangular wing and a cambered rectangular wing, are presented in the (Fig.1). In the (Fig.2) are presented, more recent designed and experimental checked GO models of fully-integrated wing-fuselage
FCs FADET I and FADET II; global optimized at \( M_\infty = 2.2 \) and, respectively, at \( M_\infty = 3 \). All these models have sharp leading edges in order to avoid the bow shock wave. The six delta FCs have the same area of their planforms and the both rectangular wings have the same planforms. The three global optimized flying configurations fulfill additionally the Kutta condition along their subsonic leading edges, in order to avoid the detachment of the flow along their leading edges, to cancel the induced drag and to increase the lift.

The measurements of the lift, pitching moment and pressure coefficients on the upper side of these models were performed in the trisonic wind tunnel of DLR Cologne, in the frame of research projects of the author, sponsored by the DFG. Correlation and interpolation software, developed by the author, were used by herself and by her young collaborators of Aerodynamics of Flight, at RWTH, Aachen University, for the evaluation and for the plotting of these experimental results. The theoretical predicted pressure, lift and pitching moment coefficients are obtained by using the non-classical three-dimensional hyperbolic potential solutions and the corresponding software of the author.

Fig. 1 Six of the models used for the exploration of supersonic flow

Fig. 2 The fully-integrated and global optimized models FADET I and FADET II

A very good agreement between the theoretical and experimental correlated values of lift and pitching moment coefficients are obtained for all the range of supersonic Mach numbers
and for the angles of attack $\alpha \leq 20^\circ$. For the pressure coefficients a good agreement between the theoretical and the experimental results is obtained for the angles of attack $\alpha \leq 10^\circ$.

The agreement between the experimental and theoretical HSAs for the pressure, lift and pitching moment of flattened FCs flying at moderate angles of attack, leads to the following important conclusions:

- the flow is laminar, as supposed here, and it remains attached in supersonic flow, for larger range of angles of attack than by subsonic flow;
- the flight with characteristic surface, which is more economic, instead of the flight with shock wave surface is confirmed;
- the validity of the three-dimensional hyperbolic analytic potential solutions for the axial disturbance velocity, with the chosen balanced minimal singularities and the corresponding developed software for the computation of the above coefficients are confirmed;
- the influence of friction upon these coefficients is neglectable;
- these analytic solutions are very useful for the computation of proposed hybrid solutions for the NSL’s PDEs, which are able to compute the total drag, including friction;

4 AEROSPACE APPLICATIONS

The designed GO shapes of FCs are used as sources of inspirations for the design of new, almost blended and high performant shapes of new generation of models of supersonic aircraft, aerospace vehicles and supersonic UAVs. One application, presented here, is related with a suborbital touristic flight in space. New GO shapes of vehicles models GEO and LEO, optimized at cruising Mach numbers $M_\infty = 2.2$ and respectively $M_\infty = 3.0$, with two congruent fuselages, only almost inserted in the wing’s thickness (in order to have windows on both sides!) and converging in the frontal part of the wing, are here proposed, as in the (Fig. 3) and (Fig. 4). GEO with a GO shape is a greater model for geostationary vehicle and a smaller one, LEO, with its GO shape, is the model for the lower earth orbit vehicle. A variant of Saenger project now with two GO space vehicles is here proposed for the touristic flight in space. The vehicle GEO can carry the smaller vehicle LEO, as presented in the (Fig. 5) during the change of passengers and for supply. LEO can up and go on GEO. During the flight of LEO in space, different UAVs can up and go from earth on GEO, for supply and exchange of passengers.
Fig. 4 The greater fully-integrated and global optimized model of space vehicle GEO

Fig. 5 The smaller, fully-integrated and global optimized model of space vehicle LEO
5 HYBRID SOLUTIONS FOR THE NAVIER-STOKES LAYER.

The proposed hybrid analytic-numeric solutions for the NSL use the non-classical HASs two times, it is: as outer flow as the NSL’s edge and to reinforce the numerical NSL’s solutions. Let us firstly introduce the coordinate $\eta$ inside the NSL, it is

$$\eta = \frac{x_1 - Z(x_1, x_2)}{\delta(x_1, x_2)} \quad (0 \leq \eta \leq 1) \quad (8)$$

The proposed hybrid solutions for the velocity components, the here introduced density function $R = \ln \rho$ and of the absolute temperature $T$ are the following:

$$u_\delta = u_e \sum_{i=1}^{N} u_i \eta^i, \quad v_\delta = v_e \sum_{i=1}^{N} v_i \eta^i, \quad w_\delta = w_e \sum_{i=1}^{N} w_i \eta^i \quad (9a, b, c)$$

$$R = R_w + (R_e - R_w) \sum_{i=1}^{N} r_i \eta^i \quad T = T_w + (T_e - T_w) \sum_{i=1}^{N} t_i \eta^i \quad (10a, b)$$

Hereby are: $\delta$ the thickness of the NSL, $u_e$, $v_e$, $w_e$ the velocity components of the hyperbolic potential flow at the NSL’s edge, $R_e$ and $T_e$ the density function and the absolute temperature of the outer flow at the NSL’s edge and $R_w$ and $T_w$ their values at the surface of the FC. The free coefficients $r_i$, $t_i$, $u_i$, $v_i$, $w_i$ are used to satisfy the NSL’s PDEs and the boundary conditions at the NSL’s edge in some points. The viscosity $\mu$ fulfills an exponential low and the pressure $p$ is
obtained from the physical equation of the ideal gas, it is

$$\mu = \mu_0 \left( \frac{T}{T_0} \right)^n , \quad p = R_x \rho T = R_x e^x T$$ \hspace{1cm} (11a, b)

All the physical entities are expressed as functions of the velocity’s coefficients, which are determined by using the collocation method and by iterative solving of the impulse PDEs. The skin friction, the friction drag and the total drag coefficients of a delta wing are the following:

$$\tau_{x_i}^{(n)} \equiv \tau_{x_i} \bigg|_{\eta = 0} = \mu_f \frac{\partial}{\partial \eta} u_\eta \bigg|_{\eta = 0} = \mu_f u_1 u_e , \quad (12)$$

$$C_d^{(f)} = 8 \int \frac{\nu_j u_j u_e \vec{x}_j d\vec{x}_j d\vec{y}}{\delta x \delta y} , \quad C_d^{(t)} = C_d^{(f)} + C_d^{(i)}$$

6 CONCLUSIONS

- The use of HASs as start solutions allow the rapid inviscid design of GO shapes of performant FCs, which are here proposed for the shapes of aerospace vehicles and as surrogate models for the IIO.
- The use of surrogate models speed up the computation time for the design of GO shapes of the FCs and are used in the first step of an iterative optimum-optimorum strategy, as in [1]-[4].
- The HASs are also used two times for the determination of hybrid solutions for the Navier-Stokes layer it is, as boundary at the NSL’s edge and in the structure of hybrid solutions, which are products of HASs with polynomials with free coefficients. These coefficients are used to satisfy the NSLs PDEs in a number of points.
- The hybrid NSL’s solutions replace the HASs up the second step of IIO and allow the computation of total drag, including friction.

5 REFERENCES

COUPLED SOLID PIEZOELECTRIC AND SHELL INVERSE-PIEZOELECTRIC ANALYSIS USING PARTITIONED METHOD FOR THIN PIEZOELECTRIC BIMORPH WITH METAL LAYERS

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Key words: Piezoelectric, Inverse-Piezoelectric, Solid Element, Shell Element, Partitioned Method, Piezoelectric Bimorph, Block Gauss-Seidel Method.

Abstract. In this study, the coupled solid piezoelectric and shell inverse-piezoelectric analysis method for a thin piezoelectric bimorph with metal layers is proposed. The piezoelectric bimorph is usually thin and includes the metal layers such as the electrode and the shim plate. In the proposed method, the solid and shell elements are used for the piezoelectric and inverse-piezoelectric analyses, respectively, since the solid elements can describe the various types of the distributions of the electric potential along the thickness, and the shell elements are suitable for analyzing the thin structure. The block Gauss-Seidel method is used to couple the solid piezoelectric and shell inverse-piezoelectric analyses. In the iterative passing of the solution variables, the transformation method is used between the solid and shell elements. The rules of mixture for the bending rigidity and the mass are used for modeling the single shell structure in the inverse-piezoelectric analysis. A pseudo-piezoelectric modeling for the conductor is proposed to consider the metal layers in the piezoelectric analysis. This modeling allows us to reuse existing programs of the piezoelectric analysis without any modification.

1 INTRODUCTION

Piezoelectric and inverse-piezoelectric effects are coupled with each other via the constitutive equations of piezoelectric materials. Thin piezoelectric bimorphs are very popular in sensor and actuator applications [1-4]. Furthermore, these bimorphs usually include metal layers such as electrode membranes and shim plates. Therefore, the coupled solid piezoelectric and shell inverse-piezoelectric analysis method for the thin piezoelectric bimorph with the metal layers is required in the design process of these applications.

The piezoelectric analysis using solid elements (solid piezoelectric analysis) is suitable for describing the various types of the electric potential distribution through the thickness, while the solid inverse-piezoelectric analysis is not suitable for solving the thin structure deformation. On the contrary, the shell inverse-piezoelectric analysis is suitable for solving the thin structure deformation, while the shell piezoelectric analysis is not suitable for describing the various types of the electric potential distribution through the thickness, since it
assumes the linear or quadratic distribution of the potential through the thickness [11]-[15]. Therefore, in this study, the solid piezoelectric analysis and the shell inverse-piezoelectric analysis are coupled using the block Gauss-Seidel method [5] [6].

Let us consider the piezoelectric analysis for the piezoelectric bimorph with the metal layers. In a specific problem, the electric potential in the metal layer is prescribed, and metal layer can be analyzed as the elastic body separately [7]. In general, however, the electric potential in the metal layer is unknown. In this study, therefore, a pseudo-piezoelectric modeling for the conductor is proposed to consider the metal layers of which potential is unknown. This modeling allows us to reuse existing programs for the piezoelectric analysis without any modification.

2 PARTITIONED SOLID PIEZOELECTRIC AND SHELL INVERSE-PIEZOELECTRIC ANALYSIS METHOD

The solid piezoelectric analysis and the shell inverse-piezoelectric analysis are coupled using a partitioned procedure as shown in Figure 1, where each field is solved separately and solution variables (electric force and structural displacement) are passed iteratively from one field to the other until convergence is achieved. In this passing, the transformation method is used between shell and solid meshes [5][6].

2.1 Finite element discretized equations for the piezoelectric material

The finite element discretized equations for the piezoelectric material are obtained using the finite element formulation for the mechanical equilibrium, the electrostatic equilibrium from the Maxwell’s equation, and the constitutive equations of piezoelectricity as

\[
\begin{align*}
\mathbf{M}\ddot{\mathbf{u}} + \mathbf{K}_{uu}\mathbf{u} + \mathbf{K}_{u\phi}\phi &= \mathbf{F}, \\
\mathbf{K}_{u\phi}^T\mathbf{u} + \mathbf{K}_{\phi\phi}\phi &= \mathbf{q},
\end{align*}
\]

where \(\mathbf{M}\) is the mass matrix, \(\mathbf{K}_{uu}\) is the mechanical stiffness matrix, \(\mathbf{K}_{u\phi}\) is the piezoelectric coupling matrix, \(\mathbf{K}_{\phi\phi}\) is the dielectric stiffness matrix, \(\mathbf{F}\) is the mechanical external force vector, \(\mathbf{q}\) is the external electric charge vector, \(\mathbf{u}\) is the mechanical displacement vector, and \(\phi\) is the electric potential vector, and the superscript \(T\) stands for transpose of matrix. \(\mathbf{K}_{u\phi}\) and \(\mathbf{K}_{\phi\phi}\) are given as

\[
\begin{align*}
\mathbf{K}_{u\phi} &= \int_\Omega \mathbf{B}_u^T\mathbf{e}\mathbf{B}_\phi d\Omega, \\
\mathbf{K}_{\phi\phi} &= \int_\Omega \mathbf{B}_\phi^T\mathbf{e}\mathbf{B}_\phi d\Omega,
\end{align*}
\]

where \(\rho\), \(\mathbf{C}\), \(\mathbf{e}\), and \(\mathbf{\varepsilon}\) are the mass density, the elastic constitutive tensor, the piezoelectric coupling tensor, and the dielectric permittivity tensor, respectively, and \(\mathbf{B}_u\) and \(\mathbf{B}_\phi\) are the gradients of the interpolation functions of the displacement and the electric potential, respectively.
2.2 Partitioned piezoelectric and inverse-piezoelectric analysis

In the inverse-piezoelectric analysis, Eq. (1) is reduced to

\[ M \ddot{u} + K_{uu} u = F + \varepsilon F , \]

where \( \varepsilon F \) is the electric force from the inverse-piezoelectric effect, and is given as

\[ \varepsilon F = -K_{uu} \phi , \]

where the superscript \( e \) stands for the electric quantity.

In the piezoelectric analysis, Eq. (2) is reduced to

\[ K_{\phi \phi} \phi = q + \varepsilon q , \]

where \( \varepsilon q \) is the electric charge from the piezoelectric effect, and is given as

\[ \varepsilon q = -K_{q\phi}^T u , \]

The piezoelectric analysis and the inverse piezoelectric analysis are coupled using the block Gauss-Seidel method as shown in Figure 1.

![Figure 1](image)

**Figure 1:** Schematic of the partitioned method for the coupled piezoelectric and inverse-piezoelectric analyses. The block Gauss-Seidel method is used as the coupling algorithm.

2.3 Transformation of the solution variables between shell and solid meshes

Solid elements are used in the piezoelectric analysis to describe the various types of the electric potential distribution along the thickness (solid piezoelectric analysis). On the contrary, shell elements are used in the inverse-piezoelectric analysis because of the thin structure (shell inverse-piezoelectric analysis). The transformation of the solution variables between the shell and solid meshes is used to couple these two analyses [5][6]:

\( \varepsilon F \) given by the solid piezoelectric analysis (6) is transformed to the equivalent force \( \varepsilon F^s \) and moment \( \varepsilon M \) acting on the shell mesh such that these forces and moment satisfy the
mechanical equilibriums. The superscript $s$ in these vectors stands for the quantity of the shell mesh. This transformation is represented using the transformation matrix $T$ as

$$\mathbf{e}^{s} = \mathbf{e}^{T} \mathbf{F}^{s}.$$ 

Then, the inverse-piezoelectric analysis (5) can be rewritten using Eq. (9) as

$$\mathbf{M}^{s} \ddot{\mathbf{u}}^{s} + \mathbf{K}^{s} \mathbf{u}^{s} = \mathbf{F}^{s} + \mathbf{e}^{s} \mathbf{F}^{s}.$$ 

Similarly, $\mathbf{u}^{s}$ from Eq. (10) should be transformed to $\mathbf{u}$ in order to calculate $\mathbf{q}$ (8) and perform the solid piezoelectric analysis (7). The transformation from $\mathbf{u}^{s}$ to $\mathbf{u}$ can be written as

$$\mathbf{u} = \mathbf{T} \mathbf{u}^{s},$$

where $\mathbf{T}$ is the transformation matrix, and is given using the displacement interpolation function of the shell element.

3 MODELING OF THIN PIEZOELECTRIC BIMORPH WITH METAL LAYERS

3.1 Rules of mixture in the shell inverse-piezoelectric analysis

In the shell inverse-piezoelectric analysis, the piezoelectric bimorph with the metal layers is modeled as the single shell structure. Therefore, the rule of mixture about the bending stiffness is used, since the first bending mode is dominant, and the rule of mixture about the mass is used.

3.2 Pseudo-piezoelectric method in the piezoelectric analysis

Let us consider the metal layers in the piezoelectric bimorph. The piezoelectric coupling tensor $\mathbf{e}$ for the conductor is equal to 0. Therefore, $\mathbf{K}_{\text{up}}$ (3) is given as

$$\mathbf{K}_{\text{up}} = 0.$$ 

Then, Eq. (2) is reduced to

$$\mathbf{K}_{\phi \phi} \phi = \mathbf{q}.$$ 

This equation is equivalent to the governing equation of the dielectric material. Furthermore, the conductor is considered as the dielectric material with an infinite value of the dielectric constant. Therefore, Eq. (13) is considered as the finite element discretized equation for the conductor in the static electric field by taking enough large value for each component of the dielectric permittivity tensor $\mathbf{e}$ in $\mathbf{K}_{\text{up}}$ (4).

It follows from the above formulation that the proposed pseudo-piezoelectric method is given as follows: (a) Evaluate the metal layers in the piezoelectric bimorph as the pseudo-piezoelectric material with $e = 0$ and $\mathbf{e} \rightarrow \infty$. (b) Execute the piezoelectric analysis (7) for the
piezoelectric bimorph with the metal layers, where the metal layers are evaluated as the pseudo-piezoelectric material. This method allows us to reuse the existing programs of the piezoelectric analysis without any modification.

4 SENSOR MODE ANALYSIS

4.1 Problem setup

Figure 2 shows the sensor mode of the piezoelectric bimorph schematically. The length and the width of the piezoelectric bimorph are 250mm and 20mm, respectively, the thicknesses of the piezoelectric and shim layers are 5mm and 0.5mm, respectively. The materials of the piezoelectric and shim layers are PVDF (Young’s modulus $E = 2.0$Gpa, Poisson’s ratio $\nu = 0.29$, the piezoelectric constant $e = 0.046$C/m$^2$, the dielectric constant $\varepsilon = 1.063 \times 10^{-10}$) and brass ($E = 110$Gpa, $\nu = 0.35$), respectively. Note that $e$ and $\varepsilon$ for the shim are set as 0 and 0.01, respectively, using the proposed pseudo-piezoelectric modeling in Section 3.2. As shown in Figure 2, the voltage $V = 0$V is applied for the upper and lower surfaces, and the external mechanical force $F = 1$mN is applied to the free end. Figure 3 shows the solid mesh used in the piezoelectric analysis. Figure 4 shows the shell mesh used in the inverse-piezoelectric analysis. As shown in these figures, the divisions along the length and the width between the solid and shell meshes are equivalent to each other. The solid elements are 20-node hexahedral elements, while the shell elements are MITC4 elements [8] [10].

---

**Figure 2:** Problem setup in the sensor mode. The upper and lower grey layers are the piezoelectric plates, and the middle white layer is the metal shim plate. The top and bottom surfaces are grounded uniformly. The arrows with $P$ refer to polarization direction. The arrow with $F$ refers the external mechanical force.

**Figure 3:** Solid mesh for the piezoelectric analysis.

**Figure 4:** Shell mesh for the inverse-piezoelectric analysis.
Figure 5: Potential distribution along the $z$-direction and the $x$-direction, where the potential is positive in the negative direction of the $y$-axis, and the magnitude is also expressed using the color contour (pink: 0.38V, blue: 0V).

4.2 Results and discussion

Figure 5 shows the electric potential distribution along the thickness and the length, where the potential is positive in the negative direction of the $y$-axis, and the magnitude is also expressed using the color contour. Note that this distribution is almost equivalent along the $y$-direction. Figure 6 shows the electric potential distributions at the fixed and free ends.

The large bending stress near the fixed end causes the large piezoelectric effect. Therefore, the quadratic distribution in each piezoelectric layer can be observed near the fixed end as shown in Figures 5 and 6. On the contrary, the small bending stress near the free end causes little piezoelectric effect, while the potential is transferred in the shim from the area near the fixed end to this area. Therefore, the linear potential distribution between the top or bottom surface and the shim in each piezoelectric layer can be observed near the free end.

Note that the shape of the potential distribution is continuously changed from the quadratic function at the fixed end to the linear function at the free end along the $x$-direction. The shell piezoelectric analysis assumes the linear or quadratic function as the potential distribution through the thickness [11]-[15]. However, it is not applicable to the present problem.

The equivalent potential in the shim is simulated using the proposed pseudo-piezoelectric method as shown in Figure 6. The numerical solution of this potential is $3.474\times10^{-1}$V, while the theoretical solution is $3.524\times10^{-1}$V [9]. Their relative error is about 1.4%. Therefore, the proposed method can analyze the thin piezoelectric bimorph with the metal layers accurately.

5 CONCLUSIONS

The solid piezoelectric and shell inverse-piezoelectric analyses are coupled using the block Gauss-Seidel method and the transformation of the solution variables between the shell and solid meshes. The rules of mixture are used in the shell inverse-piezoelectric analysis. The pseudo-piezoelectric modeling for the conductor in the solid piezoelectric analysis is proposed. This modeling allows us to reuse the existing program without any modification. The proposed method is applied for the sensor mode of the thin piezoelectric bimorph with the metal layer, and can analyze the thin piezoelectric bimorph with the metal layers accurately.
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REFERENCES

KINETIC CONSISTENT ALGORITHM FOR INCOMPRESSIBLE CONDUCTIVE FLUID

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Key words: Kinetic Methods, Kinetic Consistent Methods, High Performance Computing

Abstract. A kinetic model based on the single-particle Boltzmann-like distribution function is used to describe magneto gas dynamic phenomena. Along with the original kinetic consistent gas dynamic model, a simplified version that is more convenient for numerical implementation is considered and justified. Numerical results for a number of problems are presented, especially for the incompressible conductive fluid.

1 INTRODUCTION

The magneto gas dynamics (MGD) and magneto hydro dynamic (MHD) equations with allowance for dissipative effects (molecular and magnetic viscosity, heat conduction and others) are a mathematical models for describing technological processes and processes in fundamental science [1, 2, 3]. The modelling of many important problems requires computing technologies making use increasing capabilities of modern parallel high performance computers. Unfortunately, the use of high and ultrahigh performance of computing systems is hampered by difficulties associated with the adaptation of algorithms and software to the architecture of computers with extra-massive parallelism [4].

The novel kinetic consistent model of magneto gas and magneto hydro dynamic processes is proposed. The mathematical models are based on single-particle Maxwellian distribution function [5]:

\[ f_{0M} = \frac{\rho(t, x)}{(2\pi RT)^{3/2}} e^{-\frac{(\xi - u - iv)^2}{2RT}}, \]

(1)
here $t$ is time, $x$ is the spatial coordinate, $\xi$ is the molecular velocity, $\rho$ is the density, $u$ is the macroscopic velocity, $T$ is the temperature, $R$ is the gas constant, and $v_\alpha$ is the Alfven velocity given by

$$v_\alpha = \frac{B}{\sqrt{4\pi\rho}},$$

where $B$ is the magnetic intensity and $i$ is the imaginary unit.

In contrast to the classical locally Maxwellian statistical distribution function, the exponent in function (1) has the term $i\nu_\alpha$, which describe the relation between the charged particles in the electromagnetic field on the level of kinetic theory [6, 7].

The momentum of $f_{0M}$ gives the macroscopic variables including the magnetic field:

$$\rho(t, x) = \int m f_{0M} d\xi,$$

$$u(t, x) = \frac{1}{\rho} \int m \xi f_{0M} d\xi,$$

$$E = \int \frac{1}{2} m \xi^2 f_{0M} d\xi,$$

$$B = \frac{1}{\sqrt{\mu\rho}} \int m \xi^* f_{0M} d\xi,$$

where $E = \rho \frac{u^2}{2} + \epsilon + \frac{B^2}{8\pi}$ is the total energy, $\epsilon$ is internal energy, $\xi^*$ is the complex conjugate of the molecular velocity $\xi$ and the magnetic intensity $B$ is defined as integral with conjugated velocity.

By using function (1) and a procedure similar for deriving the Euler equations from the Boltzmann one, the ideal magneto gas dynamic equations can be obtained from the kinetic equation. In view of these possibilities of describing magneto gas dynamic phenomena, we construct a model of dissipative magneto gas dynamic processes by using approaches developed for deriving the kinetic consistent gas dynamic system in [9].

2 MODEL OF MAGNETO GAS DYNAMIC PROCESSES

We can deriving the kinetic consistent magneto gas dynamic system of equations like kinetic consistent gas dynamic equations, consider the balance equation [6]

$$\frac{f^{j+1} - f^j_{0M}}{\tau^*} + \xi_k \frac{\partial f^j_{0M}}{\partial x_k} = \frac{\partial}{\partial x_k} \frac{\tau^*}{2} \xi_k \xi_p \frac{\partial f^j_{0M}}{\partial x_p},$$

where $f^{j+1}$ is the distribution function describing the behavior of an ensemble of charged particles and the magnetic intensity at the time $t = t^{j+1}$.

In a similar manner, kinetic consistent magneto gas dynamic system of equations are obtained by multiplying the balance equation (8) by the summation invariants and integration the results over all molecular velocities. However, there is a difference from the
procedure for deriving the quasi gas dynamic system. In multiplication by \( m, m\xi, m\xi^2/2 \), we specify \( \tau \) as the time between molecular collisions as in the case of the quasi gas dynamic system. When (7) is multiplied by \( m\xi^* \), \( \tau_M \) is defined from magneto dynamic processes \( \tau_M \), the value of \( \tau^* \) will be discussed later.

As result of multiplication, whole technique is described in [6, 9], is derived the system of equations:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\tau}{2} \frac{\partial^2 \rho}{\partial t^2} + \frac{\partial}{\partial x_i} \rho u_i &= \frac{\partial}{\partial x_i} \left( \frac{\tau}{2} \frac{\partial}{\partial x_k} \Pi_{ik} \right), \\
\frac{\partial \rho u_i}{\partial t} + \frac{\tau}{2} \frac{\partial^2 \rho u_i}{\partial t^2} + \frac{\partial}{\partial x_k} \Pi_{ik} &= \frac{\partial}{\partial x_k} \Pi_{ik}^D + \frac{\partial}{\partial x_k} \left[ \left( \frac{\tau}{2} \frac{\partial}{\partial x_k} \Pi_{ik} \right) u_k \right], \\
\frac{\partial E}{\partial t} + \frac{\tau}{2} \frac{\partial^2 E}{\partial t^2} + \frac{\partial F_i}{\partial x_i} &= \frac{\partial}{\partial x_i} \Pi_{ik}^D u_k + \frac{\partial}{\partial x_i} \left[ \frac{1}{\rho} \left( E + p + \frac{B^2}{8\pi} \right) \left( \frac{\tau}{2} \frac{\partial}{\partial x_k} \Pi_{ik} \right) \right], \\
\frac{\partial B_i}{\partial t} + \frac{\tau_M}{2} \frac{\partial^2 B_i}{\partial t^2} + \frac{\partial}{\partial x_k} \Pi_{ik}^B &= \frac{\partial}{\partial x_k} \Pi_{ik}^{BB}, \\
\text{div} \mathbf{B} &= 0.
\end{align*}
\]

The left hand side of this system, including (8)-(12), like the ideal magneto gas dynamic equations. The dissipative terms on the right hand side of (8)-(12) are given by

\[
\begin{align*}
\Pi_{ik} &= \left( p + \frac{B^2}{8\pi} \right) \delta_{ik} + \rho u_i u_k - \frac{B_i B_k}{4\pi}, \\
\Pi_{ik}^D &= \frac{\tau}{2} \left[ p \frac{\partial u_i}{\partial x_k} + \frac{2}{3} \rho \frac{\partial u_m}{\partial x_k} \delta_{ik} \right] \\
&+ \frac{\tau}{2} \left[ \left( \frac{B^2}{8\pi} \delta_{m k} - \frac{B_m B_k}{4\pi} \right) \frac{\partial u_i}{\partial x_m} + \left( \frac{B^2}{8\pi} \delta_{i m} - \frac{B_i B_m}{4\pi} \right) \frac{\partial u_k}{\partial x_m} - \left( \frac{B^2}{8\pi} \delta_{i k} - \frac{B_i B_k}{4\pi} \right) \frac{\partial u_m}{\partial x_m} \right] \\
&+ \frac{\tau}{2} \left[ \left( \frac{B_m}{4\pi} \left( -\frac{B_i}{\delta_{x m}} - \frac{B_k}{\delta_{x m}} \right) \frac{\partial u_k}{\partial x_m} \right) - \frac{B_i}{\delta_{x m}} \frac{\partial u_k}{\partial x_m} + B_k \frac{\partial u_m}{\partial x_m} \delta_{ik} \right] \\
&+ \frac{\tau}{2} \left[ \rho u_i u_m \frac{\partial u_k}{\partial x_m} + u_i \frac{\partial p}{\partial x_k} + u_i \frac{\partial B^2}{\partial x_k} - B_k \frac{\partial u_m}{\partial x_m} - \frac{B_m B_k}{4\pi} \right] + \frac{\tau}{2} \left[ u_m \frac{\partial p}{\partial x_m} + \gamma \frac{\partial u_m}{\partial x_m} \right] \delta_{ik} \\
&+ \frac{\tau}{2} \left[ \frac{1}{4\pi} \left( \frac{B^2}{\delta_{x m}} - \frac{B_i}{\delta_{x m}} \frac{\partial u_m}{\partial x_m} + B_i \frac{\partial u_m}{\partial x_m} \delta_{ik} \right) ight] \\
&+ \frac{\tau}{2} \left[ \frac{1}{4\pi} \left( -\frac{B_i B_k}{\delta_{x m}} + B_i B_k \frac{\partial u_m}{\partial x_m} - B_k \frac{\partial B_k}{\partial x_m} \right) \right] \\
&+ \frac{\tau}{2} \left[ \frac{1}{4\pi} \left( -B_i B_k \frac{\partial u_m}{\partial x_m} + B_i B_k \frac{\partial u_m}{\partial x_m} - B_k \frac{\partial B_k}{\partial x_m} \right) \right].
\end{align*}
\]
The full kinetic consistent gas dynamic system of equations and magneto gas dynamic system of equations are represent more physical model, based on the relations to the kinetic Boltzmann equation and have the representation of many real physical processes which now under investigations. We can inphasise two substantial differences from their classical counterparts:

• First, the kinetic consistent magneto gas dynamic system of equations are hyperbolic type, what ensured by presence of second order derivatives in time [7], despite the presence of dissipation terms. By applying this approach, we can implement a three level explicit scheme with a better stability conditions than that in explicit schemes fore parabolic equations. This scheme has been successfully used to modeling magneto gas dynamic problem on high performance computing system [10, 11].

• Second, the continuity equation involves a dissipative term absent from the Euler and Navier–Stokes equations. Recall that, in combination with the second order derivative in time of density, the difference from the classical continuity equation consists in terms of the second order of smallness in the Knudsen number [6, 13].
However, for the practical purposes, the cumbersomeness of the kinetic consistent gas dynamic system and even more of its magneto gas dynamic version (8)-(12) make them complicated for the numerical analysis and computing. Let us describe how, relying on the kinetic consistent gas dynamic system and (8)-(17), a more compact models of gas dynamic and magneto gas dynamic processes can be obtained with the preservation of the potentials of the kinetic consistent gas dynamic description for efficient calculations on high performance computing systems.

3 COMPACT KINETIC CONSISTENT MAGNETO GAS DYNAMIC SYSTEM OF EQUATIONS

First, we note the relation between the kinetic consistent magneto gas dynamic system (9)–(13) and the classical equations of dissipative magneto gas dynamic system. Due to the cumbersomeness of system (9)–(17), this relation has not yet been analysed completely and continued. For this reason, we use an analogy with the kinetic consistent gas dynamic system, which differs from the Navier–Stokes equations in terms of the second order of smallness in the Kn number. Schematically, this relation can be expressed as

\[ \text{QGS} = \text{NS} + O(Kn^2). \]  

The closeness of the solutions to two systems has been confirmed by numerous numerical experiments and a theoretical analysis [6, 11]. This analysis is based on the fact that the solution of the balance equation

\[ \frac{f^{j+1} - f^j}{\tau} + \xi_k \frac{\partial f_0}{\partial x_k} = \frac{\partial}{\partial x_k} \frac{\tau}{2} \xi_p \xi_k \frac{\partial f_0^j}{\partial x_p}, \]  

where \( f_0 \) is given by (1), differs by terms of order \( Kn^2 \) from the solution of the Bhatnagar–Gross–Krook equation [6]

\[ \frac{\partial f}{\partial t} + \xi_i \frac{\partial f}{\partial x_i} = \frac{1}{\tau} (f_0 - f). \]

First, we consider a compact version of the kinetic consistent gas dynamic system with dissipative terms, physically this terms appears due to smoothing the solution over the mean free path, which follows from the method of deriving the balance equation [6, 13]. It is appear as the contribution made by the additional velocity \( w \), which appears on the right-hand sides of the continuity, momentum, and energy equations

\[ w_k = \frac{\tau}{\rho} \frac{\partial}{\partial x_i} (pu_k u_i + p\delta_{ik}). \]  

For this purpose, we follow a method similar to that used in continuum mechanics to derive similar equations, taking into account the gas dynamic velocity and molecular transport:
\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\tau}{2} \frac{\partial^2 \rho}{\partial t^2} + \text{div} \rho (\mathbf{u} - \mathbf{w}) &= 0, \quad (22) \\
\frac{\partial \rho \mathbf{u}}{\partial t} + \frac{\tau}{2} \frac{\partial^2 \rho \mathbf{u}}{\partial t^2} + \text{div} [\rho (\mathbf{u} - \mathbf{w}) \times \mathbf{u}] + \text{div} p &= \text{div} P_{\text{NS}}, \quad (23) \\
\frac{\partial E}{\partial t} + \frac{\tau}{2} \frac{\partial^2 E}{\partial t^2} + \text{div} [(E + p) (\mathbf{u} - \mathbf{w})] &= \text{div} \mathbf{q} + \text{div} (P_{\text{NS}} \mathbf{u}), \quad (24)
\end{align*}
\]

where \( P_{\text{NS}} \) is the Navier-Stokes viscous stress tensor and \( \mathbf{q} \) is the heat flux with components \( q_i = \kappa \frac{\partial T}{\partial x_i} \).

System (22)-(24) differs from the Navier–Stokes equations in that its left-hand side involves the generalized velocity \( \mathbf{u} - \mathbf{w} \) rather than \( \mathbf{u} \). Recall that this system of equations is derived by applying the phenomenological approach used in continuum mechanics for obtaining corresponding equations. Specifically, the original kinetic consistent gas dynamic system of equations (obtained from the balance equation (19) can be represented in the form

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\tau}{2} \frac{\partial^2 \rho}{\partial t^2} + \text{div} \rho (\mathbf{u} - \mathbf{w}) &= 0, \quad (25) \\
\frac{\partial \rho \mathbf{u}}{\partial t} + \frac{\tau}{2} \frac{\partial^2 \rho \mathbf{u}}{\partial t^2} + \text{div} [\rho (\mathbf{u} - \mathbf{w}) \times \mathbf{u}] + \text{div} p &= \text{div} \mathbf{P}^*, \quad (26) \\
\frac{\partial E}{\partial t} + \frac{\tau}{2} \frac{\partial^2 E}{\partial t^2} + \text{div} [(E + p) (\mathbf{u} - \mathbf{w})] &= \text{div} \mathbf{q}^* + \text{div} (\mathbf{P}^* \mathbf{u}), \quad (27)
\end{align*}
\]

where the tensor \( \mathbf{P} \) is given by the expression

\[
\mathbf{P}^* = P_{\text{NS}} + \rho \mathbf{u} \times \left[ \mathbf{w} - \frac{\tau}{\rho} \text{div} (\rho \mathbf{u}) \right] + \tau \left[ \text{div} p + \gamma \rho \text{div} \mathbf{u} \right], \quad (28)
\]

\[
\mathbf{q}^* = \mathbf{q} + \tau \left[ \rho \left( \text{div} \mathbf{u} + \frac{p}{\rho^2} \text{div} \rho \right) \right] \mathbf{u}, \quad (29)
\]

here \( \gamma \) is the ratio of specific heat.

Let us estimate the values of the additional terms involved in \( \mathbf{P}^* \) and \( \mathbf{q}^* \) in the two-dimensional case. The components of the tensor \( \mathbf{P}^* \) (for the equation describing the momentum along the \( OX \) axis) are

\[
\begin{align*}
P_{xx} &= \left( \frac{4}{3} u + \zeta \right) \frac{\partial u_x}{\partial x} + \frac{\tau}{\rho} (\gamma \rho + \tau \rho u_x^2) \frac{\partial u_x}{\partial x} + 2 \tau u_x \frac{\partial p}{\partial x} \\
&+ \left( -\frac{2}{3} u + \zeta + \gamma \rho \right) \frac{\partial u_y}{\partial y} + \frac{\tau}{\rho} (\gamma \rho + \tau \rho u_x u_y) \frac{\partial u_x}{\partial y} + \frac{\tau}{\rho^2} \frac{\partial p}{\partial y}, \quad (30) \\
P_{yx} &= (\mu + \tau \rho u_y^2) \frac{\partial u_x}{\partial y} + \frac{\rho}{\rho^2} \frac{\partial u_y}{\partial x} + \tau \rho u_x u_y \frac{\partial u_x}{\partial y}, \quad (31)
\end{align*}
\]
where
\[ P_{NSxx} = \left( \frac{4}{3} u + \zeta \right) \frac{\partial u_x}{\partial x} + \left( -\frac{2}{3} u + \zeta \right) \frac{\partial u_y}{\partial y}, P_{NSyx} = \mu \frac{\partial u_x}{\partial y} + \mu \frac{\partial u_y}{\partial x} \] (32)

and \( \zeta \) is the bulk viscosity.

Consider two typical cases where the dissipative terms of order \( O(Kn) \) involved in components \( P \) (28)-(29) of the tensor \( P^* \), which can determine the flow structure. First, we consider the case of a boundary layer on a surface perpendicular to the \( OY \) direction. The viscous terms become comparable with the convective ones only if they contain the derivatives \( \frac{\partial u_x}{\partial y} \) [14]. Since \( u_y \) in the boundary layer is much smaller than \( u_x \) in order of magnitude the convective terms can be comparable only with the viscous ones involved in \( P_{yx}^* \), i.e. with the components \( P_{NS} \) (28). Similarly, in the boundary layer, the work of the dissipative terms \( \text{div}(Pu) \) in the energy equation is determined by the work of the viscous forces. In turn, the additional terms involved in \( q^* \) (29) are small as compared with \( q \). This is associated with the fact that the gradients of \( \epsilon \) and \( \rho \) in the \( OY \) direction are multiplied by small values of \( u_y \).

Consider the case of flow with small \( Re \) number, when the viscous terms have the same order of magnitude as the convective terms. As a rule, such flows correspond to low Mach numbers \( M \), so the gas, let alone the fluid, is nearly incompressible.

In this case, the value of \( \text{div}u \) involved in (28) is close to zero. Let us estimate the other terms in (28) in order of magnitude:
\[ \left[ -\rho u \times \frac{\tau}{\rho} \text{div}(\rho u) + \tau u \text{div}p \right] = \frac{\tau \rho V^3}{L}, \] (33)

where \( V \) is the characteristic velocity and \( L \) is the characteristic length of the problem.

The term \( \rho u \times w \) has the same order of magnitude. Taking into account the relation between \( \mu, \tau \) and the speed of sound, a similar estimate for the components of \( P_{NS} \) is given by
\[ [P_{NS}] = \frac{\tau \rho c^2 V}{L}. \] (34)

Thus, in the case under consideration, the value of \( P^* \) is determined nearly completely by the components of \( P_{NS} \).

Now, we will analyse the relation between the energy equation (24), which was obtained using phenomenological definition, and the complete kinetic consistent gas dynamic energy equation (27), which was derived from the balance equation. From (24), the work of \( P^* \) is determined by \( P_{NS} \). Let us estimate the order of magnitude of the \( P_{NS} \) terms involved in \( q^* \) (27), \( q = \kappa \text{grad}T \), and \( \tau \left[ \rho \left( \text{udive} - \frac{\partial}{\rho} \text{div}p \right) \right] \) between the thermal conductivity \( \kappa \) and viscosity \( \nu \), and between \( T \) and the speed of sound \( c \):

the first term has the order of magnitude
\[ [q] = \frac{\tau \rho c^4}{L}, \] (35)
the second term is given by
\[
\tau \rho \left( \mathbf{u} \nabla \epsilon - \frac{p}{\rho^2} \mathbf{u} \nabla \rho \right) = \frac{\tau \rho c^2 V^2}{L}.
\] (36)

Taking into account \( c \gg |u| \), we conclude that the value of \( q^* \) is then determined by the heat flux \( q \).

In contrast to the analysis of the relation between the kinetic consistent gas dynamic system (25)-(27) and the Navier–Stokes equations, which differ by terms of the second order of smallness in the \( Kn \) number, the difference between the kinetic consistent gas dynamic system and its simplified version (22)-(24) is analysed by studying the situation when the viscosity and thermal conductivity have a large effect on the gas dynamic flows.

This conclusion is confirmed by computations, some of which are presented in the next section.

Next let’s consider the induction equation in term of compact version of the kinetic consistent magneto gas dynamic system of equations. The first dissipative term in the right hand side of (16) has a main contribution
\[
\left[ \frac{\tau_m}{2} \left( p + \frac{B^2}{8\pi} \right) \left( \frac{\partial B_i}{\partial x_k} - \frac{\partial B_k}{\partial x_i} \right) \right] \gg \left[ \Pi_{ik}^{DB^*} \right].
\] (37)

Since
\[
\text{rot} \mathbf{B} = \frac{\partial B_i}{\partial x_k} - \frac{\partial B_k}{\partial x_i}, \quad \nu_m = \frac{\tau_m}{2\rho} \left( p + \frac{B^2}{8\pi} \right),
\] (38)

where \( \nu_m \) has the meaning of magnetic viscosity.

Remark about definition of \( \tau_m \). By using (38) we can determine \( \tau_m \) in terms of the magnetic viscosity \( \nu_m \):
\[
\tau_m = \frac{2\rho \nu_m}{p + \frac{B^2}{8\pi}},
\] (39)

taking to account
\[
\nu_m = \frac{c^2}{4\pi\sigma(T,\rho)},
\] (40)

where \( c \) is the speed of light and \( \sigma \) is the conductivity.

Finally the induction equation can be represented in the form
\[
\frac{\partial \mathbf{B}}{\partial t} - \text{rot} \left( \mathbf{u} \times \mathbf{B} \right) = \nu_m \text{rot} \mathbf{B} + \frac{\partial}{\partial x_i} \Pi_{ik}^{DB^*}.
\] (41)

In view of (41) we can say that the induction equation of kinetic consistent magneto gas dynamic equations differs from the corresponding classical magneto gas dynamic equations.
by a small quantity. It has been shown previously that the numerical results based on system (8)-(17) nearly do not differ from those obtained with classical models [12].

The construction of a system for describing magneto gas dynamic processes is based on physical factors that, along with molecular transport and the magnetic field have the influence of the additional velocity \( w \) associated with smoothing the solution over the mean free path. According to (32), \( w \) is given by

\[
w_k = \frac{1}{\rho} \frac{\partial}{\partial x_i} \left[ \left( p + \frac{B^2}{8\pi} \right) \delta_{ik} + \rho u_i u_k - B_i B_k \right].
\]

This velocity, together with \( u \), affects the all magneto gas dynamic parameters and finally the compact system can be represented:

\[
\frac{\partial \rho}{\partial t} + \frac{\tau \partial^2 \rho}{\partial t^2} + \text{div} \rho (u - w) = 0, \tag{43}
\]

\[
\frac{\partial \rho u}{\partial t} + \frac{\tau \partial^2 \rho u}{\partial t^2} + \text{div} [\rho (u - w) \times u + B_k B_p] + \text{div} \left( p + \frac{B^2}{8\pi} \right) = \text{div} P_{NS}, \tag{44}
\]

\[
\frac{\partial E}{\partial t} + \frac{\tau \partial^2 E}{\partial t^2} + \text{div} \left[ \left( E + p + \frac{B^2}{8\pi} \right) (u - w) \right] = \text{div} q + \text{div} (P_{NS} u), \tag{45}
\]

\[
\frac{\partial B}{\partial t} + \frac{\tau_m \partial^2 B}{\partial t^2} = \text{rot} (u - w) \times B + \text{rot} \nu_m \text{rot} B \tag{46}
\]

\[
\text{div} B = 0. \tag{47}
\]

where \( P_{NS} \) is the viscous stress tensor, \( q \) is the flux vector, \( \nu_m \) is the magnetic viscosity and \( \tau_m \) is determined in terms of \( \nu_m \) given by (40).

4 MODELING RESULTS WITH COMPACT MAGNETO GAS DYNAMIC SYSTEM

Below, we present results obtained using compact systems (43)-(47). All computations relied on three-level explicit schemes with new values of the gas dynamic variables and the magnetic field at the time \( t = t^{j+1} \) determined from known values at \( t = t^j \) and \( t = t^{j-1} \). All spatial derivatives were approximated at the central time level \( t = t^j \) up to \( O(n^2) \).

Figure 1 presents the results obtained for the Orszag–Tang test, i.e., for the evolution of a vortex in a magnetic field [17]. The initial data and the grid for the two-dimensional problem were the same as in [18]. The figure displays the density, pressure, magnetic pressure, and kinetic at the time \( t = 0.5 \). The numerical results agree with those obtained earlier for this problem.

Second we consider solutions of hydro dynamic problems based on system (43)-(47) without magnetic field. The results of the incompressible flow in a 3D cavity with a moving upper lid [16]. To simulate an isotropic incompressible (liquid), we used the equation of state

\[
p = p_0 + \beta (\rho - \rho_0), \tag{48}
\]
where $p_0$ and $\rho_0$ are the reference values of the pressure and density and $\beta$ is a sufficiently large coefficient ensuring a large variation in pressure under minor variations in density. Figure 2 shows streamlines at $Re = 1000$, including detailed representations in the cavity corners, where vortex regions are formed. The plots do not exhibit any differences between the reference results of [16] and the results obtained on the basis of system (43)-(47).

The results of magneto hydro dynamic drive simulation is shown on Fig. 3. The representative results of magneto hydro dynamic flow in magneto hydro dynamic drive with caverna for the liquid Sodium flow. Liquid Sodium at temperature $600 \, K$ is placed in a vessel with dimensions $0.3 \times 0.3 \, m^2$. A stream of liquid Sodium is initiated by the magneto hydro dynamic drive on top of the vessel with a tube with dimension $0.02 \times 0.02 \, m^2$. The velocity provided by the magneto hydro dynamics drive is $36 \, m/s$. The analysis of the results shows the possibility of modeling of liquid flow with the kinetic consistent magneto hydro dynamic models.

5 CONCLUSIONS

The compact models (25)-(27) and ((43)-(47) for describing gas dynamic and magneto gas dynamic flows, respectively, are based on kinetic models, which lead to the kinetic consistent gas dynamic system, and on phenomenological ideas. The use of phenomeno-
logical approaches, which are visual from the point of view of physical concepts, makes the systems not only more compact in comparison with their pure kinetic consistent gas dynamic versions, but also better justified in terms of macroscopic views. Their validity was confirmed not only by theoretical estimates, but also by test computations.

The compact models preserve all positive properties intrinsic to previously proposed pure kinetic consistent gas dynamic models. Additionally, they provide a visual and simple description, which is an important factor in numerical simulation.

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REFERENCES


TRIPLY COUPLED ANALYSIS METHOD FOR THIN FLEXIBLE PIEZOELECTRIC BIMORPH IN FLUID

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Abstract. Piezoelectric–structure–fluid interaction is a complex multiphysics coupled phenomena appears wherein piezoelectric devices are in contact or surrounded by the fluid media. The piezoelectric energy harvesting using ocean waves, wind flow, and mechanical vibrations are some of the popular energy savaging methods wherein thin piezoelectric bimorphs surrounded by the fluid is used for power harvesting. With recent advances on micro air vehicles actuated by piezoelectric bimorph actuators in the fluid (surrounding media) as attracted the of piezoelectric–structure–fluid interaction. Generally, in these applications, the piezoelectric bimorph is thin, flexible, and surrounded by the fluid. The large deformation of the thin flexible piezoelectric bimorph causes strong interaction with the electric field (piezoelectric effect) and the surrounding fluid, and inversely, these two fields significantly affect the structure. The piezoelectric field–structure–fluid interaction analysis is very significant. In this work, we propose a hierarchal decomposition method to solve piezoelectric–structure–fluid interaction of a piezoelectric bimorph in the fluid. The proposed method is applied to a flexible restrictor flap in converging channel, where the rubber flap is replaced by the piezoelectric bimorphs made of PVDF or PZT–5H. The resonance frequency of the piezoelectric bimorph in the fluid agrees well with the theoretical and numerical pure FSI cases. These results show a good agreement with the previous studies.

1 INTRODUCTION

The piezoelectric bimorphs are used to actuate the flexible wings of insect–like micro air vehicles. Also, they have attracted great attention in energy harvesting due to their large electro–mechanical convertible characteristics. Generally, in these applications, the piezoelectric bimorph is thin, flexible, and surrounded by the fluid. The large deformation of the thin flexible piezoelectric bimorph causes strong interaction with the electric field (piezoelectric effect) and
the surrounding fluid, and inversely, these two fields significantly affect the structure. The electric field–fluid–structure interaction (EFSI) analysis is very significant.

A novel triply coupled analysis method is proposed to solve the thin flexible piezoelectric bimorph in the fluid. The hierarchal decomposition [1] as the theory is superior to the others in terms of the application to complicated multiphysics problems. Here, the piezoelectric–structure–fluid interaction system is decomposed hierarchically, i.e., it is partitioned into the subsystems of fluid–structure interaction (FSI) and piezoelectric field using the block Gauss–Seidel partitioned iterative method, and then the FSI is split into the fluid–structure velocity field and the pressure field using an algebraic splitting method [2], and finally, the fluid–structure velocity field is partitioned into the fluid and structure velocity fields using the explicit method for the fluid [3]. Since the structure is quite thin and flexible, MITC4 shell [4] are very well suited for the structural discretization, but modeling electric contribution is a challenging task for shell element. Therefore, the piezoelectric field is solved using 3D solid element, discussed in [5]. The fluid is solved using P1P1 element [6]. The use of these different elements remedies the shortcoming of using the same elements, i.e., the piezoelectric–structure interaction method in Ref. [5] can treat various electric configurations with almost a linear or quadratic distribution of electric potential across the thickness, whereas the shell elements, which are well suited for thin flexible bimorph, cannot treat various electric configurations. The coupled algorithm to solve piezoelectric–structure interaction using finite element methods can be found in Refs. [5,7–11]. The previous studies of the piezoelectric–structure–fluid interaction can be found in Refs. [12,13].

The proposed method is applied to a flexible restrictor flap in converging channel [14], where the rubber flap is replaced by the piezoelectric bimorphs made of PVDF or PZT–5H. The resonance frequency of the piezoelectric bimorph actuator analysis in the fluid agrees well with the theoretical and numerical pure FSI cases. However, the frequency shifts upon the connected electric resistive load can be seen for the open–and closed–circuit sensor analysis of the PVDF and PZT–5H bimorph in the fluid. This shift for PVDF is negligible, while this shift for PZT–5H is noticeable. These results show a good agreement with the previous studies [15].

2 GOVERNING EQUATIONS

2.1 Piezoelectricity

The electromechanical coupling also known as piezoelectric–structure interaction is governed by the constitutive equations written as

\[
\sigma_{ij} = C_{ijkl} S_{kl} - e_{kij} E_k, \quad (1)
\]
\[
D_i = \varepsilon_{ijkl} S_{kl} + \varepsilon^S_{ik} E_k, \quad (2)
\]

where \(\sigma_{ij}\), \(C_{ijkl}\), \(S_{kl}\), \(e_{kij}\), \(E_k\), and \(\varepsilon^S_{ik}\) denotes the stress tensor, the elastic constitutive tensor, the mechanical strain tensor, the piezoelectric coupling coefficient, the electric field vector, and the dielectric permittivity tensor, respectively. The relation between the electric field vector \(E_i\)
and a scalar electric potential $\phi_i$ is given by

$$E_i = -\phi_i.$$

### 2.2 Structure

The structure is governed by the Cauchy’s equation of motion:

$$\rho^s \frac{d^2 u^s_i}{dt^2} = \frac{\partial \sigma^s_{ji}}{\partial x_j} + \rho^s g^s_i, \text{ on } \Omega^s,$$

where $\rho^s$, $u^s_i$, $g^s_i$, and $\sigma^s_{ij}$ denotes the density of the structure, the structural displacement vector, the body force vector acting on the structure, and the 2nd Piola–Kirchhoff stress tensor, respectively. The essential and natural boundary conditions for the structure is given as

$$v^s_i = \bar{v}^s_i, \text{ on } \Gamma^s_E;$$

$$\sigma^s_{ij} n^s_j = \tau^s_i, \text{ on } \Gamma^s_N.$$

where $\Gamma^s_E$ and $\Gamma^s_N$ are complementary subsets of $\Gamma^s$, $\bar{v}^s_i$ and $\tau^s_i$ are the prescribed structure velocity and traction values on the complementary subset of $\Gamma^s$.

### 2.3 Fluid

The fluid flow is governed by the Navier–Stokes equations for incompressible Newtonian fluids. The arbitrary Lagrangian–Eulerian formulation is employed to describe the incompressible viscous fluid motion in the deformable domain [16]:

$$\rho^f \frac{\partial v^f_i}{\partial t} + \rho^f (v^f_j - \hat{v}^f_j) \frac{\partial v^f_i}{\partial x_j} = \frac{\partial \sigma^f_{ji}}{\partial x_j} + \rho^f g^f_i, \text{ in } \Omega^f.$$

The incompressibility constraint is given as

$$\frac{\partial v^f_i}{\partial x_i} = 0, \text{ in } \Omega^f,$$

where superscript $f$ indicates the fluid components, $\rho^f$, $v^f_i$, $\hat{v}^f_i$, $g^f_i$, and $\sigma^f_{ij}$ denotes the density of the fluid, the fluid velocity vector, the velocity vector of the mesh deformation in ALE co–ordinate, the body force vector acting on the fluid, and the stress tensor of the fluid, respectively.

### 2.4 Interface conditions

The interaction conditions on the interface between the fluid and the structure are imposed using the following geometric compatibility and equilibrium conditions:

$$v^f_i = v^s_i \equiv \bar{v}^s_i, \text{ on } \Gamma^{fs};$$

$$\sigma^f_{ij} n^f_j + \sigma^s_{ij} n^s_j = \tau^s_i, \text{ on } \Gamma^{fs},$$

where superscript $fs$ indicates the components of fluid–structure interface, $\bar{v}^s_i$ and $\tau^s_i$ denotes the fluid–structure interface velocity vector and the surface force vector acting on the fluid–structure interface, respectively.
3 FINITE ELEMENT FORMULATION OF PIEZOELECTRIC–STRUCTURE–FLUID INTERACTION

The piezoelectric system in 3D solid elements at time \( t + \Delta t \) is given by

\[
K^{(i)}_{\phi\phi} t+\Delta t \phi^{(i)}(t+\Delta t) + K^{(i)}_{\phi u} t+\Delta t u^{(i-1)} = q - K^{(i)}_{\phi\phi} t+\Delta t \phi^{(i)}(t+\Delta t) u^{(i-1)}.
\] (11)

where \( i \), \( K_{\phi\phi} \), \( \phi^{(i)}_{\text{solid}} \), \( q \), \( K_{\phi u} \), and \( u_{\text{solid}} \) denotes block Gauss–Seidel iteration, the matrix of dielectric stiffness matrix of piezoelectric material, the vector of electric potentials in the 3D solid elements, the vector of the external surface density charges on the piezoelectric material, the matrix of the piezoelectric coupling coefficient of the piezoelectric material, and the vector the displacement vector of the 3D solid elements which are evaluated using the displacement transformation method [5]. The displacement are transformed from the shell element to the 3D solid element to analyze the piezoelectric field given as follows [5]:

\[
u_{\text{solid}} = u_T u^s.
\] (12)

where \( u^s \) is the shell element displacement vector and \( u_T \) is the displacement transformation matrix. Applying the displacement transformation given in Eq.(12) into Eq.(11) we obtain

\[
K^{(i)}_{\phi\phi} t+\Delta t \phi^{(i)}(t+\Delta t) + K^{(i)}_{\phi u} t+\Delta t u^{(i-1)} = q - K^{(i)}_{\phi\phi} t+\Delta t \phi^{(i)}(t+\Delta t) u^{(i-1)}.
\] (13)

The induced electrical forces due to the inverse piezoelectric effect can be obtained for the known electric potential in the current BGS iteration \( i \) at each time step \( t + \Delta t \) in the 3D solid elements as

\[
(t+\Delta t) e_{\text{solid}}^{e} = - (t+\Delta t) K^{(i)}_{\phi\phi} \phi^{(i)}(t+\Delta t) u^{(i-1)}.
\] (14)

The induced electrical forces \( e_{\text{solid}}^{e} \) in the 3D solid of the piezoelectric field are transformed on the shell structure of the FSI system using the force transformation given by

\[
e_{\text{solid}}^{e} = e_T e_{\text{solid}}^{e}.
\] (15)

where \( e_T \) is the force transformation matrix. Applying the force transformation onto the shell structure of the FSI system, the external force vector acting on the FSI given in Ref. [2] (see Eq.8(f) in [2]) can be rewritten as

\[
ge^{f} = \begin{pmatrix} g_1^{f} \\ g_2^{f} \\ g_3^{f} \\ g_4^{f} \\ g_5^{f} \\ g_6^{f} \\ g_7^{f} \end{pmatrix} \quad \Rightarrow \quad \begin{pmatrix} g_1^{c} \\ g_2^{c} \\ g_3^{c} \\ g_4^{c} \\ g_5^{c} \\ g_6^{c} \\ g_7^{c} \end{pmatrix} + e^{g}_{c} = \begin{pmatrix} g_1^{d} \\ g_2^{d} \\ g_3^{d} \\ g_4^{d} \\ g_5^{d} \\ g_6^{d} \\ g_7^{d} \end{pmatrix} + e^{g}_{d},
\] (16)

where \( e_{c}^{g} \) and \( e_{d}^{g} \) are the external force or transnational force acting on the shell and the external electric moment of force or rotational force acting on the shell, respectively, i.e.,
Then the intermediate state variables and their increment are evaluated as

\[ \mathbf{g}_{\text{c}}^s = \left[ \mathbf{g}_{\text{c}}^s, \mathbf{g}_{\text{d}}^s \right]^T. \]

The external transnational force and the rotational forces acting on the shell structure of the FSI system are obtained respectively using

\[ \mathbf{g}_{\text{c}}^s = \sum_{n_r=1}^{N_r} \mathbf{g}_{\text{c}}^n + \sum_{n_s=1}^{N_s} \mathbf{g}_{\text{c}}^{ns}, \]

\[ \mathbf{g}_{\text{d}}^s = \sum_{n_r=1}^{N_r} (\mathbf{d}^{nr} \times \mathbf{g}_{\text{c}}^{nr}) + \sum_{n_s=1}^{N_s} (\mathbf{d}^{ns} \times \mathbf{g}_{\text{c}}^{ns}), \]

where \( n_r = 1, \ldots, N_r \), \( n_s = 1, \ldots, N_s \), \( \mathbf{g}_{\text{c}}^{nr} \), and \( \mathbf{g}_{\text{c}}^{ns} \) are the indices of the solid element nodes that are located along the considered director vectors \( \mathbf{V}_r^k \) of the shell nodes, the solid element nodes that are located not along the considered director vector of the shell nodes but directly adjacent to it, the nodal electric force vector at solid node \( n_r \), and the induced nodal electric force vector at solid node \( n_s \). Similarly, \( \mathbf{d}^{nr} \) and \( \mathbf{d}^{ns} \) are the position vectors of the solid element nodes \( n_r \) and \( n_s \), respectively, with respect to the shell mid-surface nodes. The details can be found in Ref. [5]. Once the force transformation is done, the FSI is analyzed inside the BGS loop using the projection method proposed by Ishihara and Horie [2]. The time integration of the FSI system is obtained through the predictor–multi–corrector algorithm (PMA) [16, 17]. The stabilization formulation streamline–upwind/Petrov–Galerkin (SUPG) formulations [17] and the pressure–stabilizing/Petrov–Galerkin (PSPG) [6] for incompressible flows are adopted to avoid numerical stability due to the fluid convection and the P1P1 element. Now the increment of intermediate acceleration is determined for the known pressure \( t+\Delta t p^{(i)(k-1)} \) using

\[ \mathbf{M}^t \Delta \mathbf{a}^{(i)} = \Delta \mathbf{g}. \] (19)

Then the intermediate state variables and their increment are evaluated as

\[ t+\Delta t \mathbf{a}^{(i)(k)} = t+\Delta t \mathbf{a}^{(i)(k-1)} + \Delta \mathbf{a}^{(i)}, \]

\[ t+\Delta t \mathbf{v}^{(i)(k)} = t+\Delta t \mathbf{v}^{(i)(k-1)} + \Delta \mathbf{v}^{(i)} = t+\Delta t \mathbf{v}^{(i)(k-1)} + \gamma \Delta t \Delta \mathbf{a}^{(i)}, \]

\[ t+\Delta t \mathbf{u}^{(i)(k)} = t+\Delta t \mathbf{u}^{(i)(k-1)} + \Delta \mathbf{u}^{(i)} = t+\Delta t \mathbf{u}^{(i)(k-1)} + \beta \Delta t^2 \Delta \mathbf{a}^{(i)}, \]

The pressure increment is obtained by solving the pressure Poisson equation (PPE)

\[ \gamma \Delta t \mathbf{T} \mathbf{G}_1 \mathbf{M}^{-1} \mathbf{G} \Delta \mathbf{p}^{(i)} = -\mathbf{T} \mathbf{G}^{t+\Delta t} \mathbf{v}^{(i)(k)}. \] (21)

The acceleration increment is obtained solving

\[ \gamma \Delta t \mathbf{T} \mathbf{G} \Delta \mathbf{a}^{(i)} + \mathbf{G}_c \Delta \mathbf{p}^{(i)} = \Delta \mathbf{h}. \] (22)

The correct phase of the PMA is executed to solve for the acceleration \( t+\Delta t \mathbf{a}^{(i)(k)} \), the velocity \( t+\Delta t \mathbf{v}^{(i)(k)} \), and the displacement \( t+\Delta t \mathbf{u}^{(i)(k)} \) at current BGS and nonlinear iterations of every
time step as follows:

\[ t + \Delta t a^{(i)}(k) = t + \Delta t a^{(i)(k-1)} + \Delta a, \]  

\[ t + \Delta t v^{(i)}(k) = t + \Delta t v^{(i)(k-1)} + \gamma \Delta t \Delta a, \]  

\[ t + \Delta t u^{(i)}(k) = t + \Delta t u^{(i)(k-1)} + \beta \Delta t^2 \Delta a, \]  

\[ t + \Delta t p^{(i)}(k) = t + \Delta t p^{(i)(k-1)} + \Delta p. \]  

At correct stage, we obtain the structural displacements in the shell structure solving Eq.(23c) which can be written as

\[ t + \Delta t u^{s(i)(k)} = t + \Delta t u^{s(i)(k-1)} + \Delta u^{s(k)}. \]  

The resultant displacements in the shell element is now transformed to the solid element using displacement transformation i.e.,

\[ t + \Delta t u^{(i)} = u^T t + \Delta t u^{s(i)}. \]  

The components of the transformation matrix \( \mathbf{u}^T \) are obtained from the displacement interpolation function at time \( t \) as in the shell [18] using

\[ t^j u^s = h^n(r_1, r_2) t^n u^n_j + \frac{r_3}{2} a h^n(r_1, r_2)(-\alpha^n V_2^n + \beta^n V_1^n), \]  

where \( t^j u^s_j, t^n u^n_j, n, h^n, \) and \( a \) indicates the displacements of a material point in a shell element at time \( t \) with natural coordinates \( (r_j) \), the displacement vector of the shell node \( n \) at time \( t \), the shell node, the element shape function, and the shell thickness, respectively. \( \alpha^n \) and \( \beta^n \) are rotations about \( V_1^n \) and \( V_2^n \), respectively.

### 4 NUMERICAL EXAMPLE

The proposed method is applied to a flexible restrictor flap in converging channel [14], where the rubber flap is replaced by the piezoelectric bimorphs made of PVDF or PZT-5H, as shown in Fig. 1. The fluid (silicone oil) properties and the fluid boundary conditions are the same with the bench mark problem [2, 14]. The material properties of PVDF and PZT-5H used in the analysis are given in [19, 20]. The theoretical solution for the transverse resonant frequency of the PVDF and PZT–5H bimorph cantilever beam in the vacuum and fluid with the geometric dimensions \( L = 0.25m, w = 0.02m \) and \( h = 0.005m \) evaluated using [21] are as follows:

- **PVDF bimorph**
  - The undamped transverse resonant frequency in the vacuum: \( \omega_{\text{vac}}^{(1)} = 85.58 \text{ rad/s} \).
  - The damped transverse resonance frequency in the fluid media: \( \omega_{\text{fld}}^{(1)} = 52.45 \text{ rad/s} \).

- **PZT–5H bimorph**
  - The undamped transverse resonant frequency in the vacuum: \( \omega_{\text{vac}}^{(1)} = 235.64 \text{ rad/s} \).
  - The damped transverse resonance frequency in the fluid media: \( \omega_{\text{fld}}^{(1)} = 198.69 \text{ rad/s} \).
Fig. 2 shows the frequency response of PVDF and PZT-5H bimorph in converging channel for 4 problem setup in Fig. 1. The simulated results depicted in Fig. 2(a) for PVDF material shows the resonance when the input frequency of the input bias voltage or the frequency of the equivalent external mechanical force $F_{ext0}$ is $\omega_0 = 50.50$ rad/sec, $\omega = 50.90$ rad/sec, $\omega = 50.10$ rad/sec, and $\omega = 50.30$ rad/sec for case 1, 2, 3, and 4, respectively. The external mechanical force $F_{ext0}$ is evaluated using the blocking force [22] which is equivalent to the electric force generated by the actuator. The vibration amplitudes of the actuator problem setup (case 1) in Fig. 2(a) have less amplitudes compared to that under the pure FSI (case 2), short–circuit sensor configuration (case 3), and the open–circuit sensor configurations (case 4) as the inverse piezoelectric effect counter plays with the mechanical excitation [23]. The resonance obtained with the pure FSI algorithm in case 2 shows a good agreement with the theoretical damped natural frequency i.e. the difference between the theoretical damped natural frequency and the simulated results in case 2 is 2.8%. Now, by taking the FSI solution as an absolute solution, the difference between the FSI (case 2) and piezoelectric-structure-fluid interaction problem (cases 1, case 3, and case 3) is within 1%. This satisfy the approximation condition for the PVDF bimorph given in [23]. This indicates that the frequency shift in the piezoelectric bimorph made of PVDF material upon the electric configuration is negligible. The proposed algorithm takes into account a small shift in the resonance frequency of piezoelectric bimorph made of PVDF which has a negligible shift in the frequency upon the external resistive loading, which also appeared in the works of Song et al. [23].
The simulated results depicted in Fig. 2(b) for PZT–5H material shows the resonance when the input frequency of the input bias voltage or the frequency of the equivalent external mechanical force $F_{ext0}$ is $\omega_\phi = 192$ rad/sec, $\omega = 195$ rad/sec, $\omega = 186$ rad/sec, and $\omega = 199$ rad/sec for case 1, 2, 3, and 4, respectively. The difference between open– and closed–circuit resonance frequency is 6.5%, thus justifying the relation given in Ref. [23] for PZT–5H material. The simulation results in [15] also shows 5% difference between the open– and closed–circuit configuration for the piezoelectric bimorph based on PZT–5H material. Therefore, the simulated results using the EFSI algorithm follow the same trends upon the shift in the resonance. Also, the resonance obtained with the FSI algorithm [2] shows a good agreement with the theoretical damped natural frequency. The connected external resistive load decrease the vibration amplitude a bit (by less than 10% [23]) compared to the pure FSI results (case 2) as the inverse piezoelectric effect counter plays the mechanical vibrations. This amplitude dependency upon the external resistive load in PZT–5H piezoelectric bimorph also follows the results presented.
5 CONCLUSIONS

A triple coupled algorithm is proposed to analyze the piezoelectric–structure-fluid interaction of a piezoelectric bimorph made of PVDF and PZT–5H material in the viscous fluid media. The proposed method takes into account the triple coupled interaction phenomena. The resonance frequency of a thin flexible piezoelectric bimorph in the fluid agrees well with the theoretical solutions. Also, the shift in the resonance frequency upon the electric boundary conditions is matched well with the theoretical approximations. It is shown that the resonance frequency difference between the open–and closed–circuit sensor mode electric configurations in PVDF piezoelectric bimorphs has a negligible shift. However, a noticeably shift upon the connected external electric resistive load can be seen in PZT–5H piezoelectric bimorphs. The simulated frequency responses and vibration amplitudes of the thin flexible piezoelectric bimorphs analyzed using the proposed EFSI method shows a good agreement with the previous studies.

REFERENCES


AEROELASTIC-STRUCTURAL COUPLING
IN ANTENNA PROTOTYPE FOR WINDY OPEN-SPACE

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Abstract. The interaction between wind and an antenna prototype for the low-frequency radio telescope of the Square Kilometer Array (SKA) is experimentally tested in the wind tunnel of the Politecnico di Torino. The tests aim to predict the antenna behaviour during working conditions, i.e. mounted by means of five contact points to a metal grid on sandy ground in the Australian desert.

The wind tunnel is characterised by a circular test section having a diameter equal to 3 m and a length equal to 5 m. The height and the distance between the lateral legs of the antenna are equal respectively to 2.2 m and 1.5 m. The tests were performed at increasing wind speed up to 110 km/h. The system under analysis is an aluminium antenna composed by four parts arranged in axial symmetry and each one made of fifteen rods and small plates/wire elements.

A numerical parametric model of the system is developed to numerically study the dynamic behaviour of the antenna in the frequency range of interest. The model is able to handle very high modal density and closed spaced modes in multiplicity of four because of the symmetric structure as well as the different shapes of the elements forming the antenna. The wind tunnel results emphasise the fluid-structure coupling of aerodynamics modes and the critical aspects of the boundary conditions for a good prediction of the oscillations amplitudes.

1 INTRODUCTION

The Square Kilometer Array (SKA) represents the near future of radio astronomy [1]. Both the low- (50-350 MHz) and mid-frequency (500-1500 MHz) instruments (to be deployed in the first and second phase of the SKA construction) will be implemented as Aperture Arrays having hundreds of thousands digitally-beamformed antenna elements.

The current baseline for the array element of the low–frequency instrument is a dual-polarized log-periodic configuration [2,4] with 16 elements, a total height from the ground of
about 2.1 m and a base width of 1.6 m, which is better described in the following. Besides the electromagnetic tests campaigns in outdoor environment [5,6] and semi-anechoic chamber, the prototype requires several qualifications for environmental parameters, as the wind-loading effect. The antenna should be able to survive a wind speed of about 100 km/h and to operate without significant deformations up to 60 km/h.

Aerodynamically speaking an antenna can be considered as a bluff boy when an interaction with an air flow takes place. The flow separation usually occurs around a body immersed in a stream. The region of detached flow (wake) is highly unsteady and contains a great variety of flow structures more or less organized and characterized by typical temporal and space scales ranging over different order of magnitude. The unsteady separated flow plays a key role in the aerodynamic excitation of the immersed body which as a consequence is characterized by a time dependent pressure distribution around the body that in turn originates time dependent forces. Particularly interesting is the shedding phenomenon characterized by the release of organized vortices that induce unsteady forces in the body [7]. The unsteadiness of the separated flow is the origin of different forms of aeroelastic instabilities such as the galloping [8], the buffeting and the flutter of the structure. The turbulence intrinsically present in the atmospheric wind influences the loads acting on a structure. Many studies are present in the literature focused on the investigation of wind-structures interaction that involves different engineering fields. Wind-bluff bodies interactions including buildings, bridges, towers, cables, are of great interest for civil engineering applications. The interaction related to antennas and the atmospheric wind is also largely analysed as shown by many papers published on this subject such as [9,11].

The aims of this work are: a) to develop and validate a structural model of the system useful to forecast the effect of antenna design changes on the dynamic behaviour of the antenna, b) to identify and to analyse the effect of aeroelastic modes given by the fluid structure interaction and c) to correlates aeroelastic modes with the antenna components.

To reach these aims, standard experimental modal analysis (EMA) is performed on the system, coupled with signature acquisition under wind excitation. Experimental modal analysis is nowadays the most used technique to acquire the dynamic behaviour of components and systems [12]. Numerical simulations on components and systems are common use in industrial fields and very often they are used for improving the design phase. EMA and other dynamics test are used to validate the numerical models and to check the actual operating conditions. Usually model updating [13] is necessary to obtain realistic model and boundary conditions are critical for the operational working condition [14]. The investigation carried out in the wind tunnel complete the validation of the whole methodology.

2 ANTENNA PROTOTYPE: EXPERIMENTAL SET UP IN THE WIND TUNNEL AND NUMERICAL MODEL

The antenna prototype under analysis, shown in Figure 1 (a), is an axially symmetric structure in Aluminum constrained to a metal grid, manufactured by Sirio Antenne [5]. A planar tree-like module is circularly repeated four times each 90 degree. The module is made several beam elements. The main body is a boxed beam 2.1 m long, cross section 25x15 mm rectangular beam and 2 mm thick walls. Nine branches are attached on the biggest face of the
main beam, in alternation between left and right side. The branches are triangular paths, created with circular cross section, diameter $\phi = 5 \text{ mm}$, their length is scaled from 0.7 m (low part) to 0.2 m (top part). The main body is supported with a bigger circular beam 0.8 m long, attached at 0.51 m of the main body and to the metal grid. The constraint with the metallic grid is a Teflon support Figure 1 (b), including two rigid kinematic hinges around the axis perpendicular to the main beam direction. This support is also linked to the main body with other two thinner circular beam, diameter $\phi = 5 \text{ mm}$. Six triangular thin plates are attached to the main beam in the top part. Support beam branches and plates are placed alternatively on left and right side of the elementary structure.

The four modules are linked together with four Teflon constraint on the main beams, shown in Figure 1 (d), located at 0.45, 0.65, 1.22, 1.75 m from the ground. The four main beams are constrained to the ground grid by means of translation constraint, shown in Figure 1 (c). The metallic grid is fixed to the ground in four points.

![Figure 1: System under analysis: a) antenna, b) supports constraints c) central constraint and d) main beam constraint.](image)

**2.1 Experimental setup**

The fluid structure interaction is experimentally investigated in subsonic wind tunnel of the Politecnico di Torino. The circuit of the wind tunnel is closed, the test section is circular characterized by a diameter of 3 m and a length of 5 m. The maximum speed available is
equal to 80 m/s. A flat plate was mounted in the test section simulating the ground of the real case. Moreover, a metal grid having the same geometric characteristics of the actual configuration was fixed to the plate through fixing points positioned on three peripheral sides simulating the same constrains conditions of the real case. In Figure 2 the antenna mounted in the test section is shown. The tests were performed at four different uniform wind speeds, without the simulation of the typical velocity distribution of the atmospheric boundary layer.

The accelerations are measured in the two points \( z_1 = 0.65 \text{ m} \) and \( z_2 = 1.22 \text{ m} \), where accelerometers PCB 356A15 are located. The measurements were performed collecting data at the sampling frequency equal to 10240 Hz. LMS Scadas mobile and Test.Lab software were used to acquire and to post-process the time domain data.

![Figure 2: The antenna mounted in the test section of the wind tunnel.](image)

The global behaviour of the antenna was monitored by means of two cameras mounted outside of the test section. The cameras were positioned so that the deformations in the vertical plane \( xz \) and in plane \( xy \) parallel to the wall were visible. Different tests were carried out with the goal of reducing the deformation of the antenna varying the constraints configuration of the antenna-grid fixing points.

Roving hammer test modal analysis is performed on the antenna structure in condition of wind off, to identify the first global structural modes of the system. LMS Scadas mobile and Test.Lab software were used to acquire data and to perform the EMA. Ten points are selected on the main beams of the structure, one each 0.3 m, and the two nodes on the second and third Teflon constraints, on which two triaxial accelerometers are located. The structure is excited in the ten points along the two directions perpendicular to the main beam, using an instrumented hammer PCB 086C03. The sample frequency is 4096 Hz, therefore the frequency response functions within 2048 Hz are measured with a frequency resolution of 0.125 Hz. Force exponential windows is applied to the input force signal and exponential windows is applied on the measured responses.

2.2 Numerical model

A finite element (FE) model is developed in LUPOS environment to perform numerical modal analysis of the structure, in condition of wind off. LUPOS is a parametric FE codes, developed in Politecnico di Torino [15], which is able to handle very well tri-dimensional...
systems which can be schematised using mono-dimensional elements. The numerical model is a FE-based model with 1D and 0D elements. Particular attention is given to the description of the main beams flexural mode shapes. The antenna model, shown in Figure 3 (left), is built by revolving a planar module, shown in Figure 3 (right).

![Figure 3: FE model: complete structure (left) and single module (right)](image)

Timoshenko 1D beam elements [16] are used to represent the central main beam, the 9 branches, the 3 supports beams of each module of the structure. Each of these components can be considered as beams. The triangular thin plates in the top part of the antenna are stiffer than branches and they are not structural components, hence they are simplified as localised equivalent added masses in the antenna upper section.

The main beam is considered fixed to the metal grid, to reproduce the boundary conditions in Figure 1 (c), while hinges are placed to the Teflon support supports, to reproduce the rotational degrees of freedom (DOF) compatible with bolt joints of the real Teflon supports in Figure 1 (b). Elastic joints are placed in correspondence of Teflon supports on the main beam Figure 1 (d), with equivalent lumped stiffness of 1000 N/m between the four adjacent main beams. The model possess in total 2600 active DOFs.

### 3 Antenna Modal Analysis

Modal analysis is performed on the antenna to identify the first global modes of the structure. The identification is performed in the frequency range $0-25$ Hz, for both experimentally and on the numerical model. The experimental modal properties of the system, natural frequency $f_{n,r}$, damping ratios $\zeta_r$ and mode shapes $\Phi$, are identified from the experimental FRFs using ML-MM algorithm [17]. Natural frequencies and mode shapes are computed from the numerical model, solving the related undamped eigen-problem. The global modes resulting from experimental and numerical modal analysis are reported and compared in Table 1. The first two modes are almost coincident eigenvalues representing the first bending global mode shapes of the antenna, shown in Figure 4. The small differences in experimental frequencies are related to not perfect symmetry of the structure in the two planes. Damping ratios are quite aligned as expected for coincident eigenvalues. The numerical mode shapes are perfectly coincident and aligned with the experimental results. The mode shapes related to experimental modes 3 and 4 and numerical 3-32 do not highlight
any contribution of the main beams of the structure, they are modes of the branches. Experimental modes 5 and 6 are the second global bending mode shapes of the antenna in the two planes, shown in Figure 5, together with the corresponding numerical modes 33-34. Also in this case natural frequencies between experimental and numerical modes are quite close and the experimentally identified damping ratios of the modes in the two planes are similar.

Branches modes are found in clusters with multiplicity 4, due to the repetitions of identical components around the main Z axis. A lot of these mode clusters are numerical found, identifying the bending of the different levels of branches. An example is reported in Figure 6, where the four bending of the first levels branches can be observed. These mode shapes cannot be experimentally identified because only the main beam is tested.

Table 1: EMA and FE antenna modes.

<table>
<thead>
<tr>
<th>Numerical</th>
<th>Experimental</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mode</td>
<td>$f_n$ [Hz]</td>
<td>Mode</td>
</tr>
<tr>
<td>1</td>
<td>5.072</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>5.072</td>
<td>2</td>
</tr>
<tr>
<td>33</td>
<td>23.53</td>
<td>5</td>
</tr>
<tr>
<td>34</td>
<td>23.53</td>
<td>6</td>
</tr>
</tbody>
</table>

![Figure 4: First global bending of the antenna: experimental (left) and numerical (right).](image-url)
Figure 5: First global bending of the antenna: experimental (left) and numerical (right).

Figure 6: Numerical 1st branches mode shapes in multiplicity four.
4 EXPERIMENTAL EVALUATION OF FLUID-STRUCTURE INTERACTION

The responses of the system during a nonstationary test, with wind speed linearly increases from 13 m/s to 23 m/s, were acquired in the wind tunnel. In particular, the air speed increases into two phases: a first phase from 13 m/s to almost 19 m/s and a second phase from 19 m/s up to 23 m/s. The auto-power spectrograms of the system response in Z direction measured at the lower accelerometer location are shown in Figure 7. The frequencies clearly move with increasing velocity, in different frequency ranges: 40-80, 150-250, 600-1100 Hz. These frequencies are the most representative of aeroelastic effects.

![Figure 7: Auto-power spectrograms during air speed transient, measured at z₁ = 0.65 m.](image)

The peaks frequencies are more prominent in steady state conditions. Four tests at different constant values of air speed are performed, while acquiring the accelerations of the measured points. The auto-powers of the three stationary signals are computed from the measured responses. The three frequency ranges highlighted before are analysed in Figure 8.

The frequencies associated with the highest energy concentration in the spectrum are clearly visible and are highlighted with vertical dotted lines.
For each wind speed several acceleration peaks emerge whose associated frequencies change according with the speed. Moreover for the three ranges of frequencies the values of the acceleration varies of about one order of magnitude. The highest frequency range involves the highest values of the acceleration, due to the higher wind speed and therefore energy given to the system.

Such frequencies can be linked to the shedding of vortices from the different components of the antenna. It has to be remarked that the antenna under investigation is characterized by different elements with different transversal shapes, lengths, and relative positioning with respect to the wind. Moreover, a very complex interactions between wakes of the components of the antenna takes place, therefore it is not simple to ascribe a specific peak of energy present in the spectrum to a precise component of the antenna from pointwise measurements. From this point of view the identification of the possible responsible is carried out considering that for bluff bodies the Strouhal number, that identifies the non-dimensional frequency associated with the peak of amplitude, is around the value 0.2 for sufficiently high Reynolds number. The Strouhal number is defined as:

$$St = \frac{fD}{V}$$  \hspace{1cm} (1)
where $f_s$ is the shedding frequency, $D$ is a characteristic dimension of the body and $V$ is the fluid speed. For a circular cylinder $D$ is the diameter of the cross section.

In the present case because of the different shapes of the cross sections, an equivalent reference length has been considered similarly to what is done for the internal flows. We adopted here the concept of hydraulic diameter defined as:

$$D = \frac{4A}{P} \quad (2)$$

where $A$ and $P$ are respectively the area and wetted perimeter of the cross section.

The ratio $f_s/V$ are evaluated for each frequency range from the peak frequencies present in the diagrams of Figure 8. In Table 2 the values of $f_s/V$ are reported. As it can be observed an almost constant value of $f_s/V$ is present varying the air speed in each frequency range.

Table 2: Frequency – air speed ratios.

<table>
<thead>
<tr>
<th>Velocity $V$ [m/s]</th>
<th>Ratio $f_s/V$ [m]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Low</td>
</tr>
<tr>
<td>13</td>
<td>3.11</td>
</tr>
<tr>
<td>23</td>
<td>3.04</td>
</tr>
<tr>
<td>27.7</td>
<td>3.01</td>
</tr>
<tr>
<td>33</td>
<td>2.98</td>
</tr>
</tbody>
</table>

Assuming that the Strouhal number associated with the shedding phenomenon, as anticipated, is approximately $St \approx 0.2$, it is possible to evaluate the equivalent diameters for the three ranges of frequencies.

$$D_1 = \frac{0.2}{(f_s/V)_1} = 6.58 \text{ cm} \quad (3)$$

$$D_2 = \frac{0.2}{(f_s/V)_2} = 1.78 \text{ cm} \quad (4)$$

$$D_3 = \frac{0.2}{(f_s/V)_3} = 4.7 \text{ mm} \quad (5)$$

The three diameters found can be correlated with the dimensions of the main parts of the antenna. The first characteristic dimension $D_1 = 6.58 \text{ cm}$ is close to the global dimensions of the four beams pack in the antenna centre. The second characteristic dimension $D_2 = 1.78 \text{ cm}$ corresponds to the size of the four supporting bars, and finally the third one $D_3 = 4.7 \text{ mm}$ can be associated to the diameter of the antenna branches. The Reynolds numbers corresponding to the values of these equivalent diameters are in the range $4200 \leq Re \leq 9700$ for $D_1$, $16000 \leq Re \leq 37000$ for $D_2$, $59000 \leq Re \leq 136000$ for $D_3$, sufficiently high to justify the assumption of $St \approx 0.2$.

In Figure 9 two pictures of the antenna for increasing wind speed are reported. As can be
observed the deformed shapes assumed by the antenna are quite close to the first bending mode, due to the transversal load of the tip of the antenna given by the interaction between the triangular surfaces on the tip and the fluid.

Figure 9: The deflection of the antenna at increasing wind speed from left to right. Maximum speed test $V = 97$ km/h.

5 CONCLUSIONS

The dynamics behaviour of an antenna prototype for gravitational waves measurements has been tested in a wind tunnel, to assess its structural deformation under wind load. A numerical model of the structural system is developed, using beam elements and validated. Structural modes of the antenna are experimentally identified in condition of wind off. The antenna presents very high modal density, with several tens of modes within the first 25 Hz. All the modes are computed from the numerical model, while only the global antenna modes are identified from experimental modal analysis. The effects of the fluid structure interaction of the dynamics behaviour of the antenna are studied in a wind tunnel under different air speed condition. Three main frequency range of interaction between the structure and the air flow are evidenced. The effects of shedding phenomena are clearly visible in the identified ranges and the components causing these effects.

Improvements of the antenna can be performed in its structural design to suppress undesirable aeroelastic effects in the low and mid frequency range if they interact with antenna functionality during antenna working conditions.

REFERENCES


DEVELOPMENT OF A CFD-BASED SCREENING TOOL FOR VIV PREDICTION

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Key words: VIV, Slice method, FSI, RANS CFD, linear FEM, strong coupling

Abstract. This paper presents an efficient screening tool, based on the 2D strip method and the CFD-based approach. The proposed method allows the study of the dynamics of the vortex-induced vibration (VIV) phenomenon with almost the same accuracy as a fully 3D Fluid-Structure interaction (FSI) model, but with a reduction in computational times by a factor of nearly 20 compared to the 3D approach. Such a large reduction makes the use of CFD-based analysis feasible on a workstation within a reasonable time frame and opens the possibility of CFD approaches in a subsea pipeline design process.

1 INTRODUCTION

When a body of circular section is subjected to flow, a vortex shedding behavior develops which can induce an oscillatory displacement of the structure that will depend on the fluctuation of the efforts. This induced displacement, known as vortex-induced vibration (VIV), can excite the natural frequencies of the structure and make the system resonate, causing a premature fatigue failure.

To evaluate the risks of fatigue, engineers use tools developed and sufficiently validated to predict the fatigue of simple structures. Nevertheless, these simplified analysis tools are not adapted to the prediction of VIV of more complex oscillating structures, such as spools and subsea jumpers which can exhibit complex, multi-modal responses. Consequently, there is an industrial need for more accurate analysis methods.
Significant improvements can be achieved using three-dimensional fluid-structure interaction (FSI) simulations, based on computational fluid dynamics (CFD). However, detailed meshes, long simulation times and high performance computing are required. Knowing that industrial design processes demand the evaluation of various geometries and different structural designs of a large number of spools, a 3D FSI simulation that takes about two days for a single spool computation, is prohibitively slow for practical design use.

It is within this context, and after confirming the lack of precision of existing design analysis methods and classification society rules, that a collaboration between Total E&P and K-Epsilon was created. The main objective consists in developing a screening tool to estimate spool vibration phenomena within affordable industrial times, with moderate computational resources. Here the stated goal is to assess VIV behavior of a spool in a few hours on a high end work station with an accuracy sufficient for design analysis.

2 STATE OF THE ART

This section focuses on previous researches and results of different methods used to model the VIV phenomena. For a detailed description of the physics of VIV, the reader can refer to the review of Le Cunff [1], or for a deeper insight, to the references given by Willden [3].

The work of Le Cunff [1] gives a global overview of models that are used to predict the lifespan of cylindrical structures subjected to a flow. The presented methods, developed at the French Petrol Institute IFP, range from a simple modal analysis approach to coupled fluid-structure computations with resolution of the Navier-Stokes equations. Three of the methods are discussed below.

The modal approach presented in [1] performs a modal analysis to determine and select the potentially excited modes of the structure. Later, the modal amplitude is calculated and the lifting force of the cylinder is obtained from a large database of empirical data. Finally, a fatigue analysis is carried out to know the fatigue lifespan of the structure and to locate the most likely failure points. Although this method is fast, it is limited to studies of cross-flow displacements (CF). In addition, codes based on modal approaches use empirical coefficients which can lead to different results depending on the software for the same case, due to the large degree of scatter observed in experimental VIV data.

Looking for more accurate results, the fluid model is improved using a wake oscillator, based on the Van der Pol oscillator equation. This second approach searches to model the fluctuating nature of a turbulent flow by considering the oscillatory release of vortices, but giving no direct indication on the fluid flow. This model is more complete than the modal methods, and is fast enough to be used during the design phase.
Finally, the results of a previous strip method approach developed at the IFP are discussed. The work of Etienne [4], fully couples a two-dimensional FSI method, using the stream function-vorticity formulation of the Navier Stokes equations, with a finite element method (FEM) approach. Although no indication is given regarding the computation time scale of any of the above methods, the validation of the strip method, with experiments, shows that this method is both qualitatively and quantitatively able to capture the VIV phenomena.

Among others researchers using the strip method, there are also the contributions of Willden [3] and Duan [2]. These two works present approaches based on a loosely coupling between a set of two-dimensional flow calculations with a three-dimensional structural dynamics model.

Establishing a benchmark, the work of Chaplin [6] presents an experimental study carried out on a vertical riser exposed to a uniform stepped current \((Re \approx 4500)\) with a set of different top tensions. In the tests, the lower 45% of the riser is subjected to the current, with the upper section in calm water. The riser is free to move in the in-line and cross-flow directions. Both the bottom and top ends are fixed using universal joints that fully constrain the displacement of the riser ends, but allow arbitrary rotation. Tension is applied to the upper end of the riser with a spring tensioning system. The experimental setup used in this work is shown in figure 1.

A parallel work of Chaplin [7], presented a comparison between the laboratory measurements and a series of different numerical models. Paraphrasing the report, it is concluded that, in general, empirical codes were more successful at predicting cross-flow displacements and curvatures than codes based on CFD. In-line curvatures, potentially the cause of the largest fatigue damage, could not be computed by any of the empirically based codes, and in general, those based on CFD were also in very poor agreement with the measurements.

3 THE STRIP METHOD

In the strip method approach, a series of two-dimensional computational planes are placed along a structure perpendicularly to the spanwise axis. Each slice or plane is solved with the same method, but is individually solved and there is no transfer of information between the planes. The motions of the series of two-dimensional flow calculations is linked through the resolution of a three-dimensional structure.
Inherent to the strip method is that the three-dimensional effects in the fluid are neglected since only the local two-dimensional dynamics is resolved. Although three-dimensional eddies may develop in the wake of a cylinder ($Re > 180$), as it is mentioned by Willden [3], the VIV lock-in effect actually increases the coherence of the flow along the cylinder and makes the local flux essentially two-dimensional. Here, the lock-in effect refers to the synchronization of the vortex shedding and structural oscillatory frequencies such that, vortex shedding occurs at the natural frequency of the structure.

As mentioned also in [3], in order to capture the excitation and damping effect of the flow, a minimum of three slices are required per half-wavelength of vibration, therefore, the number of slices of simulation can be determined by considering either the highest vibration mode that is likely to be excited or the highest mode of interest.

4 PROPOSED NUMERICAL METHOD

Through the commercial coupling tool K-FSI, the strip method proposed in this work fully couples a velocity-pressure formulation of the two-dimensional, Navier Stokes equations with a three-dimensional, non-linear FEM model of the structure.

The K-FSI tool consists of the coupling between the structural code K-Struct and the fluid solver ISIS-CFD, included in the FINE™/Marine suite. ISIS-CFD is based on the finite volume method and solves the incompressible, unsteady Reynolds-averaged Navier-Stokes equations (URANS). FINE™/Marine is coupled in a segregated manner to K-Struct, the non-linear, unsteady finite element method structure solver, which forms the core of the K-FSI fluid-structure interaction suite.

In particular, for the present work, each fluid computation slice uses the same mesh, however, each plane can be placed at different angles of incidence. The developed tool transfers information between the different 2D slices and the 3D structure through ports called sockets, using the ZeroMQ distributed message library. The use of sockets allows the communication of multiple fluid calculations, which are executed in parallel and independently, with a single structural calculation. Each fluid computation may in turn also be computed locally in parallel using the message passing interface (MPI) protocol.

The following algorithm is executed: several 2D CFD calculations are run independently on different processors. Once each of the fluid domains is resolved, the resultant
fluid efforts are sent to the structural solver at each non-linear iteration. The structural solver then uses the information obtained from each one of the fluid computations to load the structure and computes the displacements. Finally, it communicates the new displacements to each of the fluid computations. Each fluid calculation communicates independently with the structure solver using a particular socket.

5 SIMULATION SETUP

The numerical model of this paper follows the experimental setup presented in the work of Chaplin [6], and shown in Figure 1. Two FSI models are simulated, a fully 3D fluid simulation and the proposed strip method. The structural and fluid configuration, common to both models, is presented below. Information particular to each model is detailed later on.

The structural mesh consists of 180 Euler-Bernoulli beam elements. The top and bottom ends of the riser are fully constrained in translation and free in rotation to model the universal joints at each end. A constant tension of 405 N is applied at the top of the riser. The structural properties presented in Table 1 have been used for model. Both the effect of gravity and buoyancy are represented in the structure model.

For both fluid approaches, the meshes used are non-structured, hexahedral/quadrilateral meshes. A no-slip boundary condition is used on the riser surface. The meshes were designed with a target \( y^+ \) value of \( y^+ = 0.5 \). Refinement boxes are used to capture the near and far wake. The \( k - \omega \) (SST-Menter) model is used to model the turbulence, the water density is considered as \( \rho_f = 999.207 \text{ kg} \cdot \text{m}^3 \), and the dynamic viscosity is defined as \( \mu_f = 0.001002 \text{ Pa} \cdot \text{s} \).

Table 1: Structural parameters used to model the riser

<table>
<thead>
<tr>
<th>L (m)</th>
<th>Diameter (m)</th>
<th>L/D</th>
<th>EA (kN)</th>
<th>EI (N·m²)</th>
<th>GJ (N·m²)</th>
<th>Top tension (N)</th>
<th>Linear mass (kg·m⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>13.12</td>
<td>0.028</td>
<td>469</td>
<td>5880</td>
<td>29.880</td>
<td>80.660</td>
<td>405</td>
<td>1.848</td>
</tr>
</tbody>
</table>

5.1 Fully 3D fluid model

To ensure a reasonable mesh size, the cells are stretched along the \( Z \) axis, whereas an isotropic discretization is kept in the \( X \) and \( Y \) directions, to correctly capture the cylinder and the near wake. In order to match the experimental set-up, the fluid domain is confined for \( Z > 5.904 \text{ m} \) to represent the vacuum tank containing the upper 55% of the riser. A view of the lower and upper sections of the mesh is given in Figures 3a and 3b, respectively. Boundary conditions are presented in Table 2. Riser motions are captured using mesh deformation in an arbitrary Lagrangian Eulerian (ALE) approach.
Table 2: Boundary conditions imposed on the fully 3D fluid domain

<table>
<thead>
<tr>
<th>Type</th>
<th>Faces</th>
<th>Riser height</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outlet</td>
<td>Constant pressure</td>
<td>$X_{\text{max}}$, $Z &lt; 5.904 \text{ m}$</td>
</tr>
<tr>
<td>Inlet</td>
<td>Constant velocity ($0.16 \text{ m} \cdot \text{s}^{-1}$)</td>
<td>$X_{\text{min}}, Y_{\text{min}}, Y_{\text{max}}$, $Z &lt; 5.904 \text{ m}$</td>
</tr>
<tr>
<td>Wall</td>
<td>Slip condition</td>
<td>$X_{\text{min}}, X_{\text{max}}, Y_{\text{min}}, Y_{\text{max}}, Z_{\text{max}}$, $Z &gt; 5.904 \text{ m}$</td>
</tr>
<tr>
<td>Wall</td>
<td>Slip condition</td>
<td>$Z_{\text{min}}, Z_{\text{max}}$, $Z &lt; 5.904 \text{ m}$</td>
</tr>
</tbody>
</table>

(a) Lower portion of domain exposed to current (b) Upper portion of domain in vacuum tank

Figure 3: Fully 3D fluid domain

5.2 Strip method (2D Fluid calculations - 3D structure)

To assess the proposed strip method, two calculations have been executed with a total of 20 and 40 slices, respectively. Half of the slices are positioned at $Z < 5.904 \text{ m}$, and the other half at $Z > 5.904 \text{ m}$. An identical 2D mesh is used, for each and every one of the slices along the riser, even for $Z > 5.904 \text{ m}$.

This is done under the consideration that 3D interactions are neglected by the strip model, and that no confinement effect is expected, given the distance from the riser to the walls, according to the experimental set-up. The 2D fluid mesh is shown in Figure 4. Unlike, the 3D simulations, the riser motions may be treated using rigid body translations of the fluid domain and hence, the cost of mesh deformation is avoided.

To improve the capture of the vortex shedding, a slightly larger refinement box is used.
in comparison to the fully 3D model. The imposed boundary conditions are presented in Table 3.

Table 3: Boundary conditions imposed on each 2D fluid domain

<table>
<thead>
<tr>
<th>Type</th>
<th>Faces</th>
<th>Position of plane</th>
</tr>
</thead>
<tbody>
<tr>
<td>Outlet</td>
<td>Constant pressure</td>
<td>$X_{\text{max}}$</td>
</tr>
<tr>
<td>Inlet</td>
<td>Null velocity (0 m $\cdot$ s)</td>
<td>$X_{\text{min}}, Y_{\text{min}}, Y_{\text{max}}$, $Z &gt; 5.904$ m</td>
</tr>
<tr>
<td>Inlet</td>
<td>Constant velocity (0.16 m $\cdot$ s$^{-1}$)</td>
<td>$X_{\text{min}}, Y_{\text{min}}, Y_{\text{max}}$, $Z &lt; 5.904$ m</td>
</tr>
<tr>
<td>Wall</td>
<td>Mirror condition</td>
<td>$Z_{\text{min}}, Z_{\text{max}}$</td>
</tr>
</tbody>
</table>

6 NUMERICAL RESULTS

Taking as the reference the experimental results of Chaplin [6], a comparison of the two approaches is done for the in-line (IL) and cross-flow (CF) direction displacements.

A summary of the in-line displacement results is presented in Table 4. The mean IL displacement and the displacement envelopes are shown in Figures 5 and 6. Note, that the mean displacement has been filtered out of the IL response in Figure 6a to make the differences in IL oscillations more apparent.

Both, the fully 3D approach and the strip method, underestimate the maximum of the mean displacement for the in-line direction, however the 3D method provides a better representation of the IL oscillation amplitudes. The vertical position of the maximum amplitude is well predicted with both methods. See Figure 5.

Regarding the amplitudes of the in-line oscillations, the fully 3D model overestimates the envelopes but properly predicts the position of the anti-nodes and nodes. Regardless of the number of slices, a better match with the experiment is observed for the slice method. The envelopes of the cross-flow displacement are underestimated by both methods, but are slightly weaker for the strip method. The position of the nodes and anti-nodes is correct regardless of the method, (see Figure 6a and 6b).
Table 4: Comparison of the mean in-line direction results

<table>
<thead>
<tr>
<th>Method</th>
<th>Maximum displacement (D)</th>
<th>Z-Position (m)</th>
<th>Z-Position / L</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experiment</td>
<td>1.102</td>
<td>4.422</td>
<td>33.7%</td>
</tr>
<tr>
<td>3D</td>
<td>1.009</td>
<td>4.048</td>
<td>30.9%</td>
</tr>
<tr>
<td>20 Slices</td>
<td>0.857</td>
<td>4.373</td>
<td>33.3%</td>
</tr>
<tr>
<td>40 Slices</td>
<td>0.889</td>
<td>4.155</td>
<td>31.7%</td>
</tr>
</tbody>
</table>

(a) (IL) envelopes, no mean disp. (A/D)  
(b) (CF) envelopes (A/D)

Figure 6: Displacement envelopes

6.1 Spectral analysis

Examining the frequency content by spectral analysis, the dominant mode for the in-line (IL) direction of both methods is the 4th mode. Although the corresponding frequency of the 4th mode is similar, the range of frequency for the 3D method (1.4 to 2.1 Hz) is a bit wider than that of the strip method (1.7 to 2.1 Hz). The anti-node showing the maximum amplitude corresponds to the second lowest anti-node, according to the 3D method, and to the bottom most, for the strip method for both, 20 and 40 slices.

Both methods indicate that the dominant mode for the cross-flow (CF) direction corresponds to the 2nd mode. As with the in-line spectral analysis, the range of the dominant mode is somewhat larger for the 3D method (0.3 Hz for the strip method, and 0.5 Hz for the 3D method). Both methods point to the bottom anti-node as the one with maximum displacement.
6.2 Simulation time

Computational time has been measured for both methods and, as shown in Table 5, a gain has been observed with the strip method. Considering the total of the CPU hours, and compared with the full 3D method, the strip method using 20 slices is 18.6 times faster, whereas the one using 40 slices is 10.4 times faster than the 3D computation. To give an example, 9 hours are required to get a result comparable to a 3D simulation using a desktop computer, with 20 cores and 20 slices.

Table 5: Comparison of the computational cost

<table>
<thead>
<tr>
<th></th>
<th>3D</th>
<th>20 slices</th>
<th>40 slices</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simulation time for the same number of time steps (hours)</td>
<td>51</td>
<td>9</td>
<td>16</td>
</tr>
<tr>
<td>Number of processors</td>
<td>64</td>
<td>20</td>
<td>20</td>
</tr>
<tr>
<td>Total CPU hours</td>
<td>3262</td>
<td>176</td>
<td>313</td>
</tr>
</tbody>
</table>

6.3 Comparison with others tools

This section presents a comparison between the proposed strip method developed within the K-FSI suite and the results of the tools assessed in the work of [7]. These tools
are: USP, Norsk Hydro, Orcaflex vortex tracking, VIVANA, VIVIC, VICoMo, ABAVIV, and SHEAR7. The empirical and wake oscillator tools VIVANA, SHEAR7, VICoMo and ABAVIV were not developed to determine the in-line deformation of a riser.

6.3.1 In-line (IL)

All of the tools underestimate the in-line deformation, but the position of the maximum in-line deformation is globally well captured. In general, the methods developed in the present work stand out from the other ones. In particular the mean in-line displacement and the in-line envelopes are more accurately captured. Only the two K-FSI approaches and Orcaflex predicts nodes and anti-nodes, though only the two K-FSI results presented here succeed to determine the right number of anti-nodes and the proper dominant mode. In contrast, Orcaflex incorrectly predicted a fifth mode response.

(a) Minimum displacement envelopes

(b) Maximum displacement envelopes

Figure 9: Comparison mean displacement (IL) direction of the different tools

Figure 10: Comparison envelopes (IL) direction of the different tools
6.3.2 Cross-flow (CF)

The majority of the softwares gives the right mode for the cross-flow envelopes with reasonably correct amplitudes. Nevertheless, some are not suited to predict the CF displacement (Orcaflex: wrong mode, Norks Hydro: wrong mode and wrong amplitude).

![Diagram of cross-flow envelopes](image)

(a) Minimum displacement envelopes  
(b) Maximum displacement envelopes

Figure 11: Comparison of the envelopes for the different tools, (CF) direction

7 CONCLUSIONS AND FUTURE WORK

The results of the present study are compared with benchmark presented in Chaplin [6] and lead to the following conclusions:

- It emerges from all these simulations that the strip method offers results comparable to those of the 3D method while offering a significant time saving.

- In general, the strip method leads to a good agreement with the experimental data, and increasing the number of slices has been shown to yield a gain in precision though at the cost of greater computation time.

- Compared with some of the more recognized tools used in the oil industry, the K-FSI tool presented here yielded the closest results to the experiments.

- Both the fully 3D FSI and the strip approach developed were found to be reliable, robust and precise methods.

- The proposed approach makes it possible to perform an FSI simulation on a riser in a few hours, on a desktop machine dating from 2013.
Given the fact that past simulations proved to be incapable of predicting the deformations and frequencies associated with the VIV on a riser, the obtained results are very encouraging. Considering the possibility of making a specific solver for the VIV analysis, and the capacity of new processors, a drastic reduction in computational time can be expected. The developed strip method could be extended to handle more complicated geometry configurations such as spools and tandem riser configurations where the wake of one cylinder influences the behavior of the other. Examination of the case of the experimentally measured spool of [8] is the focus of ongoing work.

REFERENCES


Development of Engineering Method for Calculation of Ejected and Recirculated Air Flow Rates During Reload of Bulk Materials

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Key words: Aspiration, bulk material transfer, air suction.

Abstract. Reload of bulk materials in various industries and agriculture are accompanied by significant dust emissions. The flow of bulk materials in its fall carries air (air ejection). The study of the flow of ejected air is a complex multidisciplinary task. The maintenance costs of local exhaust ventilation systems are directly proportional to the flow rate of the ejected air. Consumption of the ejected air can be reduced by: reducing the speed of the falling bulk material flow; increase of aerodynamic drag when ejected air moves; organization of air circulation-recirculation.

The aim of the article is to develop engineering methods of calculation of aspiration systems and shelters on the basis of previously obtained results of theoretical and experimental studies of the laws of ejected and recirculated air flow.

The results and conclusions are as follows.

The technique of engineering calculation of volumes of the aspirated air during reload of dry not heated materials with natural circulation, carried out by means of the combined use of the cylindrical bypass chamber and the perforated trough is developed. Experimental and numerical studies have shown that the proposed method has sufficient accuracy.

Recommendations for the design of the developed aspiration shelter for more efficient operation with lower operating costs are proposed. The economic effect is to reduce energy intensity and the cost of cleaning dust emissions.

The values are proposed for the recirculation coefficients for the calculation of the aspiration system using the bypass chamber and the combined use of the bypass chamber and the perforated trough.

The method of calculation of the ejected air flow rate in telescopic loaders is developed.

The high energy intensity of telescopic aspiration-technological units (ATU) of reloading stations is caused by the ejection ability of gravity flows of bulk material, pumping a large amount of air into the aspiration shelters, which significantly increases the required performance of aspiration systems. Power of ATU can be significantly reduced by the use of coaxial telescopic loading troughs and corrugated impervious wall surrounding the trough and sealing the top and bottom of the cover, adjacent to the troughs.

The analytical flow rates estimation of air, moving inside the cavity of the "trough- bypass..."
chamber", can be carried out by linearization of the dynamics and inter-component interaction equations with the subsequent solution of transcendent equations in the Maple universal mathematical environment.

Numerical studies have shown that the main parameter for reducing the transit flow of ejected air and increasing the volume of recirculated air is the degree of sealing of the upper cover. For example, if the total area of the shelter leaks is reduced from 0.14 m² to 0.02 m², the flow of transit air will be reduced three times, and the recirculated air will be increased by 2.5 times. The total productivity of the local suction from the lower shelter in this case has decreased by 1.68 times.

1 INTRODUCTION

Overloading of bulk materials in various industries and agriculture is accompanied by significant dust emissions [1-3]. The flow of particles of bulk materials in its fall carries away the air (air is ejected). Reducing the flow of ejected air allows to reduce the cost of dust collection and to design effective systems of local exhaust ventilation [4,5]. To reduce the flow rate of the ejected air by reducing the rate of fall of the flow of bulk material; increasing of aerodynamic resistance during the movement of ejected air; organization of air circulation - recirculation.

The purpose of the article is to develop on the basis of previously obtained results of theoretical and experimental studies of the laws of recirculation air flow, organized in the system “loading channel - bypass chamber" of the engineering methodology for calculating aspiration installations and shelters.

2 METHOD OF CALCULATING THE VOLUME OF AIR REMOVED FROM THE ASPIRATION SHELTER

Using a dynamic approach to determine the amount of ejected air, described in the monograph [4], as well as the data obtained in the experiments [6-9], an engineering method for calculating the amount of exhaust air, which allows to take into account the flow of ejected air and the influence of the design features of the shelter on amount of aspirated air and recirculated air flow was developed.

The basis of this technique is the calculated dependencies of the amount of ejected air, one of the main parameters of which is the aerodynamic resistance of the equipment: "top shelter - overload channel - bottom shelter" [5].

The initial data for the calculation are as follows:
1. Characteristics of the material being overloaded: particle size distribution, material density $\rho$, material consumption $G$.
2. Characteristics of the overload unit: layout of the unit with heights of the fall of the bulk material, type of aspiration shelter, cross-sectional area of the loading trough $F$, loose area of the shelters.

The calculation of the volume of aspirated air is carried out in the following sequence.
1. The flow rate of the material falling along the trough at the entrance to the shelter $v$ is determined by calculating the speed of movement of the bulk material at each straight section of the loading channel:
   a) for a vertical section
b) for the inclined section

\[ v_a = \sqrt{v_s^2 + 2gh}, \]

The speed in the trough shown in Figure 2.1 will be determined as follows:

a) the speed at the beginning of the trough

\[ v_s = \sqrt{2gh}, \quad g = 9.81 \text{ m/s}^2. \]

b) speed at the end of the section

\[ v_a = \sqrt{v_s^2 + 2gh}. \]

2. The value of the volume concentration of particles in the trough, \( m^3/m^3 \):

\[ \beta = 2G_{\nu} / \left( \rho_s F_{\nu} (1 + n) v_s \right), \]

where \( n = v_s / v_a \) - the ratio of the velocity of falling of particles of bulk material at the beginning and end of the trough;

3. The average particle diameter of the bulk material, mm:

\[ d = \frac{\varphi}{\sum m_i d_i}, \]

where \( m_i \) - percentage of particles with a diameter \( d_i \) by weight.

For the value \( d \leq 14.6\sqrt{\beta} \) taken as calculated the average diameter should be taken \( d = 14.6\sqrt{\beta} \).

4. The sum of coefficients of local resistances shelters and trough aspiration system

\[ \sum \zeta = \zeta_{nu} + \zeta_{nu} + \zeta_{nu}, \]

where \( \zeta_{nu} \) - coefficient of local resistance of bottom shelter; \( \zeta_{nu} \) - coefficient of local resistance of trough (for vertical trough \( \zeta_{nu} = 1.5 \); \( \alpha = 90 \)); \( \zeta_{nu} \) - coefficient of local resistance of top shelter.

For shelters with a rigid internal partition, the value \( \zeta_{nu} \) depends on the ratio of the cross-sectional areas of the trough and the partition \( F_{nu} / F_s \) and the ratio of the heights of the partition and the shelter \( H_s / H_s \). The values for shelters are presented in table. 1. Without internal partition relies \( \zeta_{nu} = 0 \).

The value of coefficient of local resistance of the top shelter \( \zeta_{nu} \) is calculated by formula:

\[ \zeta_{nu} = 2.4 \left( F_{nu} / f_s \right)^2, \]

where \( f_s \) - area of leakage of top shelter, m².

5. The drag coefficient is determined by the formula:

\[ \psi = 1.8 \exp \left[ -1.8 \sqrt{\beta \cdot 10^7 / d} \right]. \]
Table 1: Value $\zeta_{ny}$ for shelters

<table>
<thead>
<tr>
<th>$F_{\infty}/F_{v}$</th>
<th>$H_{n}/H_{v}$</th>
<th>0.1</th>
<th>0.2</th>
<th>0.3</th>
<th>0.4</th>
<th>0.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>193</td>
<td>44.5</td>
<td>17.8</td>
<td>8.12</td>
<td>4.02</td>
<td></td>
</tr>
<tr>
<td>0.8</td>
<td>124</td>
<td>28.5</td>
<td>11.4</td>
<td>6.19</td>
<td>2.57</td>
<td></td>
</tr>
<tr>
<td>0.6</td>
<td>69.5</td>
<td>16.0</td>
<td>6.41</td>
<td>2.92</td>
<td>1.45</td>
<td></td>
</tr>
<tr>
<td>0.4</td>
<td>30.9</td>
<td>7.12</td>
<td>2.84</td>
<td>1.3</td>
<td>0.64</td>
<td></td>
</tr>
<tr>
<td>0.2</td>
<td>7.72</td>
<td>1.78</td>
<td>0.71</td>
<td>0.32</td>
<td>0.16</td>
<td></td>
</tr>
<tr>
<td>0.1</td>
<td>1.93</td>
<td>0.45</td>
<td>0.18</td>
<td>0.08</td>
<td>0.04</td>
<td></td>
</tr>
</tbody>
</table>

6. Value of the Butakov-Neykov number

$$Bu = 1500 \varphi G_v \sqrt{d \rho_f \sum \zeta}.$$  

According to this formula, the number $Bu$ is calculated for vertical troughs and for troughs with a predominance of vertical sections.

7. The value of the Euler criterion

$$Eu = P_y \sqrt{\sum \zeta \frac{v^2}{2 \rho_v}},$$  \hspace{1cm} (1)

where $P_y$ - depression in the bottom shelter, $\rho$ - density of the exhaust air.

It is necessary to add to the vacuum in the shelter the amount of pressure $P_{ob}$ generated by the working bodies of this equipment when aspirating technological equipment with ventilation capacity (roller and hammer crushers, disintegrators). In this case, the expression (1) takes the following form

$$Eu = 2(P_y + P_{ob}) / \rho_v \cdot V^2 \cdot \sum \zeta.$$  

8. With known numbers $Bu$ and $Eu$ the slip coefficient of the components with a uniformly accelerated flow of bulk material is determined by the formula:

$$\varphi = \sqrt{Eu + Bu \left|1 - \varphi^3\right| - \left|n - \varphi^3\right|} / 3.$$  \hspace{1cm} (2)

Equation (2) is solved by the method of successive approximations, with the following initial approximation

$$\varphi = 0.5 \left(0.5(1 + n) + \sqrt{Eu}\right).$$  \hspace{1cm} (3)

If $\varphi < n$, then the value $\varphi$ is determined from the quadratic equation, which follows from the expression (3):

$$\varphi = \sqrt{\left(b/(2a)^2\right) + c/a - b/(2a)},$$

where

$$a = 1 - Bu (1 - n), \quad b = (1 - n)^3 Bu, \quad c = Eu + Bu (1 - n^3)/3.$$
9. Air flow that enters in the bottom shelter by trough, m$^3$/s:
\[ Q_{\infty} = \varphi \cdot v_x \cdot F_{\infty} \cdot (1 - \beta)^2 \, . \]

10. Air flow which comes through leakages in the bottom shelter, m$^3$/s:
\[ Q = 0.65 F_{s} \left( \frac{2P_j}{\rho} \right) \, , \]
where $F_{s}$ - area of leakage of bottom shelter

11. Transit air flow, m$^3$/s:
\[ Q_{tr} = \kappa_{p} \cdot Q_{\infty} \, , \quad (4) \]

where $\kappa_{p}$ - recirculation coefficient.

Transit air flow $Q_{tr}$ shows how much air flows from the receiving part of the shelter to the aspirated part from which is removed in consequence. Transit flow depends on the amount of air entering the receiving part of the shelter along the trough. The value of the recirculation coefficient according to (4) is equal to the ratio of the transit and ejected (incoming through the trough) air
\[ \kappa_{p} = \frac{Q_{tr}}{Q_{\infty}} \, . \]

It is also possible to determine the amount of recycled air
\[ Q_{p} = Q_{\infty} - Q_{tr} \, . \]

Determination the value of the transit air flow is quite difficult. To simplify the calculation, it is proposed to use the values of the recirculation coefficient on the basis of the experimental values obtained performed during simulation and with bulk material overload with only a bypass chamber; $\kappa_{p} = 0.2-0.35$ - for the presence of a bypass chamber and perforation. These values of the recirculation coefficient were obtained for the optimal values of the cross-sectional area of the bypass chamber. According to experimental studies, the optimal ratio of the diameter of the bypass channel to the diameter of the loading pipe is 2-2.5.

For the perforation in the hydraulic path of system "top shelter - overload channel - bottom shelter" value $\zeta_{per}$ is added to the sum coefficient of local resistance $\Sigma \zeta$.

12. Suction air consumption:
\[ Q_s = Q_{tr} + Q_{p} \, . \]

The obtained values of air flow rates allows to make the hydraulic calculation of the air ducts of the aspiration system.

3 GENERAL RECOMMENDATIONS FOR THE DESIGNING ASPIRATION SYSTEM

The use of the aspiration system at the enterprises for the production of building materials, the metallurgical industry, the mining industry and the agro-industrial complex requires the solution of the following tasks.

1. The choice of a rational design of the aspiration shelter of the dusting place.
2. Calculation of the volumes of suction air required to prevent dust from escaping from the shelter.
3. Perform hydraulic calculation of air ducts.
4. Selection of a dust collector for cleaning aspirated air.

For conveyor overloads it is recommended to use the shelter design developed in this work the use of which will reduce the dust emission rate by reducing the amount of ejected air since a significant part of the air is recycled, and this in turn will reduce the loss of valuable material removed by suction.

It is recommended to use the developed shelter in the production of dry building materials (crushed stone, expanded clay), in metallurgical production (in case of pellet transshipment), and in the agricultural industry (in case of transshipment of grain materials).

Reducing the energy consumption for the operation of the aspiration system is achieved by using combined bypass and increasing the aerodynamic resistance of the receiving chamber.

The optimal ratio of the diameter of the bypass chamber $D_{b}$ to the diameter of the trough $D_a$ for the implementation of effective air recirculation is a value of 2-2.5. When $D_{b}/D_a > 2.5$ the speed of the upward recirculated air flow is reduced, which can lead to the settling of dust on the walls of the bypass chamber and its subsequent overgrowing and this in turn will adversely affect air recirculation. For smaller numbers $D_{b}/D_a < 2$ in spite of the high air velocity its hydraulic resistance in the bypass chamber will be higher than with values of 2-2.5.

For optimal implementation of the process of closed air circulation, as mentioned earlier, it is necessary to have resistance between the inlet section into the bypass chamber and the aspiration funnel. With a high bypass chamber resistance most of the air will go to the aspirated chamber and then be removed which will reduce the bypass efficiency.

Also, the presence of seal curtain on the top shelter of the aspiration system is necessary. Their presence will reduce the inflow of atmospheric air which will lead to a decrease in the volume of ejected air which will ensure the presence of additional vacuum in the top shelter and eliminate dislodging of dusty circulating air through the leakage of the top shelter.

Perforation must be applied to the trough walls in its upper part. Perforation of the bottom of the trough in the area of overpressure can lead to the formation of an air curtain when the ejected air escapes from the holes. This kind of curtain will resist the upward flow of air during its transit flow. If during the movement of the bulk material in the loading chute, the ejection pressure will decrease due to the release of air through the perforations, the air curtain in the lower part will not occur, as in the case of the telescopic chute (Figure 1).

By perforating the upper part of the trough there are certain advantages, some of which have been confirmed experimentally:

- increases the vacuum zone in the cavity of the bypass chamber, since the falling bulk material creates a vacuum inside the trough and the circulating air rushes in through the perforations;
- at real overloads of the bulk material, the pressure along the length of the chute increases and reaches high values at the entrance to the lower shelter and if there is a perforation in the upper part of the increase will not occur, this is due to the fact that the falling material will partially push the air through the perforation, and due to the low air pressure inside the trough the formation of an air curtain will be excluded.
The presence of a vertical partition or internal walls limiting the receiving chamber of the lower cover allows reducing the dusting out of the dusty air into the working area of the room and also plays the role of the main resistance between the aspiration funnel and the bypass chamber.

4 CALCULATION METHOD OF VOLUME OF ASPIRATION OF OVERLOADING OF BULK MATERIAL AT TELESCOPIC STATIONS

The most common conveyor overloading of dusting materials with ordinary closed troughs is characterized by the fact that gravitational flows of particles during a fall create ejection jets of dusty air that enter shelters of the fall site (loading points of the lower conveyors or feeders, bunkers, crushers, screens and other process equipment).

To avoid knocking out the dusty air from these shelters into the surrounding atmosphere, not only is the maximum possible compaction of these shelters, but also air suction to create a vacuum in the cavities of not only the lower shelters, but also other shelters aerodynamically associated with aspirated shelters. The required amount of aspirated air $Q_a$ (aspiration volume) for the simplest case of overload from the conveyor to the conveyor is determined by the sum of costs $Q_n$ and $Q_j$, where $Q_n$ is the flow of air entering the shelter through leakages, depends on the area of leakage ($F_m$ m$^2$) and the amount of vacuum maintained in the shelter ($P_v$, Pa) to prevent the expiration of dusty air.

$$Q_n = \mu F_m \sqrt{2P_v / \rho_o}$$

where $\mu = 1/\sqrt{\zeta}$ - the coefficient of consumption associated with the coefficient of local resistance of leakiness (for small holes $\zeta = 2.4$ and then $\mu = 0.65$); $\rho_o$ - ambient air density often taken to be 1.2 kg/m$^3$.

It is much more difficult to determine the amount of air flow $Q_j$ through the trough, often referred to as the flow rate of the ejected air. In general, the air flow rate moving through the trough depends not only on the depression in the bottom shelter ($P_v$), but also on the ejection head ($P_e$, Pa) created by the aerodynamic force of the particles falling in the chute, and also on the magnitude of the thermal head ($P_t$, Pa) arising from the heat exchange of falling heated particles and air. In the one-dimensional approximation:

$$Q_j = \mu F_e \sqrt{2(P_v + P_e + P_t) / \rho}$$

where $\rho$ - air density in the trough, kg/m$^3$; $\mu = 1/\sqrt{\sum \zeta}$ - coefficient of discharge associated with the amount of coefficient of local resistance of trough, depending on the geometry of its elements. The calculation of the ejected air in the trough of the loading telescopic stations is considerably complicated. The loading stations of small volumetric capacity (up to 250 m$^3$/h), such as the JETPACK TZS 500, as well as telescopic loaders of considerable capacity (up to 1500 m$^3$/h) of the PU-700 type, used in marine terminals, consist of loading troughs with variable loading height which are two coaxial tubes. The cavity of the inner tube, along which the feed material moves, is aerodynamically connected with the cavity of a limited impermeable outer wall and inner permeable wall. This circumstance contributes to the
organization of recirculation of the ejected air, which is quantitatively different from the ejection of air in the trough with an impenetrable wall.

### 4.1 Method of calculating the flow of ejected air in telescopic loaders

This method is based on the linearized equations of the dynamics of the ejected and recirculated air obtained in [5] (Fig. 1) with one ring of air recycling in the permeable chute with conventional (scheme a) and combined bypass (scheme b), i.e. with air recycling through two circulation rings, when the air ejected through the central channel is separated in the lower part of the telescopic trough and enters the bypass chamber (internal recycling).

Transit air flow at the exit of the chute is divided in turn into two parts, part of the air rises up through the bypass chamber 4 to the upper shelter, and the remaining part with the flow rate $Q_e$ flows through the sealing aprons into the aspirated chamber from where the aspiration pipe is removed. The overall performance of the nozzles is determined by the obvious amount: $Q = Q_o + Q_e$, where $Q_o$ is the flow rate of air entering through the leakiness of the outer sealing aprons due to the depression $P_y$ created by the fan of the aspiration system.

![Figure 1: The design scheme of aspiration of loading of the closed conveyor with use of TZS 1000 JETRAPACK](image)

- 1 - loading auger; 2 - telescopic tube (trough); 3 - corrugated outer impermeable pipe; 4 - bypass chamber with closed (scheme a) upper and lower bottoms and with open (scheme b) bottoms; 5 - aspiration shelter; 6 - lower suction nozzle; 6' - upper suction nozzle; 7 - stack of granular overloaded material; 8 - closed container; 9 - loading neck
It is necessary to determine the main component of the balance equation \( Q_g \).

Initial data for calculation: \( G_m \) - mass flow rate of the material being loaded, kg / s; \( H_l \) - trough height, m; \( d_1 \) - diameter of the upper base of the telescopic tube section, m; \( d_2 \) - diameter of the lower \((d_2 < d_1)\) base of this section, m; diameter of the outer sleeve of the trough \( D_s \), m; verage clearance between adjacent gutter sections \( z_c = (d_1 - d_2) / 2 \), m; \( D_k = (d_1 + d_2) / 2 \) - nominal diameter of the trough, m; \( S_g = \pi D_k^2 / 4 \) - the cross-sectional area of the trough, m\(^2\); \( f_m = \pi D_k z_c \) - conditional area of the living section of one gap, m\(^2\); \( N_g \) - number of sections in a telescopic tube, pcs; \( S_s = f_m N_g \) - total area of all gaps, m\(^2\); \( S_m = \pi (D_k^2 - D_1^2) / 4 \) - bypass chamber area, m\(^2\); \( r = S_n / S_g \); \( e_s = S_s / S_g \) - relative degree of permeability; \( \zeta_o \) - coefficient of local resistance of holes clearance; \( \zeta_m \) - coefficient of local resistance of opennings leakages of the outer wall of the aspiration shelter; \( E = e_s / \sqrt{\zeta_m} \) - degree of flow of air through the refraction holes of the trough; \( S_{sw} \) - area of leakages of top shelter, m\(^2\); \( S_{ak} \) - the area of leakages of bottom shelter (receiving chamber), m\(^2\); \( \zeta_{sw} = 2.4 (S_s / S_{sw})^3 \) - coefficient of local resistance to air inlet through leakage of the top shelter; \( \zeta_{ak} = 2.4 (S_s / S_{ak})^3 \) - coefficient of local resistance to air inlet through leakage of the lower cover; \( P_y \) - depression in the aspirating bottom shelter chamber, Pa; \( F_s \) - the area of leakages of the outer wall of the aspirated chamber; \( \psi_e \) - coefficient of drag of a single particle; \( \rho_s \) - particle density, kg / m\(^3\); \( \rho_g \) - air density in the trough, kg / m\(^3\); \( \rho_w \) - density of external air, kg / m\(^3\); \( d_e \) - equivalent particle diameter, mm; \( H_o \) - height of falling of particles, m; \( v_s = \sqrt{2gH_o} \) - particle velocity at the entrance to the trough, m / s; \( v_k = \sqrt{2g(H_l + H_o)} \) - particles velocity at the outlet of the trough, m / s; \( n = v_o / v_k \) the ratio of the velocity of falling of particles; \( P_r = 2P_y / (\rho g v_k^2) \) - dimensionless depression in the aspirating chamber of the bottom shelter.

After the formation of the initial data, the calculation is performed in the following sequence.

1. The volume concentration of falling particles at the end of the telescopic trough is determined: \( \beta_g = G_m / (v_s \rho_s S_g) \); and in the middle of this trough: \( \beta_s = 2G_m / (v_s (1 + n) \rho_s S_g) \).

2. Calculating the average drag coefficient of falling particles by the formula:
\[
\psi = \psi_e \exp \left[ -56.92 \sqrt{\psi_e} / d_e \right].
\]

3. Determining the ejection parameter: \( Le = \psi \beta_s H_l 1500 \) / \( d_e \).

4. Calculate the average speed of incidence of particles in a telescopic tube
\[
v_s = b_0 + b_1 \right / 2 + b_2 \right / 6,
\]
coefficients are determined by the formulas
\[
b_0 = n; b_1 = \sqrt{8(1 + n^2) - 3n - 1}; b_2 = 4(1 + n - \sqrt{2(1 + n^2)}), n = v_o / v_k.
\]

5. The averaged velocities of the ejected air in the telescopic chute \( (u_e) \), the speeds of the upward recirculated air in the bypass chamber \( (u_o) \) and the speed of air flowing from the
trough through the openings of the side wall of the chamber \( w_i \) are expressed through an unknown parameter \( u_i \):

\[
u_i = v_i - \sqrt{v_i (\zeta_i u_i - p_i) / \left(C_i \sqrt{\zeta_i E_i} \right)}; \quad w_i = u_i - \sqrt{0.25 + \zeta_i + 0.25 - \zeta_i} / \left(3 \xi_i \right), \quad \omega_i = (u_i - u_j) / r,
\]

where \( \zeta_r = \zeta_n + \zeta_k, \zeta_n = \zeta_m + 0.5, \zeta_k = \zeta_{ak} + 1 \)

6. Functions, parameters, coefficients are introduced through the values obtained at the previous stage:

\[
A = 2(u_i - \omega_i) E / \left(C_i \sqrt{\zeta_i E_i} \right); \quad B = (1 - u_i / v_i) E / \left(C_i \sqrt{\zeta_i E_i} \right); \quad k_2 = 2 b_2 A / B; \quad k_1 = (2 A (b_1 - k_2) - b_2) / B;
\]

\[
a_i = A + \sqrt{A^2 + B}; \quad a_2 = A - \sqrt{A^2 + B}; \quad a_3 = (n - k_i) / b_3 = 1 - k_i; \quad b_i = b_1 + b_2 - k_2; \quad z_i = e^x - e^{x_i};
\]

\[
C_i = C_i (1 - e^x) + a_i e^{x_i} - b_i) / z_i; \quad C_2 = (u_i (e^x - 1) - a_i e^{x_i} + b_i) / z_i
\]

and by solving a transcendental equation

\[
(\zeta_r u_i^2 - p_i) E / \left(C_i \sqrt{\zeta_i E_i} \right) - \left(C_i a_i (1 - e^x) + C_2 a_i (1 - e^{x_i}) + a_i - b_i \right) = 0
\]
determined by the dimensionless velocity of the ejected air at the inlet (and outlet) in the telescopic trough \( u_i \).

7. The velocity \( u(x) \) is calculated (in arbitrary trough sections) on a segment \( x = 0 \ldots 1: \)

\[
u(x) = C_1 e^{a_i x} + C_2 e^{b_i x} + b_1 - k_i + x(b_1 - k_2) + 0.5 b_2 x^2 \quad \text{and the mean velocity is determined by integrating the function } \nu(x) \text{ on the same segment}
\]

\[
u_i = C_i (e^{x_i} - 1) / a_i + C_2 (e^{x_i} - 1) / a_2 + b_0 + (b_1 - k_2) / 2 + b_2 / 6 - k_i.
\]

8. Cross section \( x_m \) is found by solving the equation \( C_i a_i e^{a_i x_m} + C_2 b_i e^{b_i x_m} + b_1 + b_2 - k_2 = 0 \) and calculating the maximum value of the dimensionless velocity of the ejected air \( u_m = C_i e^{a_i x_m} + C_2 e^{b_i x_m} + b_0 - k_i + x_m (b_1 - k_2) + 0.5 b_2 x_m^2 \).

9. The maximum volumetric air flow in the section \( x = x_m \) is determined. In the telescopic trough \( Q_m \) according to the formula: \( Q_m = 3600(\nu m v S) \), recirculated in the bypass chamber \( Q_r \) according to the formula: \( Q_r = 3600(u_i - u_m) v S \) and the difference between these costs \( Q_m = Q_r - Q_r \).

10. Calculate the dimensionless overpressure on the bottom of the bypass chamber \( p_u \) in accordance with the formula:

\[
p_u = 0.5 \left((\zeta_i - \zeta_u) u_i^2 - p_i\right) + 0.5 w_i \sqrt{\zeta_i E_i} \left[C_i a_i (1 + e^x) + C_2 a_i (1 + e^{x_i}) + a_i + b_i \right] / E.
\]

11. Calculations of the following dimensionless functions are performed in increments \( x = 0.1 \) (on the interval \( x = 0 \ldots 1)1:

\[
u(x) \quad \text{according to the formula: } \nu(x) = C_i e^{a_i x} + C_2 e^{b_i x} + b_1 - k_i + x(b_1 - k_2) + 0.5 b_2 x^2,
\]

\[
p_u(x) \quad \text{according to the formula: } p_u(x) = p_u - 4 a_3 (u(x) - u_i) / r,
\]

\[
p(x) \quad \text{according to the formula: } p(x) = p_u(x) - w_i \sqrt{\zeta_i E_i} \left[C_i a_i e^{a_i x} + C_2 a_i e^{b_i x} + b_1 - k_i + b_2 x \right] / E,
\]

pressure difference according to the formula: \( \Delta p(x) = -p(x) + p_u(x) \),
w(x) according to the formula: \( w(x) = \Delta p(x)/\left(\zeta_o w_x \right) \).

To analyze the changes in the above-mentioned functions, it is convenient to display the values of the argument \( x = 0; 0.1; 0.2 \ldots 1 \) in the first column, the second value \( u(x) \), the third \( w(x) \), the fourth \( p(x) \), the fifth \( p_{w}(x) \) and the sixth \( \Delta p(x) \).

12. The dimensionless velocity of the ejected air \( (u_x) \) from the equation is calculated:

\[
3 \left( n - u_x - |n - u_x| \right) + 2\Delta e/(\zeta_o u_x^2 - p_x) / (1 - n^2) = 0
\]

and its consumption \( Q_x = 3600u_x v_x S_x \) m\(^3\)/h for the case of complete sealing of the walls of the trough (that is, in the absence of air recycling in the bypass chamber).

13. The flow rate of air entering from the trough to the aspirated shelter \( Q = 3600u_x v_x S_x \) m\(^3\)/h is calculated; the flow rate of air entering the same shelter through leakages \( Q' = 3600F_p \sqrt{2\Delta p} / (\zeta_o p_x) \) m\(^3\)/h and the required flow rate of air removed from the aspiration shelter \( Q_n = Q + Q_n \).

12 CONCLUSIONS

- A method of engineering calculation of the volumes of aspirated air during overloads of dry unheated materials with natural circulation has been developed and carried out through the combined use of a cylindrical bypass chamber and a perforated trough. Experimental and numerical studies have shown that the proposed method has sufficient accuracy were performed.

- Recommendations on the design of the aspiration shelter for its more efficient operation with lower operating costs. The economic effect is to reduce energy consumption and the cost of cleaning dust emissions.

- The values of recirculation coefficients for the calculation of the aspiration system when using the bypass chamber and using the combined use of the bypass chamber and trough perforation are proposed.

- A method for calculating the flow rate of ejected air in telescopic loaders has been developed.

- The high energy intensity of telescopic aspiration-technological installations (ATI) of transfer stations is due to the ejection capacity of gravity flows of bulk material, which inject large amounts of air into aspiration shelters, which significantly increases the required performance of aspiration systems. The power of the ATI can be significantly reduced by using coaxially located loading telescopic troughs and corrugated impermeable walls located around the trough, as well as sealing the top and bottom shelters adjacent to the troughs. Coaxially located troughs and bypass chambers contribute to the formation of internal recirculation of the ejected air and a noticeable reduction in the power of transit air coming from the trench to the aspirated shelter.

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REFERENCES


DEVELOPMENT OF METHODS FOR REDUCING THE VOLUME OF ASPIRATION DURING OVERLOADS OF GRANULAR MATERIALS

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Key words: Aspiration, bulk material transfer, air suction.

Abstract. The schemes of aspiration of elevator overloads have been developing. Balance equations of ventilation of aspiration covers are compiled. The system of equations for determination of the volumes of ventilating air for a standard node overload are formulated and solved. Ways of reducing productivity of aspiration systems are offered and analytically substantiated.

Three bypass channels can be used to reduce aspiration volumes in elevator handling facilities by maintaining a smaller negative pressure inside unaspirated cowls of the elevator feeder and head. Airflows can be quantitatively decomposed using combined equations describing pressure losses in loops of a proposed aerodynamic equivalent for the assembly. These combined non-linear equations have been solved numerically using a specially developed algorithm based upon joint application of iterative and bisection procedures.

Analysis of the findings for a “standard” elevator indicates that reduction in flow rates of air entering through leakage areas of unaspirated cowls is maximized when two bypass connections are installed: the lower one, connecting feeder cowl with a buffer chamber upstream of elevator boot cowl, and the upper one, connecting elevator head cowl with the inner chamber of a double-walled cowl of the upper (receiving) conveyor. The total flow rate in the case reviewed was 1.37 times lower than (a corresponding aspiration case with identical process and design parameters of the assembly, but with no bypass ducts).

The effect cited may differ from the actual effect in every particular case. The computer program developed for the purpose can be used to provide a design-stage estimate.

1 INTRODUCTION

Relevant problems in the design of aspiration cowl for loose-matter handling facilities include devising means and techniques for reducing aspiration volumes necessary to maintain proper dedusting efficiency as well as reducing the carryover of dustlike material into the aspiration network.

In order to reduce the volume of air ejected by a flow of loose matter, the most rational and rewarding approach would be to ensure closed-loop circulation of dust-laden air streams in transfer chutes without using any additional forced-draft devices. Air circulation processes in
such chutes have not been described analytically to this day. This paper completes a series of papers [1-5].

2 REDUCING REQUIRED ASPIRATION VOLUMES IN BYPASSED ELEVATOR HANDLING SYSTEMS

Let’s now move on to examine regularities in cross-flows of air given a more complicated case, using three bypass ducts for an aspirated elevator handling facility (Fig. 1). In particular we’ll be studying the behavior of flow rates $Q_s, Q_6$ and $\Delta Q = Q_8 - Q_s$.

For this purpose we’ll put together obvious equations of air dynamics and balance for ducts and flow junction points.

\[
\begin{align*}
P_s - P_{bc} + P_1 (Q_1) &= R_c Q_1^2; \\
P_{bc} - P_s + P_1 (Q_1) &= R_c Q_1^2; \\
P_s - P_6 + P_0 (Q_0) &= R_c Q_0^2; \\
P_s - P_6 &= R_c Q_5^2; \\
P_d - P_{bc} + P_6 (Q_6) &= R_c Q_5^2; \\
P_{bc} - P_6 &= R_c Q_5^2; \\
P_{bc} - P_b &= R_c Q_5^2; \\
Q_0 &= Q_s + Q_a + Q_o; \\
Q_s &= Q_0 + Q_4 - Q_1 + Q_5; \\
Q_3 &= Q_0 + Q_7 + Q_5 - Q_2; \\
Q_7 &= Q_o - Q_0; \\
Q_a &= Q_6 + Q_a. 
\end{align*}
\]

In addition for conventions used for combined equations (12)–(24) [4], the following conventions are introduced here:

$P_s$ is absolute pressure in the outer chamber of the upper (receiving) conveyor (Pa);

$R_c, P_5$ are absolute pressures in the buffer chamber of the loading chute and in the inner chamber of the upper conveyor cowl (Pa);

$Q_4, Q_6$ are flow rates of air circulating in bypass ducts (m$^3$/s);

$Q_s, Q_6$ are flow rates of air coming in respectively from the buffer chamber into the bucket elevator boot enclosure and from the inner chamber into the outer chamber of upper conveyor cowl (m$^3$/s);

$R_s, R_6, R_t$ are aerodynamic properties of the respective bypass ducts (Pa/(m$^3$/s)$^2$) determined by their LRCs and cross-sectional areas:

\[
R_s = \rho \zeta_s / (2 S_1^2); \quad R_6 = \rho \zeta_6 / (2 S_6^2); \quad R_t = \rho \zeta_t / (2 S_t^2); 
\]
\[ \zeta_1, \zeta_2, \zeta_3 \text{ are LRCs of the respective bypass ducts referenced to dynamic heads in their cross-sections; } \]

\[ S_1, S_2, S_3 \text{ are cross-sectional areas of the respective ducts (m}^2).\]

**Figure 1:** Aspiration layout for elevator handling with a bypass connection (a) and its aerodynamic equivalent (b)
The foregoing translates into a total of 19 unknown combined equations (1)...(15) and (17), (18), (38) and (40) [4] with nineteen unknown variables in the general case. These include air flow rates in ducts $Q_0, Q_1, ..., Q_s$, air flow rates in leakage areas of cowls $Q_3, Q_4, Q_5$, air flow rates in unaspirated cowls $P_3$ and $P_4$, pressures within recirculating flow separators $P_0$ and $P_1$, and flow rates of aspirated air $Q_6$ and $Q_7$.

The number of equations may be reduced by applying the law for pressure losses in loops of complex ventilating systems as known from the aerology of mining. Let’s write down the corresponding equations:

For the loop $a$:

$$P_0(Q_0) = R_0Q_0^2 + R_4Q_0^2;$$ (16)

For the loop $b$:

$$P_1(Q_1) = R_0Q_1^2 + R_1Q_1^2 - R_0Q_1^2;$$ (17)

For the loop $c$:

$$P_1(Q_1) + P_1(Q_2) = R_2Q_2^2 + R_4Q_2^2;$$ (18)

For the loop $d$:

$$P_1(Q_1) = R_3Q_3^2 + R_4Q_3^2;$$ (19)

For the loop $e^1$:

$$P_0(Q_0) = R_0Q_0^2 + R_5Q_0^2 - R_6Q_0^2 + R_0(Q_0 - Q_4)^2;$$ (20)

For the loop $f$:

$$-R_0Q_0^2 + R_0Q_0^2 + R_1(Q_0 - Q_1)^2 - R_2Q_1^2 = 0;$$ (21)

For the loop $k$:

$$R_0Q_0^2 = R_0Q_0^2 + R_0Q_0^2 - R_0Q_0^2.$$ (22)

The ten unknown variables $(Q_0, Q_1, ..., Q_s)$ are represented with ten equations (16)...(22), (10), (14) and (12).

These combined non-linear equations will be solved iteratively. Specifically, we’ll proceed from a set negative pressure in the unaspirated cowl of elevator head (which would be equivalent to setting the initial value of $Q_4$ due to (39)) [4]. For example, let this negative pressure be $h$ ($h = 0$ or $h = h_1$ may be posited for the first approximation). Proceeding from these premises we’ll determine air flow rates in ducts $Q_0(h), Q_1(h), Q_2(h), ..., Q_s(h)$ as functions of $h$. The next step is refining the negative pressure value:

$$s_i = R_0(Q_0(h))Q_1(h);$$ (23)

where

$$Q_0(h) = Q_0(h) - Q_1(h) + Q_2(h) - Q_3(h);$$

The computation process repeats with a new value of $h_1$.

Computation can be facilitated if the following is posited for $i+1$-th approximation:

---

1 Loops $e, f, k$ are fictitious. They connect airflows in ducts by terminating them in the atmosphere of the room through leakage areas in cowls (these links are shown with dotted “ducts” in Fig. 1)
\( h_{i+1} = 0.5(h_i + s_i) \).

Computation stops as soon as the inequality is met:
\[
|s_i - h_i| \leq E,
\]  
(24)
where \( E \) is the accepted precision \( (E = 10^{-2}) \).

Now let’s derive computation formulas for \( i \)-th approximations of air flow rates in ducts: \( Q_i(h_i), Q_i(h_i), \ldots, Q_i(h_i) \).

We’ll begin with considering upper ducts adjacent to the cowl of bucket elevator “head”. Equation (19) gives:
\[
f_i = Q_i(h_i) = \frac{L_i(Q_i(h_i))}{\sqrt{R_i[L_i(Q_i(h_i))]}},
\]  
(25)
where
\[
L_i(Q_i(h_i)) = R_i(Q_i(h_i)) - R_i|Q_i(h_i)||Q_i(h_i)|.
\]  
(26)

In view of the connection between negative pressure in the cowl and air flow rates in leakage area of this cowl, equation (22) will appear as:
\[
-kh_0 + h_0 = R_u[Q_0(h_0)]^2 - R_u|Q_0(h_0)||Q_0(h_0)|,
\]
whence we can find
\[
Q_0(h_0) = \frac{L_0}{\sqrt{R_u[L_0]}},
\]  
(27)
where
\[
f_0 = L_0 = h_0 - h_0 + R_u f_i(Q_i(h_i))|f_i(Q_i(h_i))|.
\]  
(28)

(14) enables us to put forth the following equation with a single unknown variable \( Q_i(h_i) \):
\[
f_{i0} = Q_i(h_i) - Q_i(Q_i(h_i)) - Q_i(Q_i(h_i)) = 0,
\]  
(29)
which can be solved using bisection. As soon as \( (Q_i(h_i)) \) is found, formula (25) can be used to determine \( Q_i(h_i) \) and formula (27) can be used for \( Q_i(h_i) \).

Let’s now move on to the lower assembly (bucket elevator boot cowl). For the sake of clarity we’ll omit the argument of air flow rate functions. Equation (20) in view of the connection between negative pressure and air flow rate in leakage areas of the elevator boot cowl will appear as:
\[
h_0 + L_0(Q_0) = R_u Q_0^2 + R_u(Q_0 - Q_4)^2,
\]
whence
\[
f_4 = Q_4 = f_{i4}/\sqrt{|f_{i4}|},
\]  
(30)
with the following functions introduced for a more convenient notation:
\[
f_{i4} = L_{i4} = \frac{h_0 + L_0(Q_4)}{R_4} - R_u(Q_0 - Q_4)^2,
\]  
(31)
\[ f_0 = L_0(Q_0) = P_0(Q_0) - R_0|Q_0|. \] (32)

Equation (16) results in:
\[ f_4 = Q_4 = \frac{L_0(Q_0)}{\sqrt{R_L|Q_0|}}. \] (33)

In order to resolve \( Q_4 \) as a function of \( Q_0 \), we’ll use equation (21) which will be written as:
\[ h_i - R_i(Q_0 - Q_i)|Q_0 - Q_i| + R_i|Q_0| = R_i|Q_0|, \]

or
\[ L_{i1} = R_i|Q_0|, \] (34)

where
\[ L_{i1} = f_{i1} = h_i - R_i(Q_0 - Q_i)|Q_0 - Q_i| + R_i|Q_0|, \]

whence:
\[ f_6 = Q_6 = \frac{L_{i1}}{\sqrt{R_i|L_{i1}|}}. \] (35)

Substitution of (30), (33) and (35) into the air balance equation (10) results in the following functional equation for determining \( Q_0 \):
\[ f_{12} = Q_0 - Q_4(Q_0) - Q_2(Q_0) - Q_6(Q_0) = 0. \] (36)

After determining \( Q_0(h) \) and substituting it into equations (30), (33) and (35), flow rates \( Q_4(h), Q_2(h) \) and \( Q_6(h) \) will become known.

In order to determine the remaining unknown variables \( Q_6(h) \) and \( Q_6(h) \), equations (46)...(48) and (27)...(28) [3] can be used.

The resolved values of \( Q_1(h), Q_2(h), Q_3(h), Q_6(h) \) and \( Q_5(h) \) are substituted into (23) in order to determine the next iterative value of negative pressure.

The iterative process completes as soon as the condition (24) is met. A flowchart of the algorithm described above is shown in Fig. 2.

Computed flow rates of \( Q_0...Q_6 \), in addition to determining negative pressures in unaspirated cowls of elevator head \( (h) \) and in the feeder drive drum cowl,
\[ h_i = R_i(Q_0 - Q_i)|Q_0 - Q_i|, \] (37)

enable the required aspiration volumes to be computed as well.
\[ Q_6 = Q_6^* + \frac{h_i}{\sqrt{R_i}}, \] (38)
\[ Q_6 = Q_6 + Q_2 - Q_6 + \frac{h_i}{\sqrt{R_i}} \] (39)
Figure 2: Flowchart of the algorithm for computing air flow rates in ducts $Q_b, Q_1, \ldots, Q_e$ and aspiration volumes $Q_b$ and $Q_c$ of a grain-handling elevator unit equipped with bypass connections:

- $E_0 = 400 \text{ Pa} / (\text{m}^3 / \text{s})$; $L_{n0} = 1.6 \text{ m}^3 / \text{s}$; $h_n = 10 \text{ Pa}$; $R_1 = 22 \text{ Pa} / (\text{m}^3 / \text{s})$;
- $E_1 = 200 \text{ Pa} / (\text{m}^3 / \text{s})$; $E_2 = 400 \text{ Pa} / (\text{m}^3 / \text{s})$; $R_2 = 21 \text{ Pa} / (\text{m}^3 / \text{s})$; $R_3 = 22 \text{ Pa} / (\text{m}^3 / \text{s})$;
- $L_1 = 1 \text{ m}^3 / \text{s}$; $R_4 = 10 \text{ Pa} / (\text{m}^3 / \text{s})$; $R_5 = 50 \text{ Pa} / (\text{m}^3 / \text{s})$; $R_6 = 25 \text{ Pa} / (\text{m}^3 / \text{s})$;
- $R_7 = 50 \text{ Pa} / (\text{m}^3 / \text{s})$; $R_8 = 50 \text{ Pa} / (\text{m}^3 / \text{s})$; $R_9 = 36 \text{ Pa} / (\text{m}^3 / \text{s})$; $E_3 = 5 \text{ Pa} / (\text{m}^3 / \text{s})$;
- $L_{s1} = 2 \text{ m}^3 / \text{s}$; $L_{s3} = 0.5 \text{ m}^3 / \text{s}$; $h_s = 5 \text{ Pa}$; $R_s = 40 \text{ Pa} / (\text{m}^3 / \text{s})$. 

\[ \begin{align*}
Q_b &= E_0 \cdot L_{n0} / h_n; \\
Q_c &= T_1 / (T_2 + T_3) \cdot L_1 / h_1; \\
Q &= T_1 / (T_2 + T_3) \cdot L_1 / h_1. 
\end{align*} \]
The role of bypass connections can be evaluated by comparing the current values of $Q_1$, $Q_2$ and $\Delta Q$ with respective values of $Q_{\infty}$, $Q_{\infty}$ and $\Delta Q_{\infty}$ for an aspiration system without bypass connections. It would be best to choose a “standard” case of elevator facility design for this study. We’ll be using the previously considered example of elevator handling facility [4] that will be supplemented generally with three bypass channels by analogy with Fig. 1a. The following values will serve as constant parameters describing this handling facility.

Aerodynamic performance indices of bypass ducts $R_1$, $R_2$ and $R_3$ within the range of 0.5…150 $\text{Pa} / (\text{m}^3 / \text{s})^2$ will serve as variables. These values become fixed at $10^9 \text{Pa} / (\text{m}^3 / \text{s})^2$ when the respective bypass duct is closed or disconnected. For example, if $R_1 = R_2 = R_3 = 10^9$, then air flow rates in bypass ducts will be $Q_1 = Q_2 = Q_3 = 0$ i.e. bypass ducts are disconnected. Calculated values are presented on Fig. 3, 4 and 5. On these plots, air flow rates corresponding to the unbypassed case are designated with a subscript $\infty$ and their changes are plotted using straight horizontal dotted lines. Another instance of a fixed aerodynamic performance index of bypass ducts occurs at 25 $\text{Pa} / (\text{m}^3 / \text{s})^2$. For example, Fig. 3 indicates variations in air flow rates $Q_1$, $Q_2$, $\Delta Q$ and their sum total $\sum Q$ for three possible bypass layouts:

Case #1: Only a bottom bypass duct is provided (on the loading chute); its aerodynamic performance varies $0.5 \leq R_4 \leq 150$ while other bypass ducts are absent (their aerodynamic performance converges toward $\infty$ or, more precisely, is $R_1 = R_2 = 10^9$);

Case #2: Only the middle bypass duct (located on elevator enclosure) is arranged i.e. $0.5 \leq R_5 \leq 150$ and $R_1 = R_2 = 10^9$;

Figure 3: Air flow rates $Q_1$, $Q_2$, $\Delta Q$ and $\sum Q$ as functions of aerodynamic drag for an elevator equipped with a single bypass duct (H – lower, M – middle, B – upper, $\infty$ – no bypass ducts)
Figure 4: Air flow rates $Q_s$, $Q_x$, $\Delta Q$ and $\sum Q$ as functions of aerodynamic resistance for an elevator equipped with two bypass ducts (HC – lower and medium, CB – medium and upper, HB – lower and upper, $\infty$ – no bypass ducts).

Figure 5: Air flow rates $Q_s$, $Q_x$, $\Delta Q$ and $\sum Q$ as functions of aerodynamic drag $R_x$ for an elevator equipped with three bypass ducts.
Case 3: Only the upper bypass duct is provided (on the discharge chute) i.e. $0.5 \leq R_t \leq 150$ and $R_a = R_u = 10^9$ (this case is illustrated in Fig. 3).

Fig. 4 plots air flow rates for three possible design layouts of bypass ducts: case 1 – lower and middle bypass ducts are installed so that $R_a = 25 \frac{\text{Pa}}{\text{m}^3/\text{s}}$, $0.5 \leq R_t \leq 150 \frac{\text{Pa}}{\text{m}^3/\text{s}}$, $R_a = 10^9 \frac{\text{Pa}}{\text{m}^3/\text{s}}$; case 2 – middle and upper bypass ducts are installed so that $R_a = 10^9 \frac{\text{Pa}}{\text{m}^3/\text{s}}$, $0.5 \leq R_t \leq 150 \frac{\text{Pa}}{\text{m}^3/\text{s}}$; case 3 – lower and upper bypass ducts are installed, so that $R_a = R_u = 25 \frac{\text{Pa}}{\text{m}^3/\text{s}}$ and $0.5 \leq R_t \leq 150 \frac{\text{Pa}}{\text{m}^3/\text{s}}$.

Fig. 5 contains plots of air flow rates for the only possible configuration with three bypass ducts: lower, medium and upper, so that $R_a = 25 \frac{\text{Pa}}{\text{m}^3/\text{s}}$, $R_u = 25 \frac{\text{Pa}}{\text{m}^3/\text{s}}$, $0.5 \leq R_t \leq 150 \frac{\text{Pa}}{\text{m}^3/\text{s}}$.

As the plots illustrate, installation of bypass ducts noticeably decreases the total amount of air entering through leakage areas of unaspirated cowls in elevator feeder and head:

$$\sum Q = Q_a + Q_u + \Delta Q,$$

where $\Delta Q = Q_a - Q_1$.

So, with a single bypass duct installed, installation of the upper bypass duct (Fig. 3) provides the greatest effect: at $R_a = 25 \frac{\text{Pa}}{\text{m}^3/\text{s}}$, $R_u = R_s = 10^9$ the total volume of air

$$\sum Q = 0.79 \sum Q_a = 0.88 \sum Q_u,$$

that is, 1.14 times smaller than without bypass ducts installed. An even greater effect is achieved when the elevator is equipped with two bypass connections at the top and at the bottom (Fig. 3): at $R_a = 25 \frac{\text{Pa}}{\text{m}^3/\text{s}}$, $R_u = 10^9 \frac{\text{Pa}}{\text{m}^3/\text{s}}$ and $R_s = 25 \frac{\text{Pa}}{\text{m}^3/\text{s}}$ the total volume of air is

$$\sum Q = 0.66 \sum Q_a = 0.73 \sum Q_u,$$

i.e. 1.37 times less than for the case of aspiration without bypass connections installed.

It would be unwise to install three bypass connections in this case, as with $R_a = R_u = R_s = 25 \frac{\text{Pa}}{\text{m}^3/\text{s}}$, ...
\[
\sum Q_{\text{bou}} = \frac{0.73}{0.9} \sum Q_e = 0.81 \sum Q_e ,
\]
i.e. efficiency would be lower than with two (upper and lower) bypass connections. This happens because cross-flows of air from the upper cowl (at the elevator head) into the lower cowl (elevator boot cowl) increases as negative pressure in the upper cowl is reduced to 2.1 Pa \( (h_1 = 5.6 \text{ Pa for the case of upper and lower bypass ducts}). \) Meanwhile, \( \Delta Q \) increases from 0.046 m\(^3\)/s with two bypass ducts to 0.093 m\(^3\)/s with three bypass ducts.

With regard to aspiration volumes the effect of bypassing appears less prominent. For example, in the case of upper and lower bypass ducts in the example considered,

\[
Q_a = \sum Q_a + Q_b + Q_c = 0.66 + \frac{5}{36} + \frac{5}{40} = 0.66 + 0.73 = 1.39 \text{ m}^3/\text{s} ,
\]

while, absent any bypass ducts,

\[
Q_{\text{asc}} = \sum Q_a + Q_b + Q_c = 0.9 + 0.73 = 1.63 \text{ m}^3/\text{s} ,
\]
i.e. 17% higher.

It should be noted that values indicated may be higher. A specially developed computation methodology and software enable to evaluate the effect in each specific case on the design stage, making it possible to devise efficient layouts of aspiration \([6-10]\) and bypassing for elevator handling of grain.

### 3 CONCLUSIONS

- Volumes in elevator handling facilities by maintaining a smaller negative pressure inside unaspirated cowls of the elevator feeder and head. Airflows can be quantitatively decomposed using combined equations (16)-(22) describing pressure losses in loops of a proposed aerodynamic equivalent for the assembly (Fig. 1b). These combined non-linear equations have been solved numerically using a specially developed algorithm (Fig. 2) based upon joint application of iterative and bisection procedures.

- Analysis of the findings for a “standard” elevator (Fig. 3, 4 and 5) indicates that reduction in flow rates of air \( (\sum Q) \) entering through leakage areas of unaspirated cowls is maximized when two bypass connections are installed: the lower one, connecting feeder cowl with a buffer chamber upstream of elevator boot cowl, and the upper one, connecting elevator head cowl with the inner chamber of a double-walled cowl of the upper (receiving) conveyor. The total flow rate \( \sum Q \) in the case reviewed was 1.37 times lower than \( \sum Q_\infty \) (a corresponding aspiration case with identical process and design parameters of the assembly, but with no bypass ducts).

- The effect cited may differ from the actual effect in every particular case. The computer program developed for the purpose can be used to provide a design-stage estimate.
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REFERENCES


FLUID-STRUCTURE INTERACTION AND HOMOGENIZATION: FROM SPATIAL AVERAGING TO CONTINUOUS WAVELET TRANSFORM

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1 INTRODUCTION

Fluid-structure interaction (FSI) is classically modeled according a separated and local approach. It enables to take full advantage of the numerical methods specifically designed for each medium. However, it requires to take great care of the interface, and to exchange, between the algorithms, the information related to boundary conditions [1]. This treatment of the interface can quickly become too cumbersome in complex flow geometries, as in the industrial case study driving this work: an inviscid compressible flow interacting with French PWR fuel assemblies (Fig. 1a).

In such specific applications, where the solid medium exhibits a discontinuous but periodic design, an homogenized and global approach is preferred [2]. Inspired by porous media [3, 4], multiphase flows, or Large Eddy Simulation (LES), it relies on a spatial averaging of the balance equations, thus allowing to remove all interfaces. However, such filtering techniques exhibit two major limitations: first, they do not deal properly with boundary conditions, due to the non-commutativity between the filtering operator and spatial derivatives, as detailed in [5, 6, 7] for LES; second, filtering implies loss of microscopic information, and thus requires a closure model to describe interactions between resolved and unresolved scales.
In order to bypass these limitations, and especially tackle the multi-scale issue of closure, the authors hereafter put forward a new formalism to homogenize the fluid and solid media: continuous wavelet transform (CWT). Indeed, once applied to each medium balance equations, CWT allows to robustly derive a system of filtered and homogenized PDEs, while travelling back and forth between resolved and unresolved scales, thanks to its ability to reconstruct a signal from its wavelet coefficients.

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In literature, wavelets have been extensively used, for a couple decades now, in signal processing and modal identification [8], and also for the numerical computation of PDEs [9, 10, 11, 12, 13]. Nevertheless, to the authors’ knowledge, wavelets are in most cases used with the ”discrete (orthogonal) wavelet transform” (DWT) formalism, and under the assumption that the signal is known at the microscopic scale (signal processing, coarsening of a fine grid). The reference work of [14] stands among the rare examples of the use of CWT on linear differential equations, in order to derive algebraic equations.

In the current work, wavelets are used to derive filtered and homogenized equations on continuum fields, in the sense of continuum mechanics. CWT is therefore more relevant than DWT. The thorough description of the filtering process, and the numerical resolution of the filtered equations, exceed the scope of the current work. However, it can here be noted that CWT will be implemented in a 2D formalism, as the solid medium exhibits a periodic design along the transverse directions only (Fig. 1a). Moreover, the authors hereafter focus on the fluid, and consider the solid medium as a fixed and rigid body, only acting as a boundary condition for the flow. The structure displacement and deformation will be considered in further developments.

The following of the present article is hereafter divided into five parts. First, the fluid physical and mathematical modeling are described, after a brief overview of the solid medium. Second, the wavelet-based multi-scale modeling is introduced: some key points on CWT are recalled, followed by the choice of the analyzing wavelet. Third, the filtered equations are displayed, thus highlighting the key issues of closure and microscopic reconstruction. Fourth, this modeling is confronted with a 2D numerical case study, consisting in the propagation of a transverse pressure wave through rod bundles, for which a reference solution is computed with EUROPLEXUS software. These preliminary numerical investigations aim to bring a first light on the CWT ability to reconstruct the force applied by the fluid on the micro-structure. Finally, the last section is dedicated to a conclusion.
2 Physical and mathematical modeling

2.1 Solid medium

In the industrial case study, the solid medium is composed of fuel assemblies used in a French PWR. As shown in Fig. 1a, they exhibit a discontinuous but periodic design, with a beam-like geometry ($20 \text{ cm}^2 \times 4 \text{ m}$). A French 900 MW PWR possesses 157 fuel assemblies, each composed of 264 fuel rods (5 mm radius), 5 instrumentation guide thimbles, and 24 control rod guide thimbles. The latter bring stiffness and cohesion to the structure thanks to 8 spacer grids (Fig. 1b) placed along the assembly. The reader can refer to [2] for further details on the design and mechanical behavior of PWR fuel assemblies.

![Figure 1: PWR fuel assemblies design: fuel assembly (a) and spacer grid (b).](image)

2.2 Fluid

Under nominal operating conditions, the (liquid) water flow interacting with PWR fuel assemblies is almost vertical, incompressible and very turbulent, with a Reynolds number around $10^5$, at around 300 degrees Celsius and 155 bar. For this study, a fast transient compressible flow is considered, with the following modeling framework:

- monophasic compressible flow;
- inviscid fluid;
• kinetic turbulent energy, gravity effects and superficial tension are negligible compared to pressure gradients;
• conduction heat transfer is negligible;
• barotropic state law;

2.3 Local equations

The water flow is thus driven by the following Euler compressible equations:

\[
\begin{align*}
\partial_t \rho + \text{div} (\rho \mathbf{v}) &= 0 \quad \text{in } \Omega_f, \\
\partial_t (\rho \mathbf{v}) + \text{div} (\rho \mathbf{v} \otimes \mathbf{v}) &= -\nabla p \quad \text{in } \Omega_f, \\
\partial_t (\rho e) + \text{div} ((\rho e + p) \mathbf{v}) &= 0 \quad \text{in } \Omega_f,
\end{align*}
\]

(1)

which translate respectively the conservation of mass, momentum and energy.

This system of conservation laws is closed by a barotropic state law:

\[
p = p_{\text{ref}} + c^2 (\rho - \rho_{\text{ref}}),
\]

(2)

where \(\rho_{\text{ref}}\) and \(p_{\text{ref}}\) are respectively a reference density and pressure, and \(c = \sqrt{\partial_p p}\) the sound velocity in the fluid.

As for the boundary conditions, the assumption of inviscid fluid here implies:

\[
\mathbf{v} \cdot \mathbf{n} = 0 \quad \text{on } \partial \Omega_f,
\]

(3)

where \(\mathbf{n}\) is the outward unit normal vector on the boundary \(\partial \Omega_f\).

Given an initial data, the mathematical problem is thus well-posed. The fluid physical and mathematical modeling being stated, the following section can now introduce the multi-scale and homogenized modeling.

3 A multi-scale and homogenized modeling: from spatial averaging to CWT

Considering the lack of smoothness of some of the fields present in (1) (the pressure gradient and divergence operators are only defined in a distributional sense), a plain volume averaging of the equations is not mathematically robust. Moreover, a classical convolution product, as used in LES, does not enable to connect resolved and unresolved scales, and to reconstruct the force applied on the micro-structure. Continuous wavelet transform (CWT), conversely, fulfill these requirements.

In the following subsections, some key points on CWT are first recalled. The choice of the analysing wavelet is then motivated.
3.1 Continuous wavelet transform: definition and properties

Wavelets were first introduced as a tool for time-frequency analysis, in a 1D formalism. From an analyzing wavelet $\Psi$, classically defined as an oscillating function with a well-localized time-support, and a band-pass behavior $(\omega_\Psi, \Delta \omega_\Psi)$ in the Fourier domain, two parameters enable to build a family of translated ($u \in \mathbb{R}$) and dilated ($s > 0$) wavelets:

$$\Psi_{s,u}(t) = \frac{1}{\sqrt{s}} \Psi \left( \frac{t - u}{s} \right)$$ (4)

The resulting wavelet family $(\Psi_s)_{s>0}$ also exhibits a band-pass behavior. The interested reader can refer to [8, 15] for further details on wavelets and time-frequency analysis. Hereafter, wavelets are used as a spatial filtering tool. The above definition (4) is then generalized by adding one (respectively two) angular parameter(s) $\theta$ (resp. $\theta/\varphi$) in 2D (resp. in 3D). In the following, $d = 2$.

**Definition: continuous wavelet transform (2D)** Assume $\Psi \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$, with real or complex values, and satisfying a zero average condition:

$$\int_{\mathbb{R}^d} \Psi(x) \, dx = 0.$$ (5)

The continuous wavelet transform of a finite-energy signal $f \in L^2(\mathbb{R}^d)$ is defined as:

$$W[f](s, u, \theta) = \frac{1}{\sqrt{s}} \int_{\mathbb{R}^d} f(x) \Psi \left( \left( R_{\theta} \right)^{-1} \frac{x - u}{s} \right) \, dx$$ (in 2D), (6)

where:

- $W[f](s, u, \theta)$ is the wavelet coefficient;
- $\Psi$ is the analyzing wavelet, and $\Psi^*$ its complex conjugate;
- $R_{\theta} = \begin{pmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{pmatrix}$ is the 2D rotation matrix with respect to the $(O, e_1 \land e_2)$ axis, where $(e_1, e_2)$ is the orthonormal cartesian basis of $\mathbb{R}^2$;

*If $d = 1$, the $\theta$ variable and the rotation matrix $R_{\theta}$ are omitted.*

Thus, CWT can either be seen as a scalar or convolution product, between a signal and a wavelet family. But more importantly, CWT allows to reconstruct a signal at the
microscopic scale from its wavelet coefficients, assuming the analyzing wavelet satisfies the following admissibility condition (where $\mathcal{F}$ denotes the Fourier transform):

$$C_\Psi = \int_{\mathbb{R}^2} \frac{|\mathcal{F}[\Psi](k)|^2}{\|k\|^2} \, dk < +\infty \text{ (in 2D).}$$  \hspace{1cm} (7)

For further details on this property, the reader can refer to the reference book of [15]. Let us now detail the choice of the analyzing wavelet.

### 3.2 Analyzing wavelet

In literature, two major wavelet families are available: complex analytic and directional wavelets, versus real isotropic wavelets. In this work, the latter are better suited to "observe" pressure waves propagating in different directions simultaneously. The mexican hat (Fig. 2) has thus kept our attention. Its definition is recalled below (8):

$$\forall k \in \mathbb{R}^2, \mathcal{F}[\Psi](k) = 4\sigma^3 \sqrt{2\pi} \|k\|^2 e^{-\frac{\sigma^2\|k\|^2}{2}} \text{ (in 2D).}$$  \hspace{1cm} (8)

This wavelet exhibits a band-pass behavior in the Fourier domain, with a low selectivity. Besides, it satisfies the admissibility condition (7), with

$$C_\Psi = 32\pi^2 \sigma^2 \text{ (in 2D).}$$  \hspace{1cm} (9)

The mexican hat thus allows to tackle the closure issue, as detailed in the following section.
4 Filtered equations: closure and microscopic reconstruction

The wavelet-based multi-scale modeling here introduced leads to the following filtered equations on \((W[\rho], W[\rho u], W[\rho e])\) (here in 3D for the sake of generality):

Consider \(T > 0\), for all \(t \in [0, T]\), \(s > 0\), and \(\mathbf{u} \in \mathbb{R}^3\):

\[
\begin{align*}
\partial_t W[\rho](s, \mathbf{u}, t) + \text{div} (W[\rho u]) (s, \mathbf{u}, t) &= 0, \\
\partial_t W[\rho u](s, \mathbf{u}, t) + \text{div} (W[\rho u \otimes \mathbf{v}]) (s, \mathbf{u}, t) &= -\nabla W[p](s, \mathbf{u}, t) + \overline{F_{S \rightarrow F}}(s, \mathbf{u}, t), \\
\partial_t W[\rho e](s, \mathbf{u}, t) + \text{div} (W[(\rho e + p) \mathbf{v}]) (s, \mathbf{u}, t) &= 0,
\end{align*}
\]

(10)

where

\[
\overline{F_{S \rightarrow F}}(s, \mathbf{u}, t) = -\int_{\partial \Omega} \tilde{\Psi}_s^*(\mathbf{u} - \mathbf{\sigma}) p(\mathbf{\sigma}, t) \mathbf{n}(\mathbf{\sigma}) \, d\mathbf{\sigma}
\]

(11)

is a body force per unit of volume, now defined across the whole space \(\mathbb{R}^3\). In (11), the notation \(\tilde{\Psi}_s(\mathbf{x})\) refers to \(\frac{1}{\sqrt{s}} \Psi(-\frac{\mathbf{x}}{s})\). As one can notice, this filtered body force exhibits the microscopic pressure on the fluid-structure interfaces. Thanks to the CWT formalism, it is now possible to link this unresolved pressure to its resolved counterpart, i.e. the wavelet coefficients \(W[p](s, \cdot, \cdot)\), and then to the density wavelet coefficients. Indeed, the filtering of the state law results in:

\[
\forall t \in [0, T], \ s > 0, \ \mathbf{u} \in \mathbb{R}^3, \ W[p](s, \mathbf{u}, t) = c^2 W[\rho](s, \mathbf{u}, t).
\]

(12)

Nevertheless, such a solution to the closure issue exhibits two limitations. First, for the microscopic reconstruction to be exact, all wavelet coefficients, for all scales \(s > 0\), are required. The key issue is thus to assess whether or not a limited number of resolved scales can provide a satisfactory approximation of the microscopic field. Second, this need of possibly numerous scales to assess the filtered body force (11) uncover an interdependence between the different scales: when solving the filtered equations for a specific scale \(s_i\), one shall thus need the information related to other scales \(s_j\). This fact will impact the design of the numerical methods for the filtered equations (10).

In academic cases, where the solution can be computed at the microscopic scale, criteria can be introduced in order to make an "optimal" choice between the precision of the reconstruction, and the computation cost. In the following, a mechanical criterion is put forward, based on the force applied by the fluid on the micro-structure:
\[ F_{F \rightarrow S}(t) = \int_{\partial \Omega_s} p(\sigma, t) u(\sigma) \, d\sigma, \] (13)

\[ (F_{F \rightarrow S})_{N_s}(t) = \int_{\partial \Omega_s} p_{N_s}(\sigma, t) u(\sigma) \, d\sigma, \] (14)

where (14) is an approximation obtained by partially reconstructing the microscopic pressure field \( p \) with \( N_s \) scales on the range \([s_1, s_{N_s}]\).

To bring a first light on the CWT ability to recover the microscopic information with a limited number of resolved scales, the above criterion is applied on a 2D numerical case study, where the microscopic pressure field is computed with a validated code.

5 Numerical tests

This case study consists in a 2D transverse pressure wave propagating through a periodic solid medium, composed of 10 × 10 rods, as described in Fig. 3 and Tab. 1:

![Geometry and initial loading: 10 bar (yellow) and 1 bar (blue).](image)

<table>
<thead>
<tr>
<th>X-dimension</th>
<th>Y-dimension</th>
<th>rods radius</th>
<th>Nb. of rods</th>
<th>rods position</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.55 m</td>
<td>0.15 m</td>
<td>5.10^{-3} m</td>
<td>10 × 10</td>
<td>[20.25 cm, 35.25 cm]</td>
</tr>
</tbody>
</table>

Table 1: Dimensions

The fluid barotropic state law and the structure behavior, here assumed homogeneous, isotropic, and linear elastic, are detailed in Tab. 2-3:
Table 2: Fluid parameters

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference density</td>
<td>$\rho_{\text{ref}} = 1000 \text{ kg.m}^{-3}$</td>
</tr>
<tr>
<td>Reference pressure</td>
<td>$p_{\text{ref}} = 10^5 \text{ Pa}$</td>
</tr>
<tr>
<td>Sound velocity</td>
<td>$c = 1300 \text{ m.s}^{-1}$</td>
</tr>
</tbody>
</table>

Table 3: Rods parameters

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young modulus</td>
<td>$E = 210 \text{ GPa}$</td>
</tr>
<tr>
<td>Poisson coefficient</td>
<td>$\nu = 0.3$</td>
</tr>
</tbody>
</table>

The simulation of this case study is conducted with EUROPLEXUS software, a fast-transient dynamics code for fluids and structures. 3-noded triangle finite elements are used for the solid medium, while a cell-centered finite volume scheme is used for the fluid. The time discretization relies on an Euler explicit scheme. The resulting pressure field (Fig. 4) will be the reference for the mechanical criterion.

![Figure 4: Pressure field (Pa) - time = 1.6 $\times$ 10$^{-4}$ s.](image)

Considering the micro-structure geometry and the reference pressure field (Fig. 4), wavelengths around $10^{-3}$ m, $10^{-4}$ m, and smaller (because of the rods boundaries) are expected to convey a significant part of the pressure field information.

The following figure (Fig. 5) shows the evolution of the force ratio (in the horizontal direction) with the number of computed scales $N_s$, and for standard deviations $\sigma \in \{10^{-2}, 10^{-1}, 1\}$. Two scale ranges are considered: $s\sigma \in [10^{-5}, 5.10^{-4}]$ and $s\sigma \in [10^{-5}, 10^{-3}]$. Moreover, the scale discretization $\delta s$ is uniform. As can be expected, it appears that the larger range provides a better precision: the relative error indeed decreases from around 8% to 2%. Moreover, it can be noticed that, beyond the value $N_s = 10$, the number of computed scales does not have a significant impact on the reconstruction. However, a decrease to $N_s = 5$ scales has a visible influence, especially on the range
\( s \sigma \in [10^{-5}, 10^{-3}] \). Finally, a decrease in the standard deviation \( \sigma \) does not impact the reconstruction. This confirms that \( \sigma \) has a very weak impact on the wavelet selectivity.

Thus, the mechanical criterion leads to the conclusion that \( N_s = 10 \) computed scales, on the range \( s \sigma \in [10^{-5}, 10^{-3}] \), allow to recover the force applied on the micro-structure with a relative error of 2%. The corresponding wavelength range is detailed in Tab. 4:

| Wavelength range \( \sigma = 10^{-2} \) and \( s \in [10^{-4}, 10^{-1}] \) | \( \lambda_{min} \approx 2.45 \times 10^{-5} \) m | \( \lambda_{max} \approx 6.55 \times 10^{-3} \) m |

Table 4: Relevant wavelength range with respect to the mechanical criterion.

This range is consistant with the a priori estimation. In order to reduce this range, and especially increase \( \lambda_{min} \), which will drive the mesh size for the filtered equations, one should get rid of the smallest scales in the range \( s \sigma \in [10^{-5}, 10^{-3}] \). However, this would inevitably damage the precision of the reconstruction. For the sake of completeness, the following figure (Fig. 6) displays a zoom on the original and reconstructed pressure fields, with \( \sigma = 10^{-2}, s \in [10^{-3}, 10^{-1}] \) and \( N_s = 10 \) computed scales.

6 Conclusion

A new homogenization formalism, based on continuous wavelet transform, was here promoted, in the context of a fast transient FSI between an inviscid compressible flow and a periodic solid medium. It allowed to robustly derive filtered and homogenized equations, and to connect resolved and unresolved scales without relying on any model. First promising results were highlighted for a 2D transverse pressure wave propagating through \( 10 \times 10 \) rods, where the mexican hat wavelet showed its ability to reconstruct the force applied by the fluid on the micro-structure, with a limited number of computed scales.

In further developments, the focus shall be put on the derivation process of the filtered
equations, and their numerical resolution. Moreover, both the deformation and displacement of the structure shall be taken into account in the local equations.

Finally, in a will to broaden the context of the present article, this multi-scale modeling can be linked to the wide and transverse topics of reduced order modeling and sparse representation of information. This work could indeed be extended to numerous physics and engineering branches, such as multiphase and turbulent flows, porous media, or heterogeneous materials for instance. However, this modeling can only be relevant if the fields of interest exhibit well-localized spectrum. Otherwise, the computation cost required for the resolution of the filtered equations, and the microscopic reconstruction, could be equivalent to direct numerical simulation.

REFERENCES


FSI SIMULATION OF AN AXIALLY MOVING FLEXIBLE CYLINDER ENTRAINED BY A SUPERSONIC FLOW

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Key words: Air jet weaving, Fluid-structure interaction, Supersonic flow, Chimera

Abstract. Air jet weaving looms are widely used to weave fabrics because of the high production speed that can be attained. This is directly linked to the high insertion speed of the yarns. The yarn is accelerated into the reed by a main nozzle and its motion is subsequently supported by underexpanded jets emanating from relay nozzles. The contact with the reed is the only mechanical guidance that the yarn experiences along its path and its motion depends heavily on its interaction with the air flow. The yarn can thus deviate from its envisaged path and cause a failed insertion. Furthermore, the tension in the yarn, induced by the traction of the air and the inertia and resistance of mechanical components, can cause yarn breakage. Failed insertions and broken yarns are undesired as they require the machine to be restarted.

Due to the high speed of the yarn and the mechanical components, optical accessibility to the yarn inside the main nozzle is very limited. Furthermore, the complex geometry experienced by the air flow makes it hard to assess the influence of adaptations. Fluid-structure interaction (FSI) simulations might assist in understanding the behaviour of the air flow and the yarn. However, the flexibility of the yarn in combination with the high speed flow presents its own challenges.

In this research an attempt is made to simulate the launch of a yarn by a single main nozzle into the atmosphere. To better approximate reality, the yarn is considered to be stored on a drum in front of the nozzle. A two-way fluid-structure interaction simulation
is performed using Fluent for the flow side, Abaqus for the structural side and the in-house code Tango for the coupling. Continuum elements or beam elements are used for the structure. The axial motion and large transversal displacement of the yarn pose significant challenges for a single deforming grid in the flow solver. To avoid these complications a Chimera approach, which superimposes several meshes, is opted for.

The FSI simulations show that the yarn can indeed be represented by beam elements. The gain in computational time by switching to beam elements is evaluated and the results from the FSI calculation are compared to experimental results in terms of yarn velocity. Stresses in the yarn are examined to identify high tension regions.

1 INTRODUCTION

A machine used to weave a fabric is called a weaving loom. A general weaving process can basically be broken down into a repetition of 3 actions to insert a weft/pick (along the width of the fabric) in between the warp threads (along the length of the fabric):

1. Shedding: The warp threads are separated into 2 groups, an upper and a lower one. During the shedding phase the upper and lower group interchanged. This locks the previously inserted weft into the cloth and creates a space for the next insertion.

2. Picking: The weft is launched through the space created in the shedding phase.

3. Beating-Up: The inserted weft is pushed against the rest of the cloth by the reed.

Weaving looms are categorized based on their method of insertion. In the earliest weaving looms, a shuttle was used to propel the weft across the loom. Therefore, these machines are referred to as shuttle weaving looms. More modern alternatives are rapier looms (using hooks to transport the yarn) and air or water jet looms.

The simulation performed in this research is related to the field of air jet weaving looms. In such looms the yarn is accelerated by a main nozzle which generates a supersonic flow. Along its path the yarn motion is supported by auxiliary (relay) nozzles. The air flow from those nozzles is channeled by the reed which consists of a series of profiled lamellae that form a half-open tunnel. During its flight the weft is not constrained mechanically (except by possible contact with the reed). If the air flow is not tuned correctly it can cause the yarn to be blown out of the channel. Additionally, a too strong acceleration of the yarn or too abrupt braking can cause damage to the yarn. Both of the previously mentioned phenomena lead to a failed insertion requiring the bad insertion to be removed and the process to be restarted. Especially for air jet weaving looms these stops of the machine are undesirable as their high production speed is one of their key aspects. Figure 1 shows a schematic overview of an air-jet weaving machine with an open-profile reed.
Throughout the years several methods have been employed to analyze the motion of the weft or more generally the behavior of a fiber in air flow. One of the first to perform research into this topic was Uno.\textsuperscript{2} He established an equation of motion for a weft which was assumed to travel along a straight path on the centerline. For the aerodynamic forces he relied on an approximate formula for the centerline velocity decay of a jet and aerodynamic force coefficients. Similar methods were employed by Salama et al.\textsuperscript{3} and Szabó et al.\textsuperscript{4} Salama investigated the use of regular and slotted tubes for insertion, while Szabó focussed on the use of confusor drop wires. In confusor drop wire systems the air channel is formed by a series of circular openings whose circumference is not entirely closed. This allows for a better confinement of the air flow but limits the weaving width and warp density. Adanur and Mohamed\textsuperscript{5} used a similar model to compare the tension experienced by the yarn during launch for several storage systems. Later on, Celik et al.\textsuperscript{6} established a model for air jet weaving looms that also use relay nozzles to support the yarn motion.

Tang and Advani\textsuperscript{7} were among the first to employ computational mechanics on high aspect ratio fibers. They performed simulations for a single fiber and for 2 interacting fibers in a simple shear flow. As the structural motion does not influence the flow field the simulations can be classified as a one-way coupled simulation. De Meulemeester, Githaiga et al.\textsuperscript{8} used computational fluid dynamics (CFD) to calculate the flow field inside a main nozzle. A snapshot of this flow field was used to calculate the force on the yarn (using force coefficients). These forces were then passed to a 1D structural model to analyse the tension in the yarn during braking. A 3D extension of the model was then used by De Meulemeester, Puissant et al.\textsuperscript{9} to numerically simulate the unwinding of a yarn from a drum by a main nozzle. Battochio et al.\textsuperscript{10} similarly used a one-way coupling approach for simulating the motion of a long flexible fiber in a uniform turbulent flow field with an average velocity of 10 m/s. Kondora\textsuperscript{11} employed one-way coupled simulations to obtain

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Figure1.png}
\caption{Schematic overview of an air-jet weaving machine with an open-profile reed (adapted from Szabó and Szabó\textsuperscript{1})}
\end{figure}
the probability distribution function of fiber orientation in the converging channel of a papermachine headbox.

In a one-way coupling the influence of yarn motion on the flow is neglected. In some cases this interaction can have a noticeable effect on the dynamics. To capture these effects, a two-way coupling approach has to be employed resulting in fluid-structure interaction (FSI). Zeng et al.\textsuperscript{12} performed 2D two-way coupled FSI simulations inside the nozzle of an air-jet spinning machine. Similarly, Pei and Yu\textsuperscript{13} simulated the fiber motion in a Murata Vortex Spinning machine. Another 2D two-way FSI simulation was performed by Wu et al.\textsuperscript{14} who investigated the yarn whipping of a weft protruding from the main nozzle in an air-jet weaving loom. Osman, Malengier et al.\textsuperscript{15} used an immersed boundary method to perform FSI simulations for a weft launched by a main nozzle. The flow simulations were performed in a 2D-axisymmetric framework. As a structural solver an extension of the model of De Meulemeester, Puissant et al.\textsuperscript{9} was used. Following this work, Osman, Delcour et al.\textsuperscript{16} used a 3D model to simulate the oscillatory behavior of a yarn, which was clamped at the yarn inlet, inside the main nozzle. The simulation duration was, however, limited due to mesh degradation as a single deforming grid was used. In this research an attempt is made to perform a 3D two-way coupled FSI simulation of a weft, initially stored on a drum, launched into the atmosphere by a main nozzle. A Chimera technique is used to overcome the problem of mesh degradation and to facilitate the incorporation of axial yarn motion. In a Chimera technique several meshes are superimposed and the solution is obtained by interpolation between overlapping meshes. For the case at hand, a fixed background grid is used for the flow domain. On top of that a mesh containing the yarn, referred to as the component mesh, is superimposed. The component mesh moves along with the yarn but is not limited by the boundaries of the flow domain. Consequently, large yarn deformations do not severely degrade the mesh quality.

2 Methodology

2.1 Structural model

Figure 2 displays the structural model. It contains an analytical rigid body representing the main nozzle with a funnel-like attachment to guide the yarn into the nozzle. The flexible yarn itself consists of 65000 C3D8 elements (3D continuum with 8 nodes per element). The yarn is represented as if it were wound on a drum in front of the main nozzle. The drum itself has not been included in the model.
The radial dimensions of the analytical rigid body are 15% smaller than the actual nozzle geometry and contact between the yarn and the nozzle wall is taken into account. This ensures that there is always sufficient space in between the yarn and nozzle wall in the flow solver. The physical properties of the yarn correspond to those of a nylon yarn ($E = 2.5$ GPa, $\nu = 0.3$, linear density $= 464$ g/km, $D = 0.72$ mm). At the start of the winding (left end of Figure 2) the yarn is considered clamped; the right end of the yarn is free. The normal component of the contact between the yarn and the nozzle is modeled as a hard contact using a linear penalty method, which imposes a contact force proportional to the penetration distance. No friction between the nozzle and the yarn is considered so the tangential component of the contact force is set to 0. The time step size is generally the same as the one used in the flow solver. Whipping behavior of the yarn resulting in a high-speed impact between the yarn and the nozzle can, however, destabilize the structural solver. When convergence problems are encountered in the structural solver, its time step is temporarily reduced using subcycling in the structural solver. The structural simulations are performed with Abaqus 6.14.

2.2 Flow model

As mentioned in the introduction a Chimera approach is opted for. This implies that multiple meshes are superimposed in the flow solver. In this case a single background and single component grid are employed. The background grid remains fixed while the component grid deforms along with the yarn. The flow model is entirely 3-dimensional.

Figure 3 displays the background grid and its boundary conditions. This grid consists of approximately 500 000 hexahedral cells. Axial and radial expansion ratios are employed to reduce the total number of cells and as such the required computational time. In the circumferential direction 40, equally spaced, subdivisions are employed. The highest mesh densities are located in the shock region and at the exit of the nozzle.
The component mesh consists of a bent cylinder of diameter 2 mm whose centerline coincides with that of the yarn. The component mesh contains approximately 3.8 million hexahedral cells. A uniform axial and circumferential spacing is applied together with a slight radial bias. Figure 4 shows a simplified representation of the component mesh. At the start of the simulation the points A and B in Figure 4 coincide with the points A and B in Figure 3, respectively. The dashed lines in Figure 4 indicate the left outlet of the background mesh. As can be seen a large part of the component mesh is, thus, located outside of the actual computational domain. During the calculation these cells are disabled. The force on the part of the yarn located outside of the computational domain is calculated under the assumption that the pressure on the surface is uniform and equal to atmospheric pressure, the viscous force on that part is obtained from the law of the wall with a flow velocity of 0 m/s and a wall velocity as obtained from the structural solver.
The component mesh, delimited by the Chimera interface, moves along with the yarn. For the mesh deformation a spring-based smoothing method without damping is used, implying that all edges have an identical spring stiffness. Large rotational motions can introduce some skew into the cells but for the simulation at hand this was observed to be within acceptable limits. The turbulent simulations are performed with the k–ω SST model. A first-order implicit time stepping scheme was employed with a time step size of 5e-06 s. The flow was initialized as a stationary flow. At the inlet a total pressure of 4.7 bar gauge was imposed (to save on computational time the pressure build-up phase was not considered). The value for the total pressure was obtained from experimental measurements. The flow simulations are performed with Fluent 18.2.

2.3 Coupling

The flow and structural solvers are coupled using an in-house code named “Tango” which employs a partitioned approach. The coupling is implicit, using a Gauss-Seidel procedure as this converges quickly for this case. A coupling iteration is considered to be converged when the vector norm for the displacement of all interface nodes relative to the previous iteration becomes smaller than 10^{-6} m.

3 Simulation results

Using the above methodology a simulation was executed over a period of 3350 time steps (for the first 900 time steps a time step size of 1e-05 s was used). This was sufficient for the yarn tip to reach the end of the flow domain (located at 0.5 m downstream of the yarn inlet). Figure 5 shows the centerline position of the yarn at several time instants. The simulation could be continued in time without changes to the model. Forces on the
section of the yarn that exited the domain are then obtained by considering the flow variables in the wall adjacent cells to be frozen at their final value. Alternatively, a mesh section could be appended to the end of the domain or the simulation could be restarted with a longer flow domain.

Figure 5: Centerline position of the yarn at several time instants.

In Figure 6 the x(axial)-, y- and z-coordinates of the yarn tip are plotted as a function of time. The tip displays a smooth axial motion; the dashed line indicates the end of the flow domain. An oscillation can be observed in both the y- and z-directions. Towards the end of the simulation the tip starts drooping off due to gravity (which works in the negative y-direction). From the x-displacement of the yarn tip a tip velocity can be extracted, which could be compared with experiments given a suitable setup. The velocity as obtained from the displacement is plotted in Figure 7. Initially the yarn tip displays a rather linear velocity increase, towards the end of the simulation the velocity starts leveling off at about 16 m/s.
From the structural solver, data about the stresses in the material can be obtained. Figure 8 shows the maximum Von Mises stress in the yarn over time. A maximum stress of 52.3 MPa was recorded. This force can be traced back to an abrupt contact between the yarn and the funnel. Later on the location of the maximum stress value relocates to the jet entrance. A contour plot of the Von Mises stress, extrapolated to the surface nodes, at the end of the simulation is displayed in Figure 9. Due to the extrapolation the values cannot directly be compared to those in Figure 8.
4 Computational time

The largest part of the simulation was performed on the HPC-UGent infrastructure. 42 cores were assigned to the flow solver and 4 to the structural solver. The simulation had an average rate of 75 time steps per day with, on average, 2 coupling iterations per time step. This implies a total simulation time of approximately 40 days. About 70% of the time was consumed by the flow solver and 15% by the structural solver. The remainder of the time is related to the coupling and data transfer.

As the structure has a uniform cross section and a high aspect ratio, it lends itself well to the use of beam elements. This can simplify the structural model and reduce the computational cost. A preliminary test showed that beam elements are indeed suited for the structural model and that the computational time could be reduced by approximately 10% by doing so.
5 Conclusion

In this research a Chimera technique was employed to simulate the launch of a yarn by a main nozzle of an air-jet weaving loom. The Chimera technique allows large yarn deformations and axial motion to be accommodated for without severely degrading the mesh quality. Information about e.g. yarn velocity, tip displacements and stresses can be extracted from the simulation. The simulation, however, has a large computational cost. One possibility of reducing the cost is switching the structural model from continuum elements to beam elements. A gain of 10% in computational time can be attained by doing so.

6 Acknowledgments

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REFERENCES


MODELLING THE EFFECTS OF OSCILLATING STRIPE COOLING DURING A LOCA EVENT IN A VVER440/213 REACTOR PRESSURE VESSEL

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Key words: PWR, PTS, FSI, CFD, LOCA.

Abstract. A Loss of Coolant Accident (LOCA) is initiated by damage in the primary circuit and subsequent coolant leak of a pressurised water reactor (PWR). The loss of coolant is then compensated by the Emergency Core Cooling System (ECCS) [1]. This system supplies the primary circuit with cold high pressure coolant during emergencies. The mixing of this cold coolant results in stripe cooling of the RPV wall. This article focuses on the modelling of the mixing processes of this cooling stripe and their effects on the RPV wall in a VVER440/213 Russian type PWR. The mixing processes are modelled in a transient thermo-hydraulic analysis which models the mixing of the coolant flows in the reactor pressure vessel and results in the overtime temperature and pressure fields within the RPV [2]. The analysis results show that the cooling stripe is not stationary. The turbulent mixing causes an unstable oscillatory motion of the cold stripe which has a notable effect on the RPV wall temperature distribution. Selected results were subsequently transferred into a thermo-mechanical analysis via one way coupling method. This analysis was performed to evaluate the PRV loading state during the LOCA transient. Where the loading stresses were shown to correspond to the oscillatory nature of the cooling strip. In conclusion, an oscillating cooling strip can result in multiple loading cycles [3,4] of the reactor pressure vessel wall during a single LOCA transient or ECCS high pressure coolant injection.

1 INTRODUCTION

The reactor pressure vessel is considered the most reliable component of pressurised water reactors. The target of concurrent research is the extension of operating life of existing power plants and their components. The condition of the reactor pressure vessel (RPV) is a major limiting factor for the operating life of a power plant. The pressure vessel is exposed to thermo-hydraulic transients and the embrittlement effect caused by long time exposure to fast neutron radiation. The coupled impact of these effects increases the risk of structural damage to the pressure vessel during pressure thermal shock (PTS) transients. Thermal shock damage within solid materials represents high risk of structural weakening or in severe cases total structural failure and its elimination represents a significant engineering challenge.
2 PRESSURE THERMAL SHOCK ANALYSIS

Loss of coolant accidents (LOCA) represent highly transient processes within the reactor pressure vessel. The two loading conditions that influence the vessel wall are pressure and temperature, both experience rapid changes during a thermo-hydraulic transient. This makes it necessary to perform a time transient thermo-hydraulic analysis to be able to capture the dynamic loading of the RPV in sufficient quality\[4\]. Given the unstable and non symmetrical nature of the coolant flow, the analysis must also include a model without symmetrical reductions that describes the RPV and the governing coolant flow characteristics within \[5\].

As described above, a transient thermo-hydraulic analysis is necessary to capture the dynamic loading of the RPV during a Small-break LOCA event (SB-LOCA). The transient thermo-hydraulic simulation was set up to calculate coolant flow and mixing in the fluid domain and to calculate heat transfer at the RPV inner wall and the temperature field within its solid domain.

The CFD model represents the fluid domain within the RPV and the solid domain of the RPV itself. Although, the RPV and fluid layers directly in contact with it are modelled in detail, internal structures and components have been significantly simplified. The larger structural components (i.e. reactor shaft, core barrel, reactor bottom etc.) are not directly modelled, only their shape is defined in the fluid domain \[6\].

![Figure 1: Computational model with indexed bodies compared to the detailed Reactor model](image)

The structure of more complex components (i.e. fuel assemblies, perforations of reactor...
shaft and bottom etc.) were modelled as parameters of porous regions. The fully assembled model is shown in figure 1.

3 THERMO-HYDRAULIC ANALYSIS

The transient analysis simulates the initiation of high pressure coolant injection into the primary circuit cold leg. In the beginning of the simulation, the primary circuit is in nominal operational state. Water is pumped through the cold leg into the downcomer region by the main coolant pump. Cold water injection is initiated by pressure decrease at the beginning of the simulation caused by a SB- LOCA.

Specific parameters of the SB-LOCA case:
- initial condition is standard operating state
- equivalent break with a diameter of 20 mm located in Loop 1 (outside of the modelled domains)
- all other Loops are considered undamaged
- single high pressure injection pump active on CL2
- main coolant pumps and reactor shut down at t=0 s
- no coolant phase change (water-steam) during event, no water level decrease in RPV

Boundary conditions were set up based on the specific case parameters and based on data acquired from a system level thermo-hydraulic analysis:
- On undamaged loops (e.g. 2,3,4,5,6) inlet mass flows on CL are equal to the outlet mass flow on HL and are specified based on data from system code simulation (not analyzed in this paper)
- CL1 defined as pressure inlet (provides pressure information and also represents the leak), HL1 set up as mass flow according to data
- Inlet temperatures on all CLs defined based on data
- Decay heat defined from data

The above described analysis was performed using Ansys CFX on a High performance computing (HPC) cluster. The total solution time for a single 1700 s transient equalled 7 days and 14 hours. The final solution contains 270 GBs of data. As such a large database cannot be fully included in this article the following figures represent some of the most relevant result data. As the source data did not include the temperature of the ECC injected coolant, a parametric study had to be performed. Figure 2 shows the different temperature histories for the different ECC injected coolant temperature variants.
Figure 2: Outlet coolant temperature histories on HL2 for different ECC injected coolant temperatures

Variant 60C was chosen as the best fitting one, which represented ECC coolant injected at 60 °C. This variant was then used in all follow up analyses.

Figure 3: Temperature distribution on the RPV inner surface at several time marks
Figure 3 shows the overtime development and change in the temperature distribution of the RPV wall inner surface. Fluid flow and mixing creates a strip cooling effect, the RPV is cooled in a long thin strip under the nozzle. Results show that this strip is also unstable and has a slight oscillation. Sample points located on the inner surface of the RPV at different heights A(below CL2), B(Belt line weld), C (top of Core) and D(middle mark of Core) marked on figure 3 were used to plot the overtime development of the wall temperature.

Figure 4: Temperature development on the RPV inner surface at sample points

Figure 4 shows the over time temperature at the given sample points. These temperatures represent the behaviour of the cooling stripe under the cold leg. The shown temperatures represent the oscillatory nature of the cooling stripe and its effects on the inner surface temperature of the RPV wall. However the cooling is not only superficial. Figure 5 shows the cooling effects on subsurface layers of the RPV wall. The overtime transient temperatures shown in figure 5 represent the temperatures at the given depths under sample points B and C. Where depth 0mm is identical with the sample point and its time transient temperature shown in figure 4 and depth 140mm represents the time transient temperature on the outer surface of the RPV wall (wall thickness is 140mm).

As shown in figure 5, temperatures within the thickness of the wall follow and copy the inner surface temperatures and its oscillations caused by the cooling stripe. Thereby creating time transient temperature gradients in the RPV wall.
4 THERMO-MECHANICAL ANALYSIS

As shown in the previous chapter, coolant mixing during the SB-LOCA event creates highly non-uniform temperature fields within the reactor pressure vessel. Therefore, a structural analysis is required to evaluate the severity of the loading forces within the RPV. As the SB-LOCA transient is characterised by relatively slow pressure and temperature changes compared to the dynamic properties of the RPV, the Structural Analysis can be performed as a static structural problem. The structural model represents the volume and shape of the Reactor Pressure Vessel and utilises the model and element mesh already prepared for the thermo-hydraulic analysis as shown in figure 1 designated as "RPV".

However, the RPV model contains some significant simplifications compared to its real counterpart:

- Reactor Head and Closure Flange modelled as a single part together with the RPV. The model omits the effects of bolt pretension and the friction between their contact surfaces.
- The Austenitic cladding layer is not represented, it was modelled as if made from the same Bulk material. No significant difference between the relevant Material properties to merit the additional computational resources required to model the Austenitic layer.
- Material properties describing the 15Cr2MoV Steel, represent the properties of the bulk material after RPV manufacturing. The material properties do not include the effects of chemical and radiation exposure after long term operation. (These properties were unavailable in sufficient detail)
- The model does not include weld lines or residual stresses from welding.

![Figure 5: Temperature distribution in subsurface layers under sample points B and C](image-url)
• Reaction forces from pipelines are not included in the loading.

The RPV is the only "fixed" component in the primary circuit, other components in the individual coolant loops (i.e. Steam Generators, Main coolant pumps etc.) are all mounted on flexible supports to allow the free thermal expansion of pipelines. Therefore, their reaction forces were considered negligible.

Because the model does not contain the whole primary circuit, only the RPV is represented, multiple boundary conditions have to be applied to correctly support and prevent the rigid movement of the RPV.

![Figure 6: Boundary conditions and imported loads for thermo-mechanical analysis](image)

Boundary conditions are shown in figure 6 where:

A - RPV support pad - Defined as Displacement BC where vertical DOF has been set to zero

B - Outer surface of the RPV support pad - Defined as Elastic Support, implemented to prevent sideways rigid motion, but it allows thermal expansion without significant interference. The elasticity represents the friction of the RPV seating surfaces.

C - Internal surfaces of RPV - Imported Pressure loads from the Transient Thermo hydraulic analysis

D - RPV volume - Imported Temperature Distribution from Transient CFD analysis, CHT solid domain RPV.

The loads were imported for a single time point of the transient CFD results. The static structural analysis is used to calculate the state of the RPV for a given loading time point, imported from the transient CFD results.

The structural analysis was performed for a chosen time point of t=206.947 s. At this time index HPI of cold coolant is already operational and coolant mixing created stripe cooling is at its beginning.

Figure 7 shows the calculated Equivalent Strain for the given loading state at time t=206.947 s, as is evident from these results, the highest stress is located just below the cold leg nozzle. This local stress distribution is shown in a detail view in figure 7.
The highest stress region is located at CL2 with a value of 346.76 MPa. Although, the calculated stress values are relatively high, it is still within the elastic region of the modelled material with a Yield Strength of 395 MPa at 350 °C. However, all surfaces were modelled as perfectly smooth, whereas surface irregularities or cracks could create singularities that would increase stress magnitudes.

5 CONCLUSIONS

As the results show the SB-LOCA event causes strip cooling of the RPV as expected. However, the cooling strip was shown to be unstable and to oscillate over time. This oscillation could result in cyclical loading of the RPV wall and its fractures. Continued investigation into the cause of this instability and into its effects is needed. The analysis has shown that the temperature oscillations are not only superficial but propagate into the thickness of the RPV wall. Relatively high stress values calculated during the static structural analysis present an incentive to perform a fracture mechanics study to determine the loading intensity of possible initialisation fractures in the RPV, which will require a sub-modelling approach to determine localised crack loading.

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REFERENCES


NUMERICAL AND ANALYTICAL INVESTIGATION OF SUBCYCLING IN THE FLOW PROBLEM OF A STRONGLY-COUPLED PARTITIONED FLUID-STRUCTURE INTERACTION SIMULATION

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Abstract. Fluid-structure interaction (FSI) simulations can be used to quantify the frequency, damping constant and amplitude of the vibration of equipment such as piping and heat exchangers. Typically, the time step is the same in the flow and structural equations, but this causes long computational times when the time step is restricted due to stability requirements of only one solver. In that case, a more efficient approach is to use so-called subcycling with a different time step in the flow and structural solver. In this paper, only subcycling with a smaller time step in the flow solver compared to the structural solver is analyzed. The research presented here is split into two parts: an analytical study and a numerical computation of the one-dimensional flow in an elastic cylindrical tube. Firstly, a monolithic analytical FSI calculation is analyzed with a Fourier stability analysis. This allows to verify the stability of the solution by considering the eigenvalues of the problem as a function of the perturbation wavenumber. The conclusions drawn from the analytical study are subsequently verified in a partitioned numerical FSI simulation, coupling the flow solver Fluent with the structural solver Abaqus. The implicit coupling is achieved using an interface quasi-Newton method with an approximation of the inverse of the Jacobian (IQN-ILS), implemented in the in-house code Tango. The research shows that a stable solution is attained for significant subcycling in the flow problem: the results indicate that the solution remains temporally stable even if the time step in the flow solver is only one tenth of the structural time step. However, some (temporally stable) oscillations in the resulting pressure profile on the pipe wall arise when the time discretization schemes applied in the flow and structural solvers are different. These oscillations do not persist when the same time discretization scheme is applied.
1 INTRODUCTION

With the available modern-day computing power, fluid-structure interaction (FSI) simulations are becoming increasingly interesting for the study of movement-induced vibrations, in which a flow causes the motion or deformation of a structure. FSI is also used to determine the fluid-elastic properties of structural vibrations with more limited amplitude, such as to avoid fretting in tube arrays subjected to axial flow [1].

In most FSI cases, the flow and structural solver apply the same time step in transient simulations, even though the maximal time step required for stability or accuracy reasons in the flow solver is in most cases significantly smaller than in the structural solver. Since a coupling iteration happens at least once during every timestep, the required CPU time is large even though the structure barely moves during one time step. A more efficient algorithm requires the definition of a smaller time step for the flow solver and a larger time step for the structural solver. Accordingly, multiple (smaller) time steps are performed in the flow solver before performing a coupling iteration and performing one (larger) time step in the structural solver. This procedure is called subcycling.

Most previous work [2, 3] perform stability analyses on explicit subcycling. In that case, no coupling iterations occur between the flow and structural solver within a single time step. We consider a flow solver and a structural solver, respectively with time steps $\Delta t_F$ and $\Delta t_S$, such that a number $N_{S/F}$ is defined as: $N_{S/F} = \Delta t_S / \Delta t_F$. In this paper, $N_{S/F}$ is defined as a positive integer. The difficulty is to determine how the total fluid-structure interface displacement in a time step $\Delta t_S$ should be interpolated in the $N_{S/F}$ subcycles in the flow solver. Additionally, the question is what interface load should be transmitted to the structural solver at the end of the $N_{S/F}$ subcycles. In the conventional explicit subcycling procedure [3], the interface pressure at the end of the last subcycling step is transmitted to the structure. The disadvantage of this approach is that the time step required to achieve a stable solution is limited and possibly lower than the time step limit imposed by the flow solver itself. In contrast, the stability of the explicit subcycling method is preserved when two conditions are met. Firstly, the predicted displacement over one time step $\Delta t_S$ is evenly distributed among the $N_{S/F}$ subcycles. Secondly, the average interface pressure field computed during the $N_{S/F}$ subcycles is fed to the structural solver.

Contrary to explicit subcycling, little research can be found about implicit subcycling. Probably, this is due to the fact that explicit subcycling is inherently easier to define as all flow and structure variables are only calculated once. As such, explicit coupling is more flexible with respect to the use of different time steps in the solvers [4]. On the other hand, it is well-established that there are FSI problems for which the explicit coupling does not reach convergence, e.g. in high density fluids [5]. In those cases, implicit coupling is required to reach a stable solution, which is why more research into implicit subcycling is needed [6].

In this paper, the temporal stability of an implicit coupling scheme with subcycling in the flow solver is investigated. Firstly, a monolithic analytical study on a one-dimensional
model for flow in an elastic tube is presented. Secondly, a numerical partitioned strongly-coupled FSI simulation is reported. Both methods are described in Section 2. The results of both methods are subsequently compared in Section 3.

2 METHOD

2.1 Analytical monolithic FSI calculation

In order to investigate the temporal stability of the subcycling in the flow solver, the eigenvalues of the matrix relating the variables in consecutive time steps are calculated. A monolithic approach is therefore more straightforward in the analytical study than a partitioned approach, but the result of the study would be the same for a partitioned scheme (as only the temporal stability of the problem is discussed, not the stability of the coupling iterations between flow and structural solver). The fluid-structure interface condition is of the Dirichlet-Neumann type: the displacement of the structure is used as a boundary condition for the flow equations while the fluid pressure is imposed in the structural equations.

2.1.1 Governing equations

The test case is comprised of a one-dimensional flow in a straight, flexible tube shown schematically in Figure 1. The equations that describe the unsteady flow of the incompressible fluid are the continuity and the momentum equation, given by

\[
\frac{\partial s}{\partial t} + \frac{\partial s u}{\partial x} = 0 \quad (1a)
\]

\[
\frac{\partial s u}{\partial t} + \frac{\partial s u^2}{\partial x} + \frac{1}{\rho_f} \left( \frac{\partial s \hat{p}}{\partial x} - \hat{p} \frac{\partial s}{\partial x} \right) = 0 \quad (1b)
\]

in which \(s\) represents the cross sectional area of the tube, \(u\) the axial velocity, \(x\) the axial coordinate, \(t\) the time, \(\rho_f\) the fluid density and \(\hat{p}\) the pressure. In the remainder of this paper, the kinematic pressure \(p = \hat{p}/\rho_f\) will be used. It is noted that gravity and viscous terms are not considered. In the structural subproblem, the radial deformation of the elastic tube is modelled by

\[
\rho_s h \frac{\partial^2 r}{\partial t^2} + \chi \frac{\partial^4 r}{\partial x^4} - \psi \frac{\partial^2 r}{\partial x^2} + \eta (r - r_0) = \rho_f (p - p_0) \quad (1c)
\]

with \(r\) describing the inner radius, \(\rho_s\) the wall density, \(h\) the wall thickness and \(p_0\) the pressure corresponding to the reference radius at rest \(r_0\). Considering the negligence of gravity and viscous terms in the flow equations, the tube deformation in other dimensions (both longitudinal and circumferential) is not considered. As such, the proposed structural model is an extension to the so-called independent-rings model [7], as the terms containing \(\chi\) and \(\psi\) take into account the longitudinal interaction between the tube segments. \(\psi\) is equivalent to \(\kappa G h\) with \(\kappa\) the Timoshenko shear correction factor and \(G\) the shear modulus. \(\eta\) is given by \(E h/(1 - \nu^2) r_0^2\) with \(E\) the Young’s modulus and \(\nu\) the Poisson’s ratio.
2.1.2 Spatial discretization

The tube with length $L$ is discretized in $N$ spatial intervals of equal length $\Delta x$. Central discretization is used for all terms appearing in the flow and structural equations, except for the convective term in the momentum equation. For the latter, a first-order upwind scheme is applied. In the following equations, subscripts $i$ and $i \pm 1/2$ indicate cell centers and faces, respectively.

To allow for analytic manipulation, the velocity, radius and pressure are expressed as the sum of a reference value (indicated with a subscript 0) and a perturbation term (indicated with a prime). Artificial diffusion is added in the continuity equation with coefficient $[8]$:

$$\delta = \frac{s_0}{\pi} / (u_0 + \Delta x / \Delta t).$$

This term is used to stabilize the pressure equation and disappears upon convergence of the solution. After linearization of the equations, the following is obtained:

$$\Delta x \frac{\partial^2 r_i^\prime}{\partial t^2} + r_i^0 (u_i^\prime - u_{i-1}^\prime + u_{i+1/2}^\prime - u_{i-1/2}^\prime) + 2r_i^0 u_0 (r_{i+1/2}^\prime - r_{i-1/2}^\prime) - \delta (p_{i+1}^\prime - 2p_i^\prime + p_{i-1}^\prime) = 0 \quad (2a)$$

$$\Delta x \frac{\partial (r_i^2 u_i^\prime)}{\partial t} + r_i^0 (u_i^\prime - u_{i-1}^\prime + u_{i+1/2}^\prime - u_{i-1/2}^\prime + 2r_i^0 u_0 (r_{i+1/2}^\prime - r_{i-1/2}^\prime) + \frac{1}{2} r_i^0 (p_{i+1}^\prime - p_{i-1}^\prime) = 0 \quad (2b)$$

$$\rho_s h \frac{\partial^2 r_i^\prime}{\partial t^2} + \frac{\chi}{\Delta x^4} (r_{i+2}^\prime - 4r_{i+1}^\prime + 6r_i^\prime - 4r_{i-1}^\prime + r_{i-2}^\prime) - \frac{\psi}{\Delta x^2} (r_{i+1}^\prime - 2r_i^\prime + r_{i-1}^\prime) + \eta (r_i^\prime) = \rho_f (p_i^\prime) \quad (2c)$$

for $u_i \geq 0$. Subsequently, the pressure, radius and velocity perturbation are then decomposed as the sum of $N$ Fourier modes (in the spatial dimension). For example, the radius...
perturbation is defined as:

\[ r'_i = \frac{1}{N} \sum_{l=0}^{N-1} \tilde{r}_l \exp(j\omega_l \Delta x) \] (3)

with \( \omega_l = 2\pi l/L \) the wave number. Equation (3) is substituted into Equation (2). A similar procedure is applied to the velocity and pressure perturbation. Afterwards, Equation (2) is projected on \( \exp(j\omega \Delta x) \), which allows to investigate the temporal stability of each wave component independently. The latter is possible due to the linear nature of Equation (2). In the following equations, the product \( \omega \Delta x \) is substituted by \( \theta \). The tilde and subscripts are omitted.

\[
\begin{align*}
\Delta x \frac{\partial^2 r_0}{\partial t^2} + j r_0^2 \sin(\theta) u + 2 j r_0 u_0 \sin(\theta) r + 2 \delta(1 - \cos(\theta)) p &= 0 \quad (4a) \\
\Delta x \frac{\partial (r_0^2 u + 2 r_0 u_0 r)}{\partial t} + (1 - \exp(-j\theta) + j \sin(\theta)) r_0^2 u_0 u + 2 b \u_0^2 r_0 \sin(\theta) r + b^2 \sin(\theta) p &= 0 \quad (4b) \\
\rho_s \frac{\partial^2 r}{\partial t^2} + \left( \frac{4\chi}{\Delta x^4}(1 - \cos(\theta))^2 + \frac{2\psi}{\Delta x^2}(1 - \cos(\theta)) + \eta \right) r_0 &= \rho_f p \quad (4c)
\end{align*}
\]

2.1.3 Temporal discretization

The backward Euler scheme (BE) is used for the time discretization of the flow equations. Using higher-order schemes would lead to the presence of multiple older time steps in the equations, which was not desirable in the current analytical study. The BE scheme results in the following equation:

\[
\frac{2r_0 \Delta x}{\Delta t_f} (r^{n+1} - r^n) + j r_0^2 \sin(\theta) u^{n+1} + 2 j r_0 u_0 \sin(\theta) r^{n+1} + 2 \delta(1 - \cos(\theta)) p^{n+1} = 0 \quad (5a)
\]

\[
\frac{r_0^2 \Delta x}{\Delta t_f} (u^{n+1} - u^n) + \frac{2r_0 u_0 \Delta x}{\Delta t_f} (r^{n+1} - r^n) + (1 - \exp(-j\theta) + j \sin(\theta)) r_0^2 u_0 u^{n+1} + 2 b \u_0^2 r_0 \sin(\theta) r^{n+1} + b^2 \sin(\theta) p^{n+1} = 0 \quad (5b)
\]

For the temporal discretization of the structure, a logical choice is the use of the BE scheme in order to have the same time discretization in the flow and structural solver. However, the scheme defined by Hilber, Hughes and Taylor (HHT) [9] is more common for structures. Therefore, both discretization schemes will be discussed. The BE scheme for the structure yields:

\[
\rho_s \frac{h r^{n+1}}{h^2} + \left( \frac{4\chi}{\Delta x^4}(1 - \cos(\theta))^2 + \frac{2\psi}{\Delta x^2}(1 - \cos(\theta)) + \eta \right) r^{n+1} = \rho_f p^{n+1} \quad (6a)
\]
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in which the acceleration and velocity are calculated as

\[ \ddot{r}^{n+1} = \frac{1}{\Delta t_s} (\dot{r}^{n+1} - \dot{r}^n) \quad \text{and} \quad r^{n+1} = \frac{1}{\Delta t_s} (r^{n+1} - r^n). \] (6b)

For the HHT scheme, the forces in Equation (4c) are defined as a weighted average of the forces at the beginning and end of the time step, with the variable \( \alpha \) as weighting function. This discretization scheme is also imposed in the structural solver in the partitioned FSI simulation discussed in Section 2.2.

\[ \rho_s h \ddot{r}^{n+1} + (1 + \alpha) \left[ \left( \frac{4\chi}{\Delta x^2} (1 - \cos(\theta))^2 + \frac{2\psi}{\Delta x^2} (1 - \cos(\theta)) + \eta \right) r^{n+1} - \rho_f \dot{p}^{n+1} \right] - \alpha \left[ \left( \frac{4\chi}{\Delta x^2} (1 - \cos(\theta))^2 + \frac{2\psi}{\Delta x^2} (1 - \cos(\theta)) + \eta \right) r^n - \rho_f \dot{p}^n \right] = 0 \] (7a)

The operator definition is completed by the Newmark formula [10] for acceleration and velocity integration:

\[ \ddot{r}^{n+1} = \frac{1}{\beta \Delta t_s^2} (r^{n+1} - r^n) - \frac{1}{\beta \Delta t_s} \dot{r}^n - \left( \frac{1}{2\beta} - 1 \right) \ddot{r}^n \] (7b)

\[ \dot{r}^{n+1} = \dot{r}^n + \Delta t_s (1 - \gamma) \ddot{r}^n + \Delta t_s \gamma \ddot{r}^{n+1} \] (7c)

with \( \alpha \in [-1/3, 0] \) determining the numerical dissipation, \( \beta = (1-\alpha)^2/4 \) and \( \gamma = 1/2 - \alpha \).

2.2 Numerical partitioned FSI simulation

In order to verify the analytical results with a numerical simulation, a black-box flow solver is coupled to a black-box structural solver. As such, the FSI simulation is partitioned.

The flow equations are solved in an Arbitrary Lagrangian-Eulerian (ALE) formulation with the commercial code Fluent® 12.1, Ansys Inc. The fluid grid contains \( 10^4 \) cells and its deformation is computed from the solution of a system of linear springs located in between connected nodes of the mesh. The initial (undeformed) mesh is a structural mesh inside a rectangular domain. A first-order upwind scheme is used for the modelling of the convective terms. The BE scheme is selected for the temporal discretization of the flow equations. The parameters listed in Table 1 are used as numerical values for the flow in a tube. The fluid is considered incompressible and has a constant viscosity of 3 mPas. At the inlet, an axial fluid velocity of \( u_0 + \frac{u_0}{2} \sin(2\pi t)H(t) \) is imposed, where \( H \) represents the Heaviside function. Given an initial velocity field of \( u_0 = 0.1 \) m/s, the inlet velocity has a discontinuity in its derivative at \( t = 0 \) s. At this time, spurious modes can enter the solution. The temporal stability can be evaluated in the subsequent time steps. The pressure at the tube’s outlet is set to the atmospheric pressure.

The structural equations are solved in a Lagrangian frame with the commercial finite-element solver Abaqus® 6.7, Dassault Systèmes. Both the BE and HHT scheme are
applied to the structure equations. A structured grid of 2500 quadratic elements is constructed in the structural domain. Only radial deformation is allowed, similar to the analytical case described in Section 2.1.

The coupling between both solvers at the interface is done through a Dirichlet-Neumann boundary condition. As such, the flow solver computes the pressure and shear stress for a given mesh displacement. These output variables are subsequently transferred to the structural solver, which calculates the new deformation of the fluid-structure interface. The equilibrium at the fluid-structure interface is established using an interface quasi-Newton algorithm with an approximation for the inverse of the Jacobian from a least-squares model (IQN-ILS) [11]. The difference with the classical IQN-ILS algorithm is that more than 1 timestep is calculated in the flow solver before the structural solver is called. In a more mathematical description, the wrapper around the flow solver receives the data for $t^{n+1}$ from the coupling code and gives the flow solver the command to perform $N_{S/F}$ time steps, while providing boundary displacements that are interpolated in time for each of those intermediate time steps. At the beginning of the next coupling iteration, the file from time step $t^n$ is read in from the storage. A time step size $\Delta t_s$ of $10^{-4}$ s is used.

For the coupling iterations, the convergence criterion in the Euclidean norm for the residual of the interface displacement is set to $10^{-8}$ m and for the residual of the interface load to $10^{-2}$ Pa. More severe convergence criteria have no significant impact on the results. Accordingly, the coupling iterations have completely converged. Therefore, this paper does not discuss the stability of the coupling iterations. Rather, this test case is used to determine whether the subcycling procedure is temporally stable or not. Since a monolithic solver with the same convergence criteria would yield the same solution as the applied partitioned solver in the numerical simulation, the numerical and analytical results discussed in Section 3 are directly comparable.

3 RESULTS

3.1 Analytical monolithic FSI calculation

In Equations (5-7), the same time step size was used for the time integration of the flow and the structure. For the analytic study of subcycling in the flow problem, the flow time step $\Delta t_f$ is chosen equal to half of the structural time step $\Delta t_s$ or, equivalently, $N_{S/F} = 2$. Hence, the variable $\Delta t_s = \Delta t$ is called ‘a time step’ and $\Delta t_f = \Delta t/2$ is referred to as ‘a subcycle’.

An important aspect of subcycling is to determine the appropriate interpolation of the displacement of the fluid-structure interface during consecutive subcycles. In order to obtain a continuous acceleration in each node of the interface - which is desirable to obtain a numerically stable solution - a third degree polynomial per point on the interface is used to prescribe the wall displacement during time step $n + 1$. The four parameters in this polynomial are: the wall displacements at the beginning and the end of the time step ($r^n$ and $r^{n+1}$) and the wall accelerations at the beginning and the end of the time...
Table 1: Dimensions of the model and material properties.

<p>| | | |</p>
<table>
<thead>
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<tbody>
<tr>
<td>E</td>
<td>300000 N/m²</td>
<td>ν</td>
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<tr>
<td>χ</td>
<td>0 kg/m²/s²</td>
<td>ψ</td>
</tr>
<tr>
<td>ρ_s</td>
<td>1200 kg/m³</td>
<td>ρ_f</td>
</tr>
<tr>
<td>u_0</td>
<td>0.1 m/s</td>
<td>r_0</td>
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<td>L</td>
<td>0.05 m</td>
<td>h</td>
</tr>
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</table>

step (r^n and r^{n+1}) as calculated by the structural solver. The wall displacement imposed during the first subcycle is then given by:

\[
r^{n+1/2} = r^{n+1} - \frac{3r^{n+1}\Delta t^2}{16} + \frac{r^{n}\Delta t^2}{16}
\]
during the second subcycle.

Two new variables are introduced: u^{n+1/2} and p^{n+1/2}, representing the fluid velocity and the pressure at the intermediate time n + 1/2 between time step n and n + 1.

In case the BE scheme is used in both solvers, Equation (5) for the flow is changed to a corresponding system of equations at times t^{n+1/2} and t^{n+1}, respectively. The structure problem is completely described with Equation (6). Next, these equations are transformed to the following matrix form:

\[
Ay = Bz
\]

with

\[
y = [r^{n+1} r^{n+1} r^{n+1/2} u^{n+1/2} u^{n+1} p^{n+1/2} p^{n+1}]^T
\]

and

\[
z = [r^n r^n r^{n-1/2} u^{n-1/2} u^n p^{n-1/2} p^n]^T
\]

The variables r^{n-1/2}, u^{n-1/2} and p^{n-1/2} do not occur in any equation, but are added to obtain a square amplification matrix A^{-1}B. In case the BE scheme and the HHT scheme are used in the flow and the structural solver, respectively, the structure is instead governed by Equation (7). The flow equations do not change. For a more detailed description of the matrices A and B, the reader is referred to the work of De Moerloose et al. [6].

The parameters shown in Table 1 are used to calculate the eigenvalues of the amplification matrix A^{-1}B. The grid size is set to \Delta x = 10^{-4} m and the time step is chosen equal to \Delta t = 10^{-5} s. The variable α is set to −0.07. For both combinations of time integration schemes, two eigenvalues of the amplification matrix A^{-1}B are equal to one. Their eigenvectors correspond to the solution of the one-dimensional case. Additionally, three eigenvalues equal zero because the matrix B contains three zero-columns, corresponding to the variables r^{n-1/2}, u^{n-1/2} and p^{n-1/2} which do not occur in any equation. The stability of the FSI problem is thus determined by the absolute value of the remaining three eigenvalues.

3.1.1 BE-BE combination

As the variable p^n does not occur in the equations in the BE-BE combination, another eigenvalue is equal to zero, bringing the total to four (due to the absence of the variables
The amplitude of the two remaining eigenvalues is shown in Figure 2a as a function of the wave number \( \omega \). Furthermore, performing a similar analysis on the system of Equations (5-6) without subcycling, yields only one relevant eigenvalue - the other eigenvalues are either equal to zero or one. This eigenvalue determines the temporal stability of the system without subcycling and is therefore also shown in Figure 2a. Even though the amplitude of the eigenvalues comes closer to one when subcycling is used, it remains smaller than one for all wavenumbers. It can be concluded that a stable solution should be obtained.

### 3.1.2 BE-HHT combination

In case the HHT operator is used for the structure combined with the BE scheme for the flow, only three eigenvalues are equal to zero. The amplitude of the three remaining eigenvalues is shown in Figure 2b. Contrary to what was observed in Section 3.1.1, the use of subcycling reduces the amplitude of the eigenvalues of the BE-HHT scheme (compared to the calculation without subcycling). Therefore, the FSI problem also remains stable for all wave numbers.

![Figure 2](image-url)

**Figure 2:** Effect of subcycling in the flow problem on the amplitude of the eigenvalues corresponding to the spurious modes.

### 3.2 Numerical partitioned FSI simulation

The stability of the FSI simulation is investigated for two values of \( N_{S/F} \): \( N_{S/F} = 2 \) and \( N_{S/F} = 10 \). The coupling iterations are drawn schematically for \( N_{S/F} = 2 \) in Figure 3: each coupling iteration contains one time step in the structural solver and two subcycles in the flow solver. A stable solution is obtained for both combinations of time integration schemes for a flow time step size \( \Delta t_f = \Delta t_s/2 \) and a cubic wall displacement throughout.
the subcycles. This is in agreement with the results from the stability analysis shown in Figure 2.

As noted before, the inlet velocity’s derivative has a discontinuity at time 0. Consequently, a pressure oscillation occurs after time 0, which should exhibit a decreasing (or at least constant) amplitude as a function of time in case of a temporally stable solution. Therefore, the temporal evolution of the inlet pressure can be used to denote whether the simulation is stable. Figure 4 depicts the inlet pressure evolution throughout the subcycles during the first 15 time steps for a simulation using 2 (red curve) and 10 subcycles (blue curve), respectively. During the first subcycle of each time step a peak in inlet pressure can be observed. The amplitude of this peak decreases in each consecutive time step, confirming that the solution is temporally stable. Meanwhile, this peak continues to exist for the BE-HHT combination, leading to a discrepancy in pressure compared to the solution obtained with matching time steps. According to the foregoing analysis, the subcycling procedure should yield a temporally stable solution even for the BE-HHT scheme. This is in fact confirmed by the numerical simulation as the pressure oscillation does not grow over time. However, it is clear that the BE-BE scheme yields a more accurate result than the BE-HHT scheme as no pressure peaks are triggered at the beginning of each time step. It can be concluded that applying the same discretization scheme in flow and structural solver is beneficial with respect to the removal of oscillations in the solution. This could not be concluded from the analytical study presented in Section 3.1.

Figure 3: Schematic representation of the coupling iterations in the strongly-coupled FSI problem, in case $N_{S/F} = 2$. The displacement and the pressure of the fluid-structure interface are represented by $r$ and $p$, respectively. The superscript denotes the time step. The transient structure (S) and flow (F) problem are depicted as separate timelines, whereas the full lines indicate the communication between the solvers. The dotted lines show other operations not related to communication between the solvers. The ‘interpolate’ procedure denotes the distribution of the interface displacement over the subcycles.
Figure 4: Effect of subcycling in the flow problem on the evolution of the inlet pressure using (a) the BE-BE combination and (b) the BE-HHT combination.

4 CONCLUSION

The temporal stability of a subcycling procedure in the flow solver is investigated both analytically and numerically. The analytical study of a monolithic FSI calculation is used to quantify the eigenvalues of the matrix relating the flow variables in subsequent time steps. From this, it is concluded that subcycling in the flow solver is temporally stable for all values of $N_{S/F}$, for both the BE-BE and BE-HHT discretization. This conclusion was confirmed with the partitioned numerical FSI simulation, up to $N_{S/F} = 10$. It was furthermore shown that unwanted oscillations can persist in calculations where different temporal discretization schemes are applied to the flow and structural equations, despite the solution being temporally stable.

5 ACKNOWLEDGMENTS

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REFERENCES


PRESSURE-DISPLACEMENT COUPLING IN POROELASTICITY. FURTHER DETAILS OF A STABLE FINITE VOLUME FORMULATION

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Abstract. This paper further explores fundamental issues on the behaviour of a finite volume technique using staggered grids for solving poroelasticity problems. Attention is given to the well-known drawback of pressure instabilities, which arises in certain conditions, as in low permeability media, fast transients and undrained conditions. Finite volume techniques are not the first choice for solving poroelasticity problems, and the reason is cultural, since finite elements have a successful history in solving solid mechanics problems. It has been demonstrated, however, that the finite volume strategies can be successfully applied to poroelasticity problems, with the advantage of offering a single method, stable, and fully conservative for both, fluid mass and forces balance.

1 INTRODUCTION

There is a large amount of literature targeting the solution of this coupled problem using finite element for both physics, investigating deeply the reason for the appearance of pressure instabilities, since it is well known that standard Galerkin produces oscillatory pressure solutions, requiring more sophisticated finite element methods, or other strategies to obtain a stable solution [1,2,3], among others. Locking, equal order of interpolation for pressure and displacement, violation of the LBB condition has been claimed as the reason for those instabilities. Despite the origin of instabilities, stabilization techniques need to be devised in order to obtain a solution, and this is a rich field of research among the finite element practitioners, revealing, in the other hand, that the implementation of such stabilizers many times ended up in more complex and time consuming numerical schemes.

It has been shown that finite volume techniques is a viable route for the solution of the coupled fluid flow and geomechanics [4,5,6,7,8,9,10] since the enforcement, at discrete level, of mass conservation for the fluid, and momentum conservation (forces balance) for the rock, renders to the method physical consistency, and, consequently, stability and robustness.
However, even using finite volume methods, stabilization techniques are still required if pressure and displacement are co-located on the computational grid. Fortunately, since these stabilization techniques are founded on physical grounds, it is straightforward to derive them. This matter will be discussed in a following section, demonstrating that if a fully stable solution is devised, with no need of stabilization techniques at all, the use of staggered grids is the answer. This paper recapitulates the main features of a stable finite volume method for poroelasticity employing staggered grids, pointing out the similarities of the pressure-displacement coupling in poroelasticity with the pressure-velocity coupling in the Navier-Stokes equations. Results are shown for the Terzaghi’s column using non-uniform grids.

2 THE REASON FOR PRESSURE WIGGLES IN FLUID MECHANICS

In order to have a clearly understanding of the issue to be discussed, let’s just point out, by now, that the coupling between pressure and velocity, linking the mass conservations equation with the momentum conservation equations in Navier-Stokes flows, is totally similar to the coupling between pressure and displacement, linking the mass conservation equation with the momentum conservation equations (forces balance) in poroelasticity. Therefore, the remedies for avoiding pressure wiggles in Navier-Stokes flows can be readily extended to poroelasticity problems. The following section briefly discuss the origin of the wiggles in CFD and the remedy already available for more than five decades ago [11].

2.1 Pressure-Velocity Coupling in Navier-Stokes equations

Firstly, it is didactic to have in mind that the coupling we discuss herein is not related with the procedure adopted for solving the linear systems for pressure and displacements, like explicit, iterative or simultaneous (monolithic), but related to the numerical schemes used to create the linear systems, which are dependent on the type of grid used, if co-located or staggered.

Numerical analysts faced the pressure-velocity coupling difficulties in the late 60’s, when the stream function-vorticity formulation was abandoned due to its difficulty in dealing with the boundary conditions of fluid flow problems, and the primitive variables, pressure and velocity, took place. At that time, co-located grids, in which pressure and velocity are calculated at the same point, was the standard approach for any numerical scheme for fluid flow. This arrangement, however, give rise to the well-known checkerboard pressure field, situation in which a spurious decoupled pressure field may appear in the solution, as explained in [12]. There are several concurrent reasons why co-located grid creates the possibility of pressure instabilities.

Consider Figure. 1, in which a 1D grid is shown for the solution of a 1D Navier-Stokes problem using co-located variables, i.e., using the same control volume for mass and momentum conservation. Two main difficulties arise when using this grid layout.
Firstly, the integration of the momentum conservation equation will require pressure values at the interfaces of the control volume, points “e” and “w”. Since pressure variables are not stored on those points, one must count with values located at points “W”, “P” and “E”, resulting for the pressure gradient evaluation for the control volume centred at point P, \( \frac{P_E - P_W}{2\Delta x} \), disappearing the pressure value at the control volume in consideration, point \( P \), and having the pressure gradient evaluated in a coarser grid [12]. Secondly, and the strong reason why decoupled pressure fields and wiggles appear, is because momentum and mass conservation are not satisfied for the same set of velocities. When integrating the mass conservation equation, velocities at the points “e” and “w” are required to construct the approximate equation obeying the mass balance at the control volume centred at P. However, they are not available at those locations, requiring an extrapolation from the nodal values. This extrapolation is a key issue and can be done in several ways, and are, in fact, forms a family of stabilization schemes employed when solving Navier-Stokes equations using co-located variables [13,14,15]. The stability will be attained depending on the fidelity that these interface velocity represents the physics of the phenomena. If, for example, \( u_e \) is taken as a linear interpolation among \( u_P \) and \( u_E \), it will be a very poor approximation, since this averaging will consider that the physics from the point “P” to point “e” is purely diffusive, generating a scheme with pressure instabilities. Therefore, to have good stabilizing schemes, the physics between these two points must be well represented.

2.2 The remedy for the pressure wiggles and instabilities in CFD

As mentioned, Harlow and Welch, in a 1965 paper, solving free surface flows using the MAC (mark and cell) method, advanced the staggered layout of variables, as shown in Figure 2. In this case control volumes for mass and momentum conservation are no longer coincident, eliminating all difficulties, since now pressures are available at the interface of a momentum control volume for a proper evaluation of the pressure gradient, and velocities are available at the interfaces of a mass conservation control volume for mass balance. It should be observed that the important fact now is that the same set of velocities satisfying mass conservation also satisfies momentum conservation. Recalling that when the grid is co-located the specification of a physically consistent velocity at the interface of a mass balance control volume is the basis of a stabilizing scheme, it becomes clear that when the proper unknown
velocity is moved to the interface, this is the best stabilizing scheme, since the physics is represented with the highest possible fidelity. And transferring the node velocity from the center to the interface of a mass control volume is precisely the staggered grid.

Figure 2: Staggered grid for 1D situation

All schemes that find a way of better representing the nodal velocity at the interface form the family of stabilizing schemes, being the scheme that puts the nodal velocity at the interface (staggered grid) the best one. Therefore, there is no better stabilization scheme than using staggered grids. In the following section the mathematical model for the poroelasticity problem is presented, highlighting the similarities among the pressure-velocity coupling in Navier-Stokes equations and the pressure-displacement coupling in poroelasticity.

3 MATHEMATICAL MODEL FOR THE COUPLED PROBLEM

The solution of a poroelasticity problem comprises in solving the rock mechanics (momentum conservation) of the porous structure coupled with the fluid flow (mass conservation) in the porous structure. Terzaghi introduced the principle of effective stress, stating that the mechanical behaviour of the rock depends on its mechanical properties as well as of the pressure caused by the fluid flowing in the porous space. This principle is written as

\[ \nabla \sigma - \alpha \nabla p = b \]  

(1)

in which \( \sigma \) is the effective stress tensor, \( \alpha \) is the Biot coefficient, \( p \) the pressure and \( b \) stands for a possible source term. Recall that this equation, when solved, furnish the porous media displacement caused by loads and the fluid pressure. The porous pressure must be determined using the mass conservation equation, written in a convenient form for our purposes, by

\[ \frac{1}{M} \frac{\partial p}{\partial t} + \nabla \cdot (v^f + \alpha v^s) = q \]  

(2)

with \( \frac{1}{M} \) being the Biot module, \( q \) is a source term, and \( v^f \) and \( v^s \), are, respectively, the
velocity of the fluid (Darcy’s equation) and of the solid, given by

\[ \mathbf{v}^f = -\frac{k}{\mu} \cdot \nabla p \]  

(3)

and

\[ \mathbf{v}^s = \frac{\partial \mathbf{u}}{\partial t} = \frac{\partial \mathbf{e}}{\partial t} \]

Recall that in Section 2, \( \mathbf{u} \) was used for denoting the velocity vector in Navier-Stokes flows. From Section 3 forwarded, it stands for displacement of the porous media.

3.1 Coupling similarities – Navier-Stokes flows and Poroelasticity

One of the challenging aspects in solving the poroelasticity equations is to avoid pressure oscillations which appear under certain conditions resembling undrained consolidation, as in the very beginning of transients and at the interface of two media with large difference in permeability. Finite element practitioners devote a large amount of research efforts in creating stabilizing schemes to avoid those pressure wiggles, normally derived based on mathematical background, lacking, many times, the corresponding physical insight.

The characterization of an undrained consolidation process is when, by some reason, the fluid in the porous space is not flowing, situation in which Eq. (2) can be written as,

\[ \frac{1}{M} \frac{\partial p}{\partial t} + \nabla \cdot \alpha \mathbf{v}^s = q \]  

(5)

which exhibits exactly the same form as the mass conservation equation for Navier-Stokes flows, just replacing \( \mathbf{v}^s \) by the fluid velocity. It is clear, therefore, that the pressure wiggles encountered in solving Navier-Stokes flows are also present when solving poroelasticity problems under undrained conditions. Hence, the remedies are the same ones. If staggered grids are used, the stabilization is intrinsically applied since the displacement is located at the boundaries of the control volume and plays the same role as velocity in Navier-Stokes flows. Displacements in time are, in fact, solid velocity, and it plays the role of fluid velocity, as seen in Eq. (5). If co-located grids are used, finite volume techniques create stabilization schemes based on physical process, as will be described in the following section.

4 NUMERICAL APPROXIMATION

4.1 Staggered grid

In this section it will reported the numerical approximation for a 1D poroelasticity problem, highlighting the details commented previously. The finite volume approach is used, whereby the conservation equation is integrated over each control volume that subdivides the full domain. In the case under analysis the control volume for mass conservation is 1D with interfaces denoted by “w” and “e”, according to Figure 2. Interested readers may find all the
numerical developments using staggered grids for 2D problems in the context of Navier-Stokes equations with hybrid unstructured grids in [16]. Writing Eq. (2) replacing the divergence of the solid velocity by the variation in time of the displacements, and using the Darcy’s equation for the fluid velocity, one has

\[
\left( \frac{1}{M} \right) \frac{\partial p}{\partial t} - \nabla \left( \frac{k}{\mu} \nabla p \right) = q - \alpha \frac{\partial \varepsilon}{\partial t} \tag{6}
\]

Considering the 1D situation in analysis, the integration of the above equation on the grid show in Figure 2, yields,

\[
\frac{\Delta x}{M} \frac{p_e}{\Delta t} - \frac{k}{\mu} \left[ \frac{\partial p}{\partial x_e} \right] - \frac{\partial p}{\partial x_w} + \frac{\alpha}{\Delta t} (u_e - u_w) = q \Delta x + \frac{\Delta x}{M} \frac{p_e^o}{\Delta t} + \frac{\alpha}{\Delta t} (u_e - u_w)^o \tag{7}
\]

Inspecting Eq.(7) against the grid layout of Figure 2, one sees that the displacements are available were they are required for the calculation of the solid velocity, the key issue for stability in undrained conditions. The pressure gradients are calculated by

\[
\frac{\partial p}{\partial x_e} = \frac{(p_e - p_P)}{\Delta x} \tag{8}
\]

\[
\frac{\partial p}{\partial x_w} = \frac{(p_P - p_w)}{\Delta x} \tag{9}
\]

The pressure gradients in the above equations are the responsible for driving the Darcy’s velocity and for unstructured grids a gradient recovery method should be employed. Recall that in all equations reported a constant \(\Delta x\) is used. When non-uniform grids are employed, as in one of the results to be presented, the proper local dimension should be used. Substituting Eqs. (8) and (9) into Eq. (7) one gets the linear system to be solved for the pressure determination.

To complete the integration procedure, the momentum conservation equation, Eq. (1), should be integrated in time and space, using the grid shown in Figure 2. Considering the control volume for displacement centred in “e”, neglecting the source term, the integration gives,

\[
\sigma_E - \sigma_P = \alpha (p_E - p_P) \tag{10}
\]

in which one can see that the driving force for the displacement is correctly stored at the grid, another factor contributing for the stability of the scheme. The expressions for the stress tensor, for a 1D case, are given by
\[ \sigma_E = (\lambda + 2G) \frac{\partial u}{\partial x} \approx (\lambda + 2G) \frac{(u_e - u)}{\Delta x} \]  
\[ \sigma_p = (\lambda + 2G) \frac{\partial u}{\partial x} \approx (\lambda + 2G) \frac{(u_e - u_w)}{\Delta x} \]  

Introducing the above equations into Eq. (10), one gets a linear system for the determination of the u displacement with the fluid pressure present in the equation. Therefore, one has two linear systems, one for pressure and other one for displacement, which can be solved using the strategies already mentioned in this paper. Commenting on these strategies is not in the scope of this paper.

4.2 Co-located grid

Considering now the co-located grid of Figure 1, the control volumes for the integration of the mass and momentum conservation equations are the same. To clarify the difficulties with the mass conservation equation it is repeated,

\[
\frac{\Delta x}{M} \frac{p_e}{\Delta t} - k \left[ \frac{\partial p}{\partial x} \right]_w + \alpha \Delta t (u_e - u_w) = q_p \Delta x + \frac{\Delta x}{M} \frac{p_o}{\Delta t} + \frac{\alpha}{\Delta t} (u_e - u_w) \]

with the marked difference that now the displacements required at points “e” and “w”, the interfaces of the control volume for mass conservation, are not available, requiring, therefore, some stabilization scheme, as discussed in the previous section. In this paper no stabilization schemes are used in conjunction with co-located variables, since the idea is to show the appearance of pressure instabilities.

4.3 Error approximation

The evaluation of the pressure and displacement gradients is made by finite differences with 2nd order errors when the grid is uniform, and somewhere in between 1st and 2nd order when the grid is non-uniform. Therefore, few questions arise concerning the connexion between the order of approximation and stability, as

1) Are pressure and displacements 2nd order accurate?
2) Does pressure and displacement have the same order of accuracy?
3) Will the staggered grid mitigate the numerical instabilities, even in presence of low accuracy?

The following results tries to put some lights over these questions by solving a very simple 1D problem, the Terzaghi’s column using both types of grids.
5 RESULTS

The 1D Terzaghi’s problem is solved using staggered grids with equally and unequally grid sizes. Consider a domain with length $L$ divided into $n$ subdomains with equally spaced grids, $\Delta x = \frac{L}{n}$, resulting in $(n+1)$ grid points. The coordinates for the equally spaced grids are given by

$$x_i = x_1 + (i-1)\Delta x, \quad i = 1\ldots n+1$$  \hspace{1cm} (14)

in which $x_1$ is the coordinate of the first grid point, normally made equal to zero. The coordinate $x_i$ of the grid points in the non-uniform grid is calculated based on the equally spaced grid, by

$$x_i = x_1 + \theta \beta \Delta x, \quad i = 1\ldots n+1$$  \hspace{1cm} (15)

with $\beta$ being a number between 0 and 1, and $\theta$ the random parameter that controls how much distortion the grid will be subjected to. By the way, $\theta = 0$ recovers the equally spaced grid and $\theta = 0.9$ generates a highly non-uniform grid, as can be seen in Figure 3.

![Figure 3: Generation of a non-uniform grid based on equally spaced intervals](image)

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As depicted in Figure 4, the solution domain has its bottom boundary fixed and impermeable and the top boundary is fully-permeable \((p_{\text{top}} = 0 \text{ kPa})\) and subjected to a compressive load of \(\sigma_{\text{top}} = 10 \text{ kPa}\). The structure is initially non-deformed and the initial pore pressure equals to zero. The fluid phase properties are: \(\rho = 998.2 \text{ kg/m}^3\), \(\mu = 1,002 \times 10^{-3} \text{ Pa.s}\) and \(c_f = 1,0 \times 10^{-4} \text{ MPa}^{-1}\). The solid phase properties are: \(G = 1,732 \text{ MPa}\), \(\lambda = 2,597 \text{ MPa}\), \(\phi = 0.3\), \(\alpha = 1.0\) and \(K = 1,0 \times 10^{-4} \text{ m/s}\), where \(K\) represents the hydraulic conductivity.

To begin presenting the results, a validation is done comparing the numerical and analytical solutions, as shown in Figures 5 for highly distorted grid. The results for \(\theta = 0.1\) are not shown for lack of space. As can be seen, the numerical results agree very well with the corresponding analytical ones for highly non-uniform grid.

**Figure 4:** Geometry and boundary conditions for the 1D Terzaghi’s problem

**Figure 5:** Pressure and displacement fields for \(\theta = 0.9\)
Concerning the convergence rate, two sets of grids were used. The first and second sets consider randomly spaced grids with $\theta = 0.1$ and $\theta = 0.9$, respectively. For each set of grids, pressure and displacement profiles are taken at $t = 500$ seconds. These profiles are compared with the analytical solutions and the Euclidean norm ($L_2$-norm) of the error vector is computed. Four different time step sizes are considered: 0.1, 1, 10 and 100 seconds.

The behavior of the pressure and displacement error as the grid is refined is presented in Figure 6 for randomly spaced grids with $\theta = 0.9$. As can be verified, a second order decay of the error is obtained and a 2nd order approximation is clearly obtained for the displacement. For pressure, however, the figure suggests that this variable is somehow affected by the grid distortion, but it can still be regarded as a second order approximation.

Figure 6: Convergence analysis for the grid $\theta = 0.9$. (a) Pressure, and (b) displacement convergence

Figure 7: Analytical, staggered and co-located grid results for $\theta = 0.1$ - 16 nodes
Figures 7 and 8 show results for the Terzaghi’s column using very small time steps in the beginning of the computations creating conditions for the appearance of instabilities. The co-located grid results are, of course, without stabilization schemes, since tests already performed in other works demonstrate that the use of the PIS scheme in conjunction with co-located grids eliminates the pressure wiggles [14,7]. It is well known that non-uniform grids deteriorate the order of the finite difference approximations when the non-uniformity increases, but in this problem, even using highly non-uniform grids, it was demonstrated that the stability is not influenced by the grid non-uniformity.

6 CONCLUSIONS

This paper presented a discussion about the stabilization schemes required for avoiding pressure wiggles and instabilities in poroelasticity problems when the flow conditions resemble an undrained situation. The similarities among the pressure-velocity coupling in Navier-Stokes flows and pressure-displacement coupling in poroelasticity is clearly stated, and it is shown that when co-located grids are used, despite the method used, stabilization schemes are required. It is also pointed out that when the stabilization algorithm is seen under a physical perspective, the quality of the schemes is dependent on the fidelity in which the interface displacement is related to the nodal point displacement. Few results were shown in which it is possible to verify that the use of staggered grids contains intrinsically the best stabilization scheme.

REFERENCE


SOIL-STRUCTURE INTERACTION SIMULATIONS TAKING INTO ACCOUNT THE TRANSIENT PROPAGATION OF SEISMIC WAVES

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Key words: Soil-Structure Interaction, Finite Element Method, Scaled Boundary Finite Element Method, Wave propagation, Earthquake, Time Domain Analysis

Abstract. In this contribution we present a strategy to investigate the vibrations of buildings subjected to a transient seismic excitation, including the soil-structure interaction. The proposed simulation method can be helpful during the design of earthquake-resistant structures in seismic active areas as well as for the design of vibration reduction measures for buildings subjected to surrounding emissions like vibrations induced by traffic or machine foundations. The structures and their foundation as well as parts of the soil are modeled by Finite Element Method (FEM). The far field is idealized as an infinite half-space and modeled with the Scaled Boundary Finite Element Method (SBFEM). Both methods are coupled at the common interface. This approach fulfills exactly the Sommerfeld radiation condition. The seismic excitation is idealized as a plane wave propagating toward the structure with an arbitrary angle with respect to the soil surface. The 3D seismic wave field, caused by the wave passage at the near field boundary, is transformed into boundary tractions, which are then applied at the interface between the near and far fields. We present an application of the proposed method for a group of three buildings, which interact with each other through the soil during the propagation of the transient seismic waves. Although not shown here, the proposed method can handle nonlinear material properties assigned to any element of FEM part.
1 INTRODUCTION

During a seismic event, the excited buildings interact with the soil and with each other through the soil, leading to a complex highly scattered oscillation response. A realistic representation of the seismic soil-structure interaction (SSI) requires a high computational workload, especially when computing the transient nonlinear response of the coupled soil-structures system. The main questions of seismic SSI investigations are: 1) How is the seismic excitation estimated and applied to the SSI system? 2) How is the seismic response of one or more buildings influenced by the interaction with the flexible soil?

The two questions are intrinsically related because the propagation of seismic waves from a source and the response of the near field underneath the structure are both governed by the same mathematical description, the Lamé equations, and therefore cannot be solved independently.

However, the most common approach to answer the two questions is to treat them separately. Indeed, the seismic SSI can be seen as a multiresolution problem: the far-field scale for the simulation of the propagation of seismic waves in the free field and the near-field scale for the simulation of the SSI system. This assumption is at the heart of the Domain Reduction Method (DRM) [21, 7, 5]. In the DRM, the problem is solved in two steps: in a first step, the displacement field of the soil due to a far field source is computed for a specific region at the boundary of the near field; in a second step, equivalent seismic loads are derived from this displacement and applied as input to a small-scale model, which includes the near field and the buildings.

At the far-field scale, the free field motions caused by a seismic event are mainly characterized by a low-frequency content, because short-wavelength waves are dissipated during the propagation towards the structure through large distances. Analytical solutions for the Lamé equations only exist for very idealized soil profiles and, therefore, numerical approaches are preferred. Currently, the most-established method for computing the large-scale three-dimensional 3D far field is the Finite Element Method (FEM) with several extensions such as high order elements [17], spectral elements [6] and discontinuous Galerkin method [8]. These models deliver the seismic input at a certain near field surface (either at the SSI interface or at the near field boundary). Depending on the size of the considered far field, in many cases the maximum considered frequency in the simulation is between 2 and 5 Hz, to keep the element number affordable.

Once the first step is performed, the seismic excitation is applied to the small-scale model for the near field scenario, which couples the buildings with each other through the soil and, at the same time, satisfy the radiation conditions. At the near-field scale, a higher maximum frequency is necessary and, therefore, a much finer mesh is required. One common option for the modelling of the infinite soil in the small-scale model is the FEM extended with transmitting boundaries (TB) [1]. These are special elements at the boundaries of the FEM domain: paraxial boundaries, perfectly-matched layers (FML), infinite elements or scaled boundary finite elements (SBFEM). The FEM can account for
nonlinearities in the structure as well as in the soil near field and can be solved using direct time integration methods such as central difference method or Newmark method. The soil’s far field is assumed to remain linear. An alternative to the transmitting boundaries, the boundary element method [18], the discrete wavenumber method [16] and the integral transform method [3] have been popular for problems with relatively simple geometry and geological conditions. These are based on the fundamental solution of the Lamé equations and can be coupled to the FEM using the substructure approach, but their application is limited to linear cases and homogeneous or horizontally layered soils.

One drawback of the DRM is that the type of earthquake source of the seismic event must be known in detail and this is not always possible. Moreover, two different models (with different scales) need to be generated and run. In this contribution we propose an efficient 3D method for the simulation of the seismic SSI. The substructuring method is used, where the problem is subdivided into two sub-systems (cf. figure 1). The near field, which contains the structure and its foundation as well as parts of the soil, is modeled by FEM. The far field of the infinite half-space is discretized by the SBFEM. Both sub-systems are coupled at the common interface of FEM and SBFEM $\Gamma$ [20].

We assume that the buildings are at great distance from the sources and the wavefront can be considered plane. In this case the seismic excitation is simulated as a transient plane wave that propagates through the far field at a constant speed inclined with a certain angle with respect to the free field surface. The accelerations due to the passing plane wave are computed for the free field (without buildings) at the outer nodes of the near field boundary and are translated into equivalent seismic loads. These loads are used in the full seismic SSI system to transfer the plane wave to the near field. The main assumptions are that the seismic input is not strongly affected by the presence of the buildings and that the seismic input reaches the near field as a plane wave.

2 FEM-SBFEM COUPLING

The FEM-SBFEM coupling is described briefly; more information about the theoretical background and its efficient implementation can be found in Schauer et al. [11, 13]. The
equation of motion is given by

\[
\begin{bmatrix}
M_{\Omega\Omega} & M_{\Omega\Gamma} \\
M_{\Gamma\Omega} & M_{\Gamma\Gamma}
\end{bmatrix}
\ddot{u}
+ \begin{bmatrix}
C_{\Omega\Omega} & C_{\Omega\Gamma} \\
C_{\Gamma\Omega} & C_{\Gamma\Gamma}
\end{bmatrix}
\dot{u}
+ \begin{bmatrix}
K_{\Omega\Omega} & K_{\Omega\Gamma} \\
K_{\Gamma\Omega} & K_{\Gamma\Gamma}
\end{bmatrix} u
= \begin{bmatrix}
p_{\Omega\Omega} \\
p_{\Gamma\Gamma}
\end{bmatrix}
+ \begin{bmatrix}
0 \\
p_b
\end{bmatrix},
\] (1)

which is divided up, so that \(\Omega\Omega\) contains all near field nodes and \(\Gamma\Gamma\) contains all far field nodes. \(\Omega\Gamma\) and \(\Gamma\Omega\) represent the coupling nodes of near field and far field. \(M, C\) and \(K\) represent mass, damping and stiffness matrix and the vectors \(u, \dot{u}\) and \(\ddot{u}\) denote displacement, velocity and acceleration. The vector \(p\) represents the applied nodal forces. \(p_b\) contains the influence of the infinite half-space, which is described by SBFEM. The interacting forces at the interface \(\Gamma\) are given by the vector

\[
p_b(t_n) = \gamma \Delta t M_0^\infty \dot{u}_n + \sum_{j=1}^{n-1} M_{n-j}^\infty (\dot{u}_j - \dot{u}_{j-1}).
\] (2)

Here \(\gamma\) and \(\Delta t\) are parameters introduced by the time integration scheme. The unit acceleration impulse matrices or influence matrices \(M^\infty\) are assumed to be constant within each time step. This matrices are computed in a pre-process applying model reduction techniques to reduce numerical effort [14]. Inserting equation (2) into equation (1) yields a direct and bidirectional coupled FEM-SBFEM formulation

\[
\begin{bmatrix}
M_{\Omega\Omega} & M_{\Omega\Gamma} \\
M_{\Gamma\Omega} & M_{\Gamma\Gamma} + \gamma \Delta t M_0^\infty
\end{bmatrix}
\ddot{u}
+ \begin{bmatrix}
C_{\Omega\Omega} & C_{\Omega\Gamma} \\
C_{\Gamma\Omega} & C_{\Gamma\Gamma}
\end{bmatrix}
\dot{u}
+ \begin{bmatrix}
K_{\Omega\Omega} & K_{\Omega\Gamma} \\
K_{\Gamma\Omega} & K_{\Gamma\Gamma}
\end{bmatrix} u
= \begin{bmatrix}
p_{\Omega\Omega} \\
p_{\Gamma\Gamma} - \sum_{j=1}^{n-1} M_{n-j}^\infty (\dot{u}_j - \dot{u}_{j-1})
\end{bmatrix}.
\] (3)

The damping matrix is a combination of weighted mass matrix and stiffness matrix according to the Rayleigh representation

\[
C = c_m M + c_k K.
\] (4)

The calculation in the time domain is performed by executing the generalized-\(\alpha\) time integration scheme [2].

3 TRANSIENT WAVES

To simulate transient waves through the far field we consider: at first seismic wave propagates through the far field at a constant speed inclined with a certain angle, as shown in figure 2 and secondly the seismic forces as external loads contained in the vector \(p_{\Gamma\Gamma}\) in equation (3). This approach is an efficient approximation to avoid the computation of the interaction forces at the interface \(\Gamma\), which would require the relative quantities in equation (3) in place of \(\dot{u}_j\).
Figure 2: Simplified sketch of propagation of inclined wave fronts as represented in the numerical model [15].

The movement of the particle of the wave front can be governed by an arbitrary time-dependent accelerogram \( a(t) \). When the wave front reaches the near field the nodes at the interface \( \Gamma \) are accelerated at different time steps, depending on the nodes position, e.g. figure 2. For the computation of the boundary tractions, only the outer nodes are considered, so that the wave front is transferred homogeneously to the near field. The nodes which are located in the shadowed areas are not loaded, to avoid inhomogeneous effects due to waves travelling in opposite direction w.r.t the wavefront. The loads are computed by \( \mathbf{p}_{TT} = \mathbf{M} \mathbf{1} a(t) \), where \( \mathbf{M} \) is the mass matrix e.g. equation (1). \( \mathbf{1} \) is a vector that contains ones at the degrees of freedom accelerated by the wave front and \( a(t) \) contains the scalar information of nodal acceleration.

4 APPLICATION

Figure 3 shows the considered near-field as well as three buildings, to which the seismic waves are applied. The seismic wavefront is vertical and it propagates in horizontal direction (its ray is the \( x \)-axis) with constant speed equal to \( c_p \) and the particles move in horizontal direction. The transient wavefront accelerates the outer nodes of the near field boundary at different time steps and the resulting boundary tractions at the interface between near and far field generate a spatially scattered seismic field at the soil surface. Even if the plane wavefront gives an input in \( x \)-direction where all the particles in the vertical plane are in-phase, the resulting ground motions at the surface for the SSI system have non-zero components also in \( z \)- and \( y \)-direction. This is the consequence of both the combination of body and surface waves and the scattering effect of the oscillating buildings (asymmetric w.r.t. the \( x \)-axis) on the free field motions.

The domain of interest is a half sphere with a radius of 100 [m]. The discretization is done by FEM as described before and the finite element mesh consists of 20989 nodes, 18744 elements and so 62967 degrees of freedom. To gain results in a reasonable time, mapping methods are utilized to transfer state variables like velocity, acceleration and forces between FEM and SBFEM discretization. This has the advantage that non-matching
meshes in space can be used and the computational effort is reduced significantly \[16\]. Here, the time discretization is the same in FEM and SBFEM. While the interface (the surface of the FEM domain) has 2370 nodes, 2316 elements and 7116 degrees of freedom the SBFEM domain comes out with only 287 nodes, 229 elements and 861 degrees of freedom.

![Figure 3: Views of the near field with three buildings \[12\].](image)

The buildings in this example are designed as solid blocks and are therefore very much simplified, they serve only for illustrative purposes. The buildings geometric dimensions like width, depth and height as well as the chosen material parameters like Young’s modulus, Poisson ratio and density are summarized in Table 1. The cylindrical opening inside the third building has a radius of 10 [m]. Young’s modulus, Poisson ratio, and density of the soil are \(100 \cdot 10^6\) [Nm\(^{-2}\)], 0.30 [-], and 2200 [kgm\(^{-3}\)], respectively. This leads to a \(p\)-wave velocity \(c_p\) of 247.36 [ms\(^{-1}\)].

**Table 1: Summary of buildings geometric dimensions and material characteristics.**

<table>
<thead>
<tr>
<th></th>
<th>width [m]</th>
<th>depth [m]</th>
<th>height [m]</th>
<th>Young’s modulus [Nm(^{-2})]</th>
<th>Poisson [-]</th>
<th>density [kgm(^{-3})]</th>
</tr>
</thead>
<tbody>
<tr>
<td>building 1</td>
<td>5</td>
<td>5</td>
<td>80</td>
<td>(200 \cdot 10^6)</td>
<td>0.30</td>
<td>1000</td>
</tr>
<tr>
<td>building 2</td>
<td>30</td>
<td>5</td>
<td>60</td>
<td>(10 \cdot 10^6)</td>
<td>0.15</td>
<td>500</td>
</tr>
<tr>
<td>building 3</td>
<td>40</td>
<td>40</td>
<td>40</td>
<td>(10 \cdot 10^6)</td>
<td>0.15</td>
<td>450</td>
</tr>
</tbody>
</table>

In order to set up the damping coefficients of the Rayleigh damping (see equation (4)) a modal analysis is conducted. Therefore the eigenvalue problem

\[
det [M \lambda^2 + K] \mathbf{x} = 0
\]

(5)
is solved to compute the unknown eigenvalues $\lambda$ and the corresponding natural frequencies $\omega$. Some vibration modes are illustrated in table 2. Table 3 lists a specification of the vibration modes for natural frequencies within the range of 0.2 to 3.0 [s$^{-1}$]. Higher natural frequencies are a combination of modes and can not be clearly assigned.

**Table 2:** Illustration of some modes. The mode description is given in table 3.

![Illustration of some modes](image)

**Table 3:** Natural frequencies and corresponding modes within the range of 0.2 to 3.0 [s$^{-1}$].

<table>
<thead>
<tr>
<th>Natural freq. $\omega$ [s$^{-1}$]</th>
<th>Frequency $f$ [Hz]</th>
<th>Period $T$ [s]</th>
<th>Mode</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2468</td>
<td>1.5507</td>
<td>0.6449</td>
<td>building 1 first bending mode x-direction</td>
</tr>
<tr>
<td>0.2469</td>
<td>1.5513</td>
<td>0.6446</td>
<td>building 1 first bending mode y-direction</td>
</tr>
<tr>
<td>0.4134</td>
<td>2.5975</td>
<td>0.3850</td>
<td>building 2 first bending mode x-direction</td>
</tr>
<tr>
<td>1.0300</td>
<td>6.4717</td>
<td>0.1545</td>
<td>building 2 first bending mode y-direction</td>
</tr>
<tr>
<td>1.4680</td>
<td>9.2237</td>
<td>0.1084</td>
<td>building 1 second bending mode x-direction</td>
</tr>
<tr>
<td>1.4684</td>
<td>9.2262</td>
<td>0.1084</td>
<td>building 1 second bending mode y-direction</td>
</tr>
<tr>
<td>1.5321</td>
<td>9.6265</td>
<td>0.1039</td>
<td>building 2 first torsion mode</td>
</tr>
<tr>
<td>1.9282</td>
<td>12.1152</td>
<td>0.0825</td>
<td>building 2 second bending mode x-direction</td>
</tr>
<tr>
<td>2.2632</td>
<td>14.2201</td>
<td>0.0703</td>
<td>building 1 third bending mode x-direction</td>
</tr>
<tr>
<td>2.2701</td>
<td>14.2635</td>
<td>0.0701</td>
<td>building 2 third bending mode x-direction</td>
</tr>
<tr>
<td>2.3763</td>
<td>14.9307</td>
<td>0.0670</td>
<td>building 1 first tension mode</td>
</tr>
<tr>
<td>2.9115</td>
<td>18.2935</td>
<td>0.0547</td>
<td>and higher are combined modes, not clearly assignable</td>
</tr>
</tbody>
</table>

To determine $c_m$ and $c_k$ we chose from building 1 and 2 the natural frequencies of the first bending modes $\omega_1 = 0.2468$ [s$^{-1}$] and $\omega_3 = 0.4134$ [s$^{-1}$]. The damping ratio $\varsigma$ is set to 5% since we assume the buildings to be reinforced concrete structures. This leads to the Rayleigh damping coefficients [9]

$$c_m = \varsigma \frac{2\omega_1 \omega_3}{\omega_1 + \omega_3} = 0.015 \text{ [s]}$$

$$c_k = \varsigma \frac{2}{\omega_1 + \omega_3} = 0.151 \text{ [s$^{-1}$]} \quad .$$

(6)
As described in section 3 seismic loads are considered in $p_{\text{FF}}$. Here the numerical analysis is conducted with a strong earthquake event. Figure 4 shows the acceleration-time-plot of the Kobe, Japan earthquake in 1995. It has a moment magnitude scale of $M_w = 7.2$. The major acceleration takes place within the range 7 to 15 seconds, which means a time slot of 8 seconds.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{acceleration_plot.png}
\caption{Earthquake acceleration Kobe, Japan, 1995.}
\end{figure}

Since the acceleration-time-plot of Kobe earthquake has a duration of 50 [s] and the p-wave needs approximately 1 [s] to run through the domain of interest, 60 [s] of simulation time are conducted. The time step length in both domains FEM and SBFEM is chosen to $\Delta t = 1.0 \cdot 10^{-3}$ [s], so that $60 \cdot 10^3$ time steps are evaluated. The Generalized-$\alpha$ Methods time integration parameter is set to $\rho^\alpha = 0.8$.

To discuss the solution representative nodes are chosen, as shown in table 4a. For each building one node at its foundation as well as one node at its top is observed. For these observed nodes the nodal displacement for each spatial direction is shown in tables 4b-d. In the upper part of the pictures the results at the buildings top and in the lower part the results at the interface between ground and building are presented. The excitation reaches the buildings at different time steps, depending on their position with respect to the propagation direction, which points from the negative to the positive x-axis. First, the seismic load affects node 424, then node 115, and finally node 5789. Thus, the simulation shows a correct sequence of events. Even though the seismic excitation is computed independently from the presence of the buildings, the SSI interaction has an influence on the motion of the ground surface. This can be seen in table 5, which shows the Fourier transformed displacements of the Kobe earthquake as well as the buildings top and base displacements: the displacements at the ground level of the buildings have modified frequency content w.r.t. the input. The FEM-SBFEM coupling allows to simulate the passage of waves through the near field without being reflected at its boundary and therefore fulfilling the radiation condition.
Table 4: Components of the displacement field versus time, at the base and top nodes of the buildings.

a) Observed nodes.

b) Building 1 nodes 424 and 288.

c) Building 2 nodes 115 and 15.

d) Building 3 nodes 5789 and 20512.

5 CONCLUSION

The proposed approach allows to simulate one or more buildings coupled to the underlying soil subjected to 3D plane ground-born seismic wave fronts, including the SSI effects. Such simulations can be used to determine maximum displacements, velocities, accelerations, stress and strains of buildings or other constructions, which can be used
Table 5: Spectra of the displacements in x-direction for the input and the outputs.

a) Input displacements of the wavefront.

b) Output displacements of building 1.

c) Output displacements of building 2.

d) Output displacements of building 3.

for seismic design verifications or for the improvement of the usability/comfort. It is assumed that the buildings are a large distance from the excitation source, where the wavefront becomes plane and the ray has a certain inclination w.r.t. the soil surface. The FEM/SBFEM coupling combined with the approximated methodology for the simulation of transient ground-borne wavefront provides good physical insights into the complex problem with reasonable results, a practical implementation of the input for the seismic excitation and a limited calculation time. For future improvement, the FEM/SBFEM coupling will be used to investigate nonlinear processes in the near field due to strong earthquakes.

REFERENCES


A NOVEL METHOD FOR MAGNETOHYDRODYNAMIC SIMULATIONS AND ITS FIRST APPLICATIONS IN ASTROPHYSICS AND COSMOLOGY ON HIGH PERFORMANCE COMPUTATIONAL SYSTEMS

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Key words: kinetic consistent schemes, high performance computing, galactic winds, intergalactic magnetic fields

Summary Magnetic fields are one of the most important phenomena in science and engineering, as they are present on almost every scale in nature, ranging from atomic magnetic moments to the intergalactic space, and are used in applications ranging from Magnetic Resonance Imaging to nuclear fusion.

In this work we first present a novel powerful method for high performance magnetohydrodynamic (MHD) calculations which is based on kinetic schemes. In particular, using it, it is possible to derive the MHD equations directly from the Boltzmann Equation without the necessity of an ad hoc introduction of terms related to electromagnetic interactions.

With that at hand, we were then able to apply the method to one of the most important problems in present day astrophysics and cosmology, namely to the question of the origin and time evolution of Intergalactic Magnetic Fields. As for their origin, there are mainly two scenarios discussed in the literature – on the one hand the cosmological one, where the magnetic field is produced by some process in the very early Universe, and on the
other hand the cosmological one, where a seed of the magnetic field is created during structure formation and then amplified by some dynamo effect.

Here, we show first results of the aforementioned application of our method – on the one hand, concerning the astrophysical scenario, the simulation of galactic winds, i.e. the ejection of matter from galaxies which might also carry magnetic energy, and on the other hand, for the cosmological scenario, the time evolution of primordial magnetic fields and their possible imprints on the Cosmic Microwave Background (CMB).

1 INTRODUCTION

The interaction of magnetic fields and matter via the Lorentz Force is one of the most fundamental phenomena in physics. If conducting fluids and gases are considered, the corresponding branch of physics is called Magnetohydrodynamics (MHD) and is basically bringing together the equations of fluid dynamics (continuity and momentum equations together with energy conservation) and electromagnetism (Maxwell’s Equations).

The fluid dynamics quantities and equations can be derived from the distribution function \( f \) which is governed by the Boltzmann equation which, without external forces, reads

\[
\frac{\partial f(x, \xi, t)}{\partial t} + \xi \cdot \nabla f(x, \xi, t) = C_f(x, \xi, t),
\]

where \( x \) and \( \xi \) are the position and velocity vector, respectively, and \( C_f \) is the collision integral.

The relevant quantities can be obtained by taking the so-called moments of \( f(x, \xi, t) \), i.e. by calculating the integral

\[
M_i f(x, \xi, t) = \iiint \phi_i(\xi) f(x, \xi, t) d^3\xi,
\]

using the invariants \( \phi_i = (1, \xi, \xi^2/2) \), therefore obtaining

\[
M_1 f(x, \xi, t) = \iiint \phi_1(\xi) f(x, \xi, t) d^3\xi = \iiint f(x, \xi, t) d^3\xi = \frac{\rho}{m},
\]

\[
M_2 f(x, \xi, t) = \iiint \phi_2(\xi) f(x, \xi, t) d^3\xi = \iiint \xi f(x, \xi, t) d^3\xi = \frac{\rho}{m} u,
\]

\[
M_3 f(x, \xi, t) = \iiint \phi_3(\xi) f(x, \xi, t) d^3\xi = \iiint \frac{\xi^2}{2} f(x, \xi, t) d^3\xi = \frac{e}{m},
\]

where \( \rho \) is the mass density, \( m \) is the particle mass, \( u \) is the velocity field and \( e \) is the (total) energy density.

Solving the general form of the Boltzmann Equation, (1), is a rather complicated task which is usually done numerically. However, for the collisionless case, i.e. for \( C_f(x, \xi, t) \),
an analytical solution can be found, given by

\[ f_M(x, \xi, t) = \frac{\rho m^{\frac{3}{2}}}{[2\pi k_B T]^\frac{3}{2}} \exp \left\{ -\frac{m}{2k_B T(x, t)} [\xi - u]^2 \right\}, \]  

(6)

where \( k_B \) is the Boltzmann Constant and \( T \) is the temperature.

On the other hand, the electromagnetic contribution is given by Ohm’s Law,

\[ j = \sigma [E + u \times B], \]  

(7)

where \( \sigma \) is the (local) conductivity and \( j \) is the electric current density, Faraday’s Law,

\[ \frac{\partial B}{\partial t} = -\nabla \times E, \]  

(8)

Ampère’s Law,

\[ \nabla \times B = \mu j + \frac{1}{c^2} \frac{\partial E}{\partial t} \]  

(9)

and the monopole condition of the magnetic field,

\[ \nabla \cdot B = 0. \]  

(10)

As it turns out, combining the fluid and electromagnetic equations in a natural and consistent way is rather difficult. Usually, it is done by an \textit{ad hoc} introduction of electromagnetic terms, resulting in, for example, the Vlasov Equation [1].

In this work we present a novel method for the derivation of the MHD equations in a more consistent way by introducing complex velocities, such that all electromagnetic terms can be derived directly from the Boltzmann equations. We then proceed to develop an algorithm to solve the resulting equations numerically and apply it to problems in astrophysics and cosmology.

In particular we are interested in the physics of Intergalactic Magnetic Fields (IGMF), i.e. the magnetic fields in the voids between galaxies and galaxy clusters [2]. Since it is difficult to measure them, little is known about their origin, evolution and even magnitude, such that a lot of effort has to be put into investigating them.

These difficulties arise due to the scales which are involved. On the one hand, being present on the largest scales of the Universe and being created in each early stages (s. below), while potentially being created on much smaller scales, numerical simulations of the phenomenon are difficult as they have to involve such large range of spacial and temporal scales. There are mainly two ways to solve this problem: Either carrying out (semi)analytical computations [3, 4, 5, 6] which, due to their nature, drastically reduce the computational time, or performing large scale numerical MHD simulations [7, 8, 9, 10] which may not have the full range, but, with the increasing computational power, are getting more and more detailed and feasible for extrapolation.
On the other hand, being thought to have a very small magnitude of nG or below [2], IGMF are difficult to measure experimentally since in any cosmic object (Galaxies, stars, etc.) they are overlaid by this object’s own much stronger magnetic, hence being undetectable. Therefore, one has to measure them inside the voids or to rely on more indirect methods. The former is, for example, done by cosmic (and gamma) ray observation, since they (or their parent particle, respectively) are charged and hence are subject to the Lorentz Force resulting in imprints of the IGMF seen in observations [11, 12, 13, 14]. The latter is done for example by calculating the impact of the IGMF on some cosmological parameters and then comparing this predicted value to measurements, hence being able to set constraints (see [15] and the references therein). However, it should be noted that while several well-established upper limits exist, the lower limits, derived from the first method, are still under debate [2], hence making the zero IGMF hypothesis a conclusion which has not been ruled out yet.

Finally, another important, but still not fully known aspect of IGMF is their origin. Currently there are two scenarios being discussed in the literature: On the one hand the Cosmological Scenario, where the IGMF are created in the very early Universe in a cosmological process such as Inflation [16, 17, 18, 19] or a cosmological phase transition (for example the electroweak [20, 21, 22, 23, 24] or the quantum chromodynamic [25, 26, 27, 28] one). Since it is a cosmological process, strong small-scale magnetic fields are created all over the universe and then decay, thus transporting energy to larger scales, resulting in the present day large-scale IGMF. On the other hand there is the Astrophysical Scenario, where the magnetogenesis is thought to be happening later in time, during structure formation, for example due to protogalactic density perturbation [29], cosmic ray currents [30] or galactic outflows [31].

This work is structured as follows: After explaining the novel method of complex distribution functions which allow it to derive the MHD equation in an elegant way in Sec. 2, we show, in Sec. 3, two of its applications for EGMF, namely the simulation of galactic winds (Sec. 3.1), and some first results for cosmological simulations of EGMF with their implications for CMB observations (Sec. 3.2).

2 A NOVEL METHOD FOR MAGNETOHYDRODYNAMIC SIMULATIONS

2.1 Complex Distribution Function

In this work we propose a new model to derive the MHD equations by introducing a complex-valued distribution function [32, 33, 34] which in the equilibrium case is given by

\[ f_M(x, \xi, t) = \frac{\rho m^2}{[2\pi k_B T]^2} \exp \left\{ -\frac{m}{2k_B T(x, t)} \left[ \xi - \left( u + i v_A \right) \right]^2 \right\} \],

(11)

where \( v_A \) is the Alfven Velocity given by

\[ v_A = \frac{B}{\sqrt{\mu_0 \rho}}, \]

(12)
$\mu$ being the (local) magnetic permeability. As one can see, (11) maintains the general form of the real-valued equilibrium distribution function (6), while at the same time introducing the electromagnetic contributions.

This complex distribution function is an elegant, consistent and natural extension of the classical distribution function. Introducing the magnetic field into the distribution function in the way it is done above is motivated by several aspects. First of all, since magnetic fields cause a circular movement of charged particles due to the Lorentz Force, using complex variables is a natural and well-known way to take that fact into account, by that also considering the axial vector behaviour of the magnetic field \[35\]. Second, it has been proven that the concept of both the distribution function and the Boltzmann Equation remain valid even after the introduction of electromagnetic fields \[36\]. Finally, as can be shown by explicit calculations, the formalism of the section above remains valid if one generalizes Eq. (4) to

\[
\Re M_2 f(x, \xi, t) = \Re \int \int \int \phi_2(\xi) f(x, \xi, t) d^3 \xi = \Re \int \int \int \xi f(x, \xi, t) d^3 \xi = \frac{\rho m}{\mu} u, \tag{13}
\]

\[
\Im M_2 f(x, \xi, t) = \Im \int \int \int \phi_2(\xi) f(x, \xi, t) d^3 \xi = \Im \int \int \int \xi f(x, \xi, t) d^3 \xi = \frac{\rho m}{\mu} v_A, \tag{14}
\]

where the operators $\Re$ and $\Im$ denote the real and imaginary part, respectively.

2.2 Balance Equation

After obtaining the distribution function including the electromagnetic contributions we now proceed to obtain the time evolution equations for the relevant MHD quantities.

This is done, in analogy with the procedure for the pure hydrodynamic case from \[37\], by considering the change of the distribution function (11) over a short period of time $\tau$, which is taken to be the relaxation time, such that after this period of time the distribution function is in equilibrium again. We, hence, are able to carry out a Taylor expansion:

\[
f_M(x, \xi, t + \tau) = \sum_{n=0}^{\infty} \frac{\tau^n}{n!} \frac{\partial^n f_M(x, \xi, t)}{\partial t^n} = \sum_{n=0}^{\infty} \frac{(-1)^n \tau^n}{n!} (\xi \cdot \nabla)^n f_M(x, \xi, t). \tag{15}
\]

Considering only the first three terms on both sides we obtain

\[
f_M(x, \xi, t) + \tau \frac{\partial f_M(x, \xi, t)}{\partial t} + \frac{\tau^2}{2} \frac{\partial^2 f_M(x, \xi, t)}{\partial t^2} = f_M(x, \xi, t) - \tau (\xi \cdot \nabla) f_M(x, \xi, t) + \frac{\tau^2}{2} (\xi \cdot \nabla)^2 f_M(x, \xi, t), \tag{16}
\]

from which the hyperbolic differential time evolution,

\[
\frac{\partial f_M(x, \xi, t)}{\partial t} + \frac{\tau}{2} \frac{\partial^2 f_M(x, \xi, t)}{\partial t^2} + (\xi \cdot \nabla) f_M(x, \xi, t) = \frac{\tau}{2} (\xi \cdot \nabla)^2 f_M(x, \xi, t), \tag{17}
\]
may be derived, while considering only the first two terms on each side results in the parabolic equation

\[
\frac{\partial f_M(x, \xi, t)}{\partial t} + (\xi \cdot \nabla) f_M(x, \xi, t) = 0. \tag{18}
\]

Taking the moments \(M_1, M_2,\) and \(M_3,\) this results in the following system of equations [38, 39, 40]:

\[
\frac{\partial \rho}{\partial t} + \frac{\tau_m \rho}{2} \frac{\partial^2 \rho}{\partial t^2} + \text{div}(\rho (\mathbf{u} - \mathbf{w})) = 0, \tag{19}
\]

\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \frac{\tau_m \rho}{2} \frac{\partial^2 \rho \mathbf{u}}{\partial t^2} + \text{div} \left[ \rho (\mathbf{u} - \mathbf{w}) \times \mathbf{u} + \frac{B_i B_k}{\mu} \right] + \nabla \left( p + \frac{B^2}{2\mu} \right) = \text{div} \mathbf{P}_{NS}, \tag{20}
\]

\[
\frac{\partial E}{\partial t} + \frac{\tau_m E}{2} \frac{\partial^2 E}{\partial t^2} + \text{div} \left( \left( E + p + \frac{B^2}{2\mu} \right) (\mathbf{u} - \mathbf{w}) \right) = \text{div} \mathbf{q} + \text{div} (\mathbf{P}_{NS} \mathbf{u}), \tag{21}
\]

\[
\frac{\partial \mathbf{B}}{\partial t} + \frac{\tau_m \mathbf{B}}{2} \frac{\partial^2 \mathbf{B}}{\partial t^2} = \text{rot} \left[ (\mathbf{u} - \mathbf{w}) \times \mathbf{B} + \nu_m \text{rot} \mathbf{B} \right] \tag{22}
\]

\[
\text{div} \mathbf{B} = 0, \tag{23}
\]

where

\[
w_k = \frac{1}{\rho} \frac{\partial}{\partial x_i} \left[ \left( p + \frac{B^2}{2\mu} \right) \delta_{ik} + \rho u_i u_k - \frac{B_i B_k}{\mu} \right], \tag{24}
\]

\(P_{NS}\) is the viscous stress tensor, \(\mathbf{q}\) is the heat flux vector, \(\nu_m\) is the magnetic viscosity and \(\tau_m\) is defined via the relation

\[
\frac{\tau_m}{2\rho} \left( p + \frac{B^2}{2\mu} \right) = \nu_m. \tag{25}
\]

### 3 APPLICATIONS

In this section we present first results of the application of the method described above to the problem of EGMF.

#### 3.1 Simulating Galactic Winds

The simulations presented here are based on the idea that supernova (SN) explosions inside the galaxy produce enough energy to eject matter and energy from the galaxy. This phenomenon is what is usually known as Galactic Wind. Here we use the same initial conditions as in [41], namely a gas mass density profile given by

\[
\rho(z) = \frac{\Sigma_g}{2z_0 \cosh^2 \left( \frac{z}{z_0} \right)}, \tag{26}
\]

where the \(z\) axis is pointing in the direction perpendicular to the galactic disk, \(\Sigma_g\) is the surface density of the gas in \(z\) direction, and \(z_0\) is a measure for the distribution of mass along the \(z\) axis.
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Figure 1: Simulation of Supernova-driven Galactic Wind after \( t = 5 \) Myr. From left to right: Temperature, gas mass density, velocity along the \( z \) axis and pressure.

The gravitational potential (which we assume to be static for now) is given by

\[
\Phi(z) = \frac{2\pi G \zeta_0 \Sigma_g}{\alpha_g} \ln \cosh \left( \frac{z}{z_0} \right),
\]

where \( \alpha_g = \rho/\rho_{\text{tot}} \), i.e. the ratio of the gas mass density to the total mass density and \( G \) is the Gravitational Constant. With the assumption of initial hydrostatic equilibrium and the proton mass \( m_p \), one gets \( z_0 = \alpha_g k_B T_0 / (\pi m_p G) \), where for the results presented here we have used \( \alpha_g = 0.1 \), \( \Sigma_g = 11.6 M_\odot/pc^2 \) and \( T_0 = 10^4 K \).

The SN formation rate and energy were taken from [42], where they were found to be \( \nu_1 = 1/330 \) yr\(^{-1} \) and \( \nu_2 = 1/44 \) yr\(^{-1} \) for SN Type I and II, respectively, such that for the simulated time of \( t_{\text{sim}} = 5 \) Myr and the simulation box used (256 \( \times \) 256 \( \times \) 1280 nodes for the size 200 pc \( \times \) 200 pc \( \times \) 1000 pc) the expected amount of SN is \( N_{\text{NS}} = 15.9 \) [43, 44].

After some basic astrophysical simulations using the proposed new method have been carried out before [45], here we present the results of the first full-scale simulation of an actual physics problem for which the input parameters used were taken from observations. In Fig. 1 one can see a cross-section of the galaxy after \( t = 5 \) Myr. The results we obtain are in good agreement with previous results and will be used in the future to calculate how much of magnetic field energy is ejected along with the matter outflows.

3.2 Simulating the Time Evolution of Primordial Magnetic Fields and its impact on the Cosmic Microwave Background

Since in this case we want to simulate the Early Universe on the largest scales, the initial conditions are rather simple since we have to consider a isotropic and homogeneous
MHD system in an Expanding Universe. Furthermore, in order to take into account the interaction of the medium with free photons, we introduce a drag term $\propto \alpha v$, where $\alpha$ is antiproportional to the photon mean free path [46]. Finally, the last component is a stochastic magnetic field $\mathbf{B}$.

Since a magnetic fields effectively acts as a pressure term, it causes density perturbations of the medium, which we measure by the so-called clumping factor $b$ defined as

$$b = \left\langle \frac{\delta \rho}{\rho} \right\rangle^2 = \frac{1}{V} \int \frac{\rho(x) - \langle \rho \rangle}{\langle \rho \rangle} \, dV$$

(28)

As it turns out, from the size of the density perturbations, which are imprinted on the Cosmic Microwave background (CMB), one can deduce upper limits on the magnitude of the magnetic fields [47]. With the results from our simulations, presented in Fig. 2, we therefore were able to derive upper limits on the EGMF in the order of picogauss, which is better than most of the previous constraints by several orders of magnitude.

4 CONCLUSIONS AND OUTLOOK

In this paper we have presented a novel method for the derivation of the MHD equations directly from the distribution function by introducing complex velocities. We then applied it to two important problems in the physics of EGMF, namely galactic outflows and the imprints of the time evolution of EGMF on the CMB.

Figure 2: Dependence of the maximal clumping factor $b$ on the ratio between the Alfven velocity $c_A$ and the sound of speed $c_s$. 
In the future we will explicitly include magnetic fields in the galactic wind simulations and compare them to our present estimates of the outflow of magnetic energy from the galaxy. This, in turn, can then be used to investigate the astrophysical scenario of EGMF magnetogenesis.

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REFERENCES


HIGHLY PARALLEL MULTI-PHYSICS SIMULATION OF MUSCULAR ACTIVATION AND EMG

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Abstract. Simulation of skeletal muscle activation can help to interpret electromyo-
graphic measurements and infer the behavior of the muscle fibers. Existing models con-
sider simplified geometries or a low number of muscle fibers to reduce the computation
time. We demonstrate how to simulate a finely-resolved model of biceps brachii with a
typical number of 270,000 fibers. We have used domain decomposition to run simulations
on 27,000 cores of the supercomputer HazelHen at HLRS in Stuttgart, Germany. We
present details on opendihu, our software framework. Its configurability, efficient data
structures and modular software architecture target usability, performance and extensi-
ibility for future models. We present good parallel weak scaling of the simulations.

1 INTRODUCTION

The neuro-muscular system allows humans to perform a wide range of tasks. A skeletal
muscle, with its adaptable neural recruitment process and numerous muscle fibers can
perform fine, coordinated movements such as gripping a small needle, powerful actions
such as lifting weights, and enduring, repetitive actions such as running a marathon.

Due to the difficulty of observing internal activities in in-vivo experiments, simulation
plays an important role in understanding the neuro-muscular system. What can indeed
be measured on a live subject is the electric potential over time. This process, known
as electromyography (EMG), can be performed either on the surface or intramuscularly
via needle electrodes. Although signal-processing techniques can help us understand the
functioning of the neuromuscular system [1], weak signals, shifting of electrodes during
movement, and muscle fiber cross-talk [2] make it difficult to identify precisely which muscle fibers have been activated. Simulating the muscle activation process can thus help improve post-processing techniques for interpreting high-density EMG measurements and provide insights into those processes not detectable via measurements.

Both analytical and numerical models exist to perform in-silico experiments regarding the electromyography of a skeletal muscle. Analytical models provide closed formulas for the resulting signal [3] and are typically limited to simplified geometries (e.g. cylinders) and homogeneous material properties. For example, the authors in [4] derive a formulation for a single fiber and a plate electrode. A finite-element-based numerical model that also includes bone, fat and skin tissue is presented by [5]. Here, however, the domain is cylindrical and only a single action potential is simulated. In [6] the authors consider an axis-symmetric muscle geometry and simulate prescribed fiber shortening by adjusting the diffusion tensor. The electric conduction through the tissue volume is discretized with 100,000 finite elements using a commercial solver. However, this work does not account for the actual muscle geometry and for the activation of fibers organized into motor units.

The authors of [7] describe a framework to model biophysically motivated muscle activation and contraction and the resulting EMG. They study 390 fibers in a cuboid geometry. They also illustrate a realistic geometry by simulating the tibialis anterior muscle with 2700 fibers. However, the latter simulation is presented only for a short time span with little contraction. They report long computation and file I/O times using the open-source software OpenCMISS. In our previous work [8] we parallelized the OpenCMISS code to run on up to 768 cores. We detected issues with the memory consumption, which prevented further parallel scaling.

In this work, we present the computational framework opendihu to perform parallel simulations of the neuro-muscular system. We implement a highly-resolved, physically based, multi-scale model of muscular activation and intramuscular EMG. Our approach uses the same models for the action potential and predicting the intramuscular EMG as in [7]. However, we do not include the model for tissue contraction. We use the real geometry of the musculus biceps brachii and simulate 273,529 muscle fibers, which is a typical number for the biceps brachii [9]. The overall problem contains 1.6 billion degrees of freedom for the activation model and 37 million for the computation of the EMG. Our code executes on 27,744 cores of the supercomputer HazelHen in Stuttgart and allows simulations with runtimes in the range of several hours.

In section 2 we describe the model used in our simulation. We motivate the design goals of our software framework opendihu and describe the software components in section 3. In section 4 we perform weak scaling studies that are evaluated in section 5.

2 MODEL

A skeletal muscle comprises numerous muscle fibers. These fibers are innervated by axons of the nervous system at the innervation zone, which is located at the center of the fibers. Motor neurons in the spinal cord generate stimuli that lead to electric action
potentials on the muscle fibers. Upon activation of a fiber, the action potential travels from the innervation zone to both ends of the fiber.

All muscle fibers that are connected to the same motor neuron are excited simultaneously and form a motor unit (MU). In our simulations, we assumed 100 MUs. The number of fibers per MU was distributed exponentially. We employed a recruitment model that activated smaller MUs more frequently than larger MUs, as in [7].

In the following, we describe the model of action potential propagation and contribution to intramuscular EMG signals.

### 2.1 The model of activation and electromyography

Our simulation is based on the framework described in [7], which is briefly summarized here. The multi-scale model is comprised of the following three ordinary and partial differential equations, solved on 0D, 1D and 3D domains, respectively:

\[
\frac{\partial y}{\partial t} = f(y, V_m), \tag{1}
\]

\[
\frac{\partial V_m}{\partial t} = \frac{1}{A_mC_m} \left( \sigma_{\text{eff}} \frac{\partial^2 V_m}{\partial x^2} - A_m I_{\text{ion}}(y, V_m) \right) \quad \text{in } \Gamma_t, \tag{2}
\]

\[
\text{div} \left( (\sigma_e + \sigma_i) \text{grad} (\phi_e) \right) + \text{div} \left( \sigma_i \text{grad} (V_m) \right) = 0 \quad \text{in } \Omega_t, \tag{3}
\]

where \( y \) and \( V_m \) are the vector of subcellular states and transmembrane potential, respectively. \( A_m \) is the fibers’ surface to volume ratio. \( C_m \) is the capacitance of the membrane and \( \sigma_{\text{eff}} \) is the effective conductivity of the muscle fibers. \( I_{\text{ion}} \) describes the ionic current passing across the membrane. The conductivity tensors in the extra and intracellular domains of the bidomain model are represented as \( \sigma_e \) and \( \sigma_i \) and the extracellular potential is \( \phi_e \).

The first equation, eq. (1), describes subcellular processes and is a system of ordinary differential equations (ODEs) with state vector \( y \). We use the Hodgkin-Huxley model [10], which contains 4 state variables. In the following, we refer to it as the 0D model.

The second equation, eq. (2), is the 1D monodomain equation. We model each muscle fiber as a 1D domain \( \Gamma_t \) embedded in the 3D muscle domain \( \Omega_t \). We solve the monodomain equation, eq. (2), for each of these 1D domains. The connection to the 0D model is made through the states \( y \), which are computed at equidistant points on the 1D domains by solving the system of ODEs, eq. (1).

The third equation of the model is the bidomain equation, eq. (3), which provides the extracellular potential, \( \phi_e \), in the 3D muscle domain, \( \Omega_t \). This is in fact the electric signal that could be measured by the intra-muscular electromyography. The required transmembrane potential, \( V_m \), in the 3D domain is projected from the values of \( V_m \) in the embedded 1D domains using a trilinear interpolation.
2.2 Discretization and solution

We solve the coupled 0D and 1D equations of the model, eqs. (1) and (2), with the Strang operator splitting approach [11]. The time derivatives are discretized using finite differences. We integrate the 1D reaction-diffusion equation by the Crank-Nicolson scheme and the 0D equations with Heun’s method. Thus, the splitting scheme would be second order consistent.

For the spatial discretization of eq. (2), we use the Finite Element Method with linear 1D elements and solve eq. (1) at each node. We solve the 3D part, eq. (3), with the Finite Element Method using 3D linear hexahedron elements. The 3D and 1D discretizations share some nodes, such that the 1D fiber meshes are aligned with the edges of the nearby 3D elements, which they pass through. The 3D elements have a coarser discretization than the 1D elements. A visualization of the meshes is given in fig. 1a.

For the 3D model, eq. (3), the intra and extra-cellular conductivity tensors, $\sigma_i$ and $\sigma_e$, are chosen such that the conductivity is 10 times higher in the direction of fibers than in the transverse direction. We estimate the fibers’ directions by considering streamlines of a potential flow, which we solve inside the muscle geometry, a valid approach approved by the literature [12, 13]. The potential flow problem is described by a Laplace equation for the pressure with Dirichlet boundary conditions of 0 and respectively 1 at the longitudinal ends of the muscle.

This auxiliary potential flow problem above, the 1D monodomain and 3D bidomain equations involve solution of linear systems of equations. Only the Crank-Nicolson scheme of the 1D equation yields a symmetric positive definite system matrix, for which we use a conjugate-gradient solver. For the solution of the other two system of equations, we employ a GMRES solver.

3 SOFTWARE

We implement a solver for the described model within our novel software framework, named opendihu. This framework provides functionality to solve static and dynamic multi-physics problems, spatially discretized in 1D, 2D and 3D by the finite element method. Our core design goals of the framework are usability, performance and extensibility. In the following section, we describe how these goals are realized in our framework.

3.1 Design goals

The first design goal is usability. From the user’s perspective, running and examining a simulated scenario is possible without altering the technical C++ implementation. Changing the geometry, tuning discretization parameters or evaluating different model parameters can be done in a python script, which will be parsed by the simulation program at runtime.

The second design goal is performance. Parallel execution reduces runtime by distributing the computational workload to multiple CPUs. Vectorization allows to calculate
multiple values at once with single instructions. The internal data representations enable these paradigms and avoid time-consuming data copy. The framework runs efficiently on supercomputers as well as normal workstations with a smaller numbers of CPUs.

The third design goal is extensibility, which allows to create solvers for new models. The object-oriented architecture allows to combine existing components to new solvers and to implement new ones. A testing infrastructure ensures that existing functionality is preserved.

3.2 Software components

Opendihu is an open-source software framework\(^1\). To remain lightweight, it is closely built upon established open-source projects. The parallel message passing interface (MPI) is used to enable distributed memory parallelism. Linear algebra and solvers are provided by OpenBLAS\(^2\) and PETSc\(^3\). A Python interpreter with Numpy and Scipy is included for the configuration interface.

Installation on different linux systems, supercomputers as well as workstations, is managed by a SCons\(^4\) based build system. Supported compilers are GNU, Intel and Cray. Compliance to the C++14 standard is enforced by compiler flags that disallow warnings and add pedantic errors, which ensure high code quality.

The code comprises four parts: data representation, finite element method related functionality, solvers, and I/O functions.

**Data representation.** Native parallel PETSc data structures of vectors and sparse matrices are used. Vector fields have the “Struct of Array” layout, where each component is stored consecutively in the memory. This allows cache-efficient data accesses and enables instruction-level parallelism.

**Finite Element discretization.** As the base for the Finite Element Method, opendihu implements assembly of the stiffness and mass matrices for the generalized Laplace operator. Quadratures for 1D, 2D and 3D domains are performed using Gauss, Newton-Cotes and Clenshaw-Curtis schemes. Ansatz functions can be chosen as linear and quadratic Lagrange and cubic Hermite functions.

We have implemented three mesh types: (i) the general, unstructured mesh with arbitrary topology, (ii) the structured mesh, whose elements can be efficiently iterated over by nested for loops and (iii) the regular mesh with a fixed mesh width in all dimensions, for which the system matrix assembly uses time-efficient, pre-computed stencils.

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\(^1\)https://github.com/maierbn/opendihu, release 1.0 is used for the studies in this paper
\(^2\)https://www.openblas.net
\(^3\)https://www.mcs.anl.gov/petsc/
\(^4\)https://scons.org/
Data can be mapped linearly between arbitrary meshes that occupy the same physical space, e.g. between one-dimensional muscle fibers and a 3D continuum representation of the tissue.

**Solvers.** Solvers and time stepping schemes are implemented as C++ class templates. Multiple schemes can be nested at compile-time to create multi-physics solution schemes. Examples of implemented schemes are the forward and backward Euler integration, Heun’s method, Crank-Nicolson scheme, and Godunov and Strang operator splittings.

The main C++ program of every simulation consists of the definition of a compound class of such nested solvers and a "run" command. This allows users to get a quick overview over how the model is solved, by inspecting the minimalist main source file.

**Input and output.** Inputs to the simulation program include the configuration, geometry data and subcellular model. The configuration is done in a python script, where all parameters can be computed and specified. The script is initially parsed by the simulation program. During the time stepping, callback functions allow to alter parameters and boundary conditions, which we use for stimulating the MUs at prescribed physical times. The geometry data can be either specified in this script or provided as a binary file, which is then loaded in parallel using the distributed MPI read functions. This is needed to input large amounts of data in highly parallel runs.

The subcellular model, eq. (1), is loaded from a CellML file, a standard description for biomechanical ODE models. **OpenDihu** implements a novel source-to-source compiler, which combines the code for multiple instances of such models and, by enabling vectorization, reduces the solution time.

Output of simulation results can be written in various formats. A binary, python-pickle-based format and the ASCII-based Exfile format are used for small amounts of data, to be postprocessed with the **OpenDihu** matplotlib scripts and the OpenCMISS-Zinc based utility, respectively. For large amounts of data, **OpenDihu** implements MPI-parallel output to binary VTK files to be viewed with ParaView or can use the adaptable IO System 2 (ADIOS2) for parallel output in a binary-packed format.

### 3.3 Parallelization and solver structure

In our muscle simulations, we use structured grids for the spatial discretization. A structured grid is divided by planar cuts into subdomains for multiple processes, as depicted in fig. 1a. Thus, each subdomain contains parts of multiple fibers, where each fiber is handled by multiple processes.

The parallel solver structure is depicted in fig. 1b. The innermost solvers are the Heun scheme operating on the 0D model, eq. (1) using the CellML description, and the Crank-Nicolson scheme for solving the diffusion equation, eq. (2), for which the spatial operator is discretized by the finite element method. These schemes are wrapped in
MultipleInstances classes, which subsequently call them for all fibers in the subdomain. Thus, all processes that participate in the computation of fibers can solve the diffusion equation in parallel. Figure 1b at the bottom right visualizes the used data in this step. The Strang splitting scheme uses these two solution schemes to solve the propagation of the action potential in a set of fibers that share processes. The surrounding MultipleInstances class calls the splitting scheme subsequently for all of these sets of fibers, as visualized at the top right of fig. 1b. Finally, the solver for the 3D bidomain equation, eq. (3), is called after a specified time span by the top-level Coupling class.

4 RESULTS

To examine the efficiency of our software framework, we compare runtimes with the simulation of the tibialis anterior muscle in [7]. It consists of 2700 fibers, each comprising 50 instances of the Shorten subcellular model [14]. We replicate the discretization but only consider a cuboid geometry, since this does not influence the runtime. Moreover, we only solve the electrophysiology without the model for contraction, which in [7] was discretized using only 12 3D elements. We run our simulation using a single processor on a computer with an Intel(R) Xeon(R) CPU E7-8880 v3, which features the same microarchitecture (Ivy Bridge) but a lower frequency (2.3 GHz instead of 3.2 GHz) compared to the hardware used in [7]. Whereas the authors in [7] reported 3h runtime to solve for 0.2 ms, opendihu computes the same time span in 4 min 40 s overall runtime, including file output, which is
a reduction by a factor of 38. On a modern laptop with an Intel Core i5-6300U CPU and frequency of 2.4 GHz the runtime using a single processor reduces to 80 s.

4.1 Weak scaling

In the following, we present studies of parallel scalability. Our scenario is the action-potential propagation in the biceps brachii muscle. The geometry is extracted from the Visible Human Male of the Visible Human Project [15]. The model is described in section 2. The stimulation times and material parameters are the same as in [7].

We compile our program with the Cray compiler and execute it on the supercomputer HazelHen in Stuttgart, Germany. This is a Cray XC40 computer with a total of 7712 compute nodes, each with 2 Intel Haswell E5-2680v3 CPUs at 2.5 GHz and 24 cores per node. Figure 2 shows the simulation results using 4489 fibers at time $t = 100$ ms.

The weak scaling studies are depicted in fig. 3a. The runtimes are measured while increasing the size of problem and number of processes at the same time as listed in table 1. The size of problem is increased by increasing the number of muscle fibers. Each fiber is discretized by 1479 1D elements, leading to an element length of approximately 100 $\mu$m. The number of 3D elements is coupled to the number of fibers. In the $x$ and $y$ spatial directions, there are $3 \times 3$ fibers going through each of the 3D elements and in the $z$ direction (direction of the fibers) there are 3 1D elements per each 3D element.

The time steps are 1.5 $\mu$s for Heun’s method, 1 $\mu$s for the Crank-Nicolson scheme and 3 $\mu$s for the Strang splitting. The 3D bidomain equation is solved with 10,000 iterations of the GMRES solver in the interval of 1 ms. The simulation time for the weak scaling study is also 1 ms, which corresponds to one time step of the outermost loop.

We choose the number of fibers such that there are approximately 10 fibers per process for every measurement. We start from 4 processors and increase the number of processors up to the last data point of 27,744 processes for 273,529 fibers.

The parallel partitioning is performed based on the following two conditions. First, the number of subdomains in the fiber direction has to be a factor of 24, which is the number of cores per each compute node. Second, the number of subdivisions in the three
coordinate directions should be similar. The first condition ensures that each fiber is computed on only one computational node, the second condition reduces the surface between neighboring subdomains and thus minimizes the communication in the solution of the 3D model.

The weak scaling shows a perfect behavior for the 0D model, as can be seen from the yellow curve in fig. 3a. This is expected, since all instances of the 0D model are independent of each other. The runtimes for solution of the 1D model, shown by the red curve in fig. 3a, is only dependent on the numbers of processes per fiber, which are given in the first column of table 1. The runtime increases slightly for higher process counts. This is also expected, as the solution of the 1D model requires communication of all processes of the respective fiber.

The duration of the 3D problem increases, because all processes are involved in the solution using the GMRES solver, although the processes’ subdomains are constructed as cuboids in order to make the communication surfaces as small as possible. This supports a fast solution of the 3D solver, because of the small amount of communication required between the processes. On the other hand, this partitioning increases the runtime for the 1D solver, as the elements of the 1D domains are distributed to multiple processes. However, this is acceptable, because the 3D solver takes a longer runtime.

The runtime for initialization, which includes e.g. parallel reading of the geometry files, assembly of the stiffness matrices and compilation of the CellML code, is the largest portion of the overall runtime. This is because the study only considers the runtimes for one (the first) timestep. For an enough long simulation time, the portion of initialization
Table 1: Parameters of the weak scaling study

<table>
<thead>
<tr>
<th>partitioning</th>
<th>fibers</th>
<th>fibers per process</th>
<th>total degrees of freedom</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2 \times 2 \times 1 = 4$</td>
<td>49</td>
<td>12.3</td>
<td>297,984</td>
</tr>
<tr>
<td>$3 \times 3 \times 2 = 18$</td>
<td>169</td>
<td>9.4</td>
<td>1,032,160</td>
</tr>
<tr>
<td>$4 \times 4 \times 4 = 64$</td>
<td>625</td>
<td>9.8</td>
<td>3,797,216</td>
</tr>
<tr>
<td>$5 \times 5 \times 6 = 150$</td>
<td>1369</td>
<td>9.1</td>
<td>8,303,280</td>
</tr>
<tr>
<td>$7 \times 8 \times 8 = 448$</td>
<td>4489</td>
<td>10.0</td>
<td>27,201,100</td>
</tr>
<tr>
<td>$10 \times 10 \times 12 = 1200$</td>
<td>11,881</td>
<td>9.9</td>
<td>72,124,720</td>
</tr>
<tr>
<td>$17 \times 17 \times 12 = 3468$</td>
<td>34,969</td>
<td>10.1</td>
<td>212,187,268</td>
</tr>
<tr>
<td>$18 \times 18 \times 24 = 7776$</td>
<td>76,729</td>
<td>9.9</td>
<td>464,686,624</td>
</tr>
<tr>
<td>$27 \times 27 \times 24 = 17,496$</td>
<td>182,329</td>
<td>10.4</td>
<td>1,102,902,304</td>
</tr>
<tr>
<td>$34 \times 34 \times 24 = 27,744$</td>
<td>273,529</td>
<td>9.9</td>
<td>1,656,579,616</td>
</tr>
</tbody>
</table>

would become negligible.

4.2 Process placement

In the next study, we investigate the effect of placing MPI processes on hardware cores in different ways. We use the same parameters as in the weak scaling study and consider the duration of solving the 1D model for two different rank placement strategies. The red curve in the results in fig. 3b shows a scenario, where for each 1D domain all processes are located on the same compute node. This strategy is also used in the weak scaling study. For the orange curve all processes are placed in a round-robin fashion. Thus, the processes that compute a fiber are all located on different nodes. Although the two strategies are almost the same for small number of cores, as the number of cores increases, the difference becomes prominent in the order of 25 times higher runtimes, if the processes for an instance of the 1D problem are no longer on the same computational node.

5 DISCUSSION

The modular structure of opendihu and the use of C++ class templates allows to create composite solver combinations for multi-scale problems, as demonstrated with the simulations in this paper. As the compiler knows the final structure of solvers and meshes, it can optimize for performance. This is a difference to OpenCMISS Iron, where procedural programming is used and composite solvers are only selected at runtime.

We have demonstrated that by targeting efficiency, runtimes can be reduced by a significant factor in comparison to the OpenCMISS Iron used in [7]. This enables us to solve problems of large sizes and allows for studying some effects that are not visible in small-sized scenarios.

The Finite Element meshes used for High Performance Computing have a regular structure. Therefore, subdividing the cuboids by planar cuts allows us to generate a
parallel domain decomposition with equally sized subdomains. Unlike for tetrahedral or unstructured quadrilateral grids, the neighbor information for each subdomain and element is given implicitly, which avoids time-intense lookup operations and improves memory consumption. Considering a regular grid is sufficient when simulating the belly of a fusiform muscle, like the biceps brachii. For more irregular geometries, unstructured grids have to be used, which opendihu supports for serial execution so far.

Our weak scaling study demonstrates that the High Performance Computing is applicable to the type of multi-physics problems considered. The considered multi-physics formulation contains numerous instances of the 0D and 1D models, which can be solved independently of each other. This allows to simulate the realistic number of fibers for biceps brachii in about 4 min runtime per millisecond simulation time, excluding initialization and file output. The study of process placement emphasizes the importance of a proper placement on the supercomputer.

6 CONCLUSION

We have presented the novel open-source software framework opendihu for multi-physics simulation of skeletal muscle. By employing C++ and Python codes, it combines usability and performance. For serial execution, we achieved a speedup of 38 for a particular simulation, compared to simulation software OpenCMISS.

On the supercomputer HazelHen, we simulated the propagation of the action potentials and resulting intramuscular EMG signals using a highly-resolved, multi-physics activation model of a realistic biceps brachii with a typical number of 273,529 muscle fibers. We have run simulations on 27,744 cores and examined the weak scaling behavior providing reasonable runtimes.

REFERENCES


A ROBUST 3D PARTICLE TRACKING SOLVER FOR IN-FLIGHT ICE ACCRETION USING ARBITRARY PRECISION ARITHMETIC

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Key words: Particle laden flows; Particle tracking; Arbitrary Precision Arithmetic; in-flight icing

Abstract. A particle tracking code is presented to compute droplet trajectories within a known Eulerian flow field for in-flight ice accretion simulations. The implementation allows for hybrid or unstructured meshes used by common CFD solvers. A known vicinity algorithm was devised to identify particles inside the mesh by computing the intersection between the particle trajectory and the faces of the mesh elements. Arbitrary precision arithmetic is used in the intersection evaluation in order to avoid errors when selecting the exit face if the intersection point is close to or coincident with a vertex or an edge. State-of-the-art wall interaction models are used to take into account droplet rebound, splash and spread at the walls. Non planar surface elements are assumed to improve the accuracy in evaluating the trajectory of secondary re-emitted particles. The software exhibits almost linear scaling when running in parallel on a distributed memory system. The particle tracking code is assessed against the experimental results regarding the impingement of Supercooled Large Droplets over a wing.

1 Introduction

In-flight ice accretion is a relevant issue in aircraft design and aviation safety [1]. If an aircraft flies through cold wet air, the water particles from clouds can freeze after impacting upon its surfaces, possibly creating ice build-ups in the most exposed zones. Freezing occurs because impinging droplets are in a metastable state called supercooled state. Supercooled droplets exist in water form well below 0°C and can freeze if their equilibrium is perturbed, as it happens when they impinge against the surface of an aircraft. Ice formations have a detrimental effect on aircraft performance as they modify the aerodynamic shape of wings and blades, and can also affect aircraft stability as they
modify the weight distribution. Moreover ice build up on control surfaces and sensors can prevent the pilot or the control system from correctly manoeuvring the plane, which has led in the past to many accidents, some of which led to casualties. Ice accretion concerns also aircraft engines, as ice accumulation on the fan and spinner may eventually lead to ice shedding which can cause mechanical damage. Also, ice accretion on turbofan splitters and fan and booster vanes can result in slow acceleration and lead to compressor stall [4].

Ice accretion software are nowadays a fundamental tool in aircraft design. They are used to predict ice shapes, to investigate performances degradation and to aid the design of anti or de-icing systems. Diverse ice-accretion software can be found both in academy and industry [5, 6, 7]. The simulation of in-flight ice accretion requires the computation of the multiphase flow surrounding the aircraft. The flow is made up by a gaseous phase, namely, air, carrying the water particles, or droplets, in the liquid phase. From the solution of the flow field and of particle trajectories, the rate of mass of water impinging on the surfaces is extracted. Ice accretion is then computed by solving the energy and mass balance on the surface of the plane. Ice accretion is a time dependent problem: as ice starts to form, the shape of the surface changes and therefore the aerodynamic flow field around the body is altered. Since droplet trajectories strongly depend on the local value of the flow velocity and density, each trajectory is modified and the impact point is displaced, thus eventually altering the ice accretion rate. The ice accretion characteristic time is much larger than the aerodynamic one and therefore the ice accretion problem can be solved alternating the aerodynamic flow computation and the ice accretion computation. The output of the aerodynamic solver, including e.g. rate of mass impinging on the boundaries, heat transfer coefficient, shear stress, is fed into the accretion tool which computes the ice accretion modifying the geometry of the boundary. The (deformed) domain mesh is then regularized or the domain is re-meshed in order to comply with the deformed surface and the process is repeated until the total exposure time is reached.

The goal of the present contribution is to improve the Lagrangian particle tracking capabilities of PoliMiIce by adding a robust tracking solver by including a known vicinity algorithm and by taking advantage of arbitrary precision arithmetic techniques to compute the intersection points of the droplet trajectories and the mesh edges. PoliMiIce is an in-flight ice accretion framework developed at Politecnico di Milano capable of predicting rime and glaze ice formation on both 2D and 3D geometries [7].

The present paper is structured as follows. In Section 2, particle-laden flow equations are recalled and the particle solver is outlined. In Section 3, the tracking algorithm is described. To conclude, numerical results are reported in Section 4 and final comments are given in Section 5.

2 Particle-laden flow solver

Particle laden flows are multi-phase flows in which a carrier phase, liquid or gas, is mixed with a particulate of another phase. The carrier phase is continuously connected while the other is made of small, immiscible particles. An aircraft flying through a cloud
of supercooled water droplets is indeed a typical example of particle laden flows.

The concentration of droplets in the cloud is expressed via the Liquid Water Content (LWC), namely the measure of the mass of water in a cloud in a specified amount of dry air. It is usually measured in grams per volume of air. The LWC of a cloud varies significantly depending on the type of clouds present in the atmosphere: typical values range from 0.002 to 3 g/m$^3$. A representative value for the size of droplets in a cloud is the Median Volume Diameter (MVD). It is defined as the median value of the drop diameter in the drop size distribution, averaged by the liquid water content. Particle concentration is a key parameter in determining coupling between phases in particle laden flows. If the dispersed phase does not alter the dynamics of the continuous fluid the flow is said to be one-way coupled; otherwise it is two-way coupled.

Given the low volume fractions of droplets in clouds, the particle laden flow encountered in the ice-accretion problem can be described as a one-way coupled flow. Therefore, the carrier flow equations can be solved independently from the particles, using an e.g. Eulerian formulation of the flow equations, and the particle trajectories can be later solved as a post processing of the continuous flow solution, using either an Eulerian or a Lagrangian description of the particle dynamics. In this work, the compressible RANS equations governing the carrier fluid are solved in the Eulerian frame using the open-source solver SU2 [8].

The Discrete Parcel Method (DPM) is used to compute the particulate phase. Each computational particle, or parcel, represents a set of $N$ neighbouring droplets having an average velocity $u_p$ and average diameter $d_p$. Each parcel trajectory is solved in a Lagrangian frame by integrating the following

$$
\begin{align*}
\frac{dx_p}{dt} &= u_p \\
\frac{dV_p}{dt} &= \frac{\pi}{8} \mu d_p Re_p (u - u_p) \cdot C_D + V_p g (\rho_p - \rho)
\end{align*}
$$

where $\mu$, $\rho$, $u$ are the gas viscosity, density and velocity at the particle position, $V_p$ is the volume of the average particle in the parcel and $C_D$ its drag coefficient and where only forces acting on the particle are gravity and drag forces since the droplet density is much larger than the gas density ($\rho_p >> \rho$) [9]. $Re_p$ is the Reynolds number computed using the relative droplet-flow velocity,

$$
Re_p = \frac{\rho (u - u_p) d_p}{\mu}
$$

The model used for the drag coefficient takes into account the deformations that can occur for larger droplets. For a spherical particle the model by Morrison [10] is linked to that reported by Clift, Grace, and Weber [11] at $Re_p = 10^6$ to best fit experimental data:

$$
C_D = \begin{cases} 
24 \frac{Re_p}{Re_p} + 2.6 \frac{Re_p}{Re_p + \delta} + 0.411 \frac{Re_p}{Re_p + \delta}^{-7.94} + 0.25 \frac{Re_p}{Re_p + \delta} + 0.19 - \frac{8 \times 10^4}{Re_p} & \text{if } Re_p \leq 10^6 \\
0.19 - \frac{8 \times 10^4}{Re_p} + \delta & \text{if } Re_p > 10^6
\end{cases}
$$
Droplet deformation can be modelled as a shape change from a sphere to an oblate disk; the parameter governing this transformation is the Weber number,

$$\text{We} = \frac{\rho p u_p \cdot \hat{n}}{\sigma} \left( u_p \cdot \hat{n} \right)^2$$  \hspace{1cm} (4)

where $u_p$ is the droplet velocity at the moment of impact and $\hat{n}$ is the surface normal at the impingement point, which is a measure of the external forces acting on a droplet relative to its surface tension. The value for the droplet eccentricity is given as a function of the Weber number as $e_f = \left( 1 + 0.07 \sqrt{\text{We}_b} \right)^{-6}$ where $e_f$ is the spheroid eccentricity [12]. The deforming droplet drag coefficient can be obtained by a weighted average of that of a rigid sphere and that of a disk:

$$C_D = \begin{cases} 
(1 - f)C_{D_{\text{Sphere}}} + fC_{D_{\text{Disk}}} & \text{if } We_b \leq 12 \\
C_{D_{\text{Disk}}} & \text{if } We_b > 12 
\end{cases} \hspace{1cm} (5)$$

where the disk drag coefficient is reported in [11].

Modelling of droplet-wall interactions is of paramount importance to compute the amount of water collected at the wall boundaries. The impingement of a droplet against a solid surface can result in different behaviours, whose occurrence depends on a large set of parameters, such as the properties of the droplet (size, density, viscosity, surface tension), its impact velocity and direction relative to the surface, in addition to the properties of the surface, including the temperature. Bai and Gosman [13] identify four different mechanisms of droplet-wall interactions that can happen in the in-flight icing framework: stick (complete adhesion and deposition), rebound (complete bouncing), spread (on the surface) and splash (partial deposition with formation of secondary droplet). In order to simulate all possible interactions, semi-empirical models are used to discriminate between the different regimes. In our implementation, the rebound mechanism is not included and bouncing is considered as a special case of splashing, when only one secondary droplet
is formed and no water is left on the wall. This choice is consistent with the scientific literature concerning the wall interaction problem, as many authors [14] identify only two results of the impingement: deposition and splashing. The model adopted is based on the observations made by Cossali [15] and Trontin and Villedieu [16] and defines two different conditions for which a splash/rebound can happen. The first is based on the amount of normal impact energy and is expressed as a lower limit for what is called the Cossali parameter. A second splashing regime is observed at low incidence angles, defined as the complimentary of the angle between the droplet velocity and the surface normal. At low incidence, the normal impact velocity is not high enough to activate the splashing condition; nonetheless splashing can still be observed. Indeed, in this case the droplet does not spread much on the surface and a part of the particle results not to be attached to the wall during the impact. Hence, the tangential kinetic energy is not efficiently dissipated by the viscous forces and the liquid droplet may partially or completely bounce off the wall.

The splashing mass is divided in a number $N_s$ of secondary droplet fragments proportional to the square of the impact velocity [17]. The splashing droplets are re-emitted inside the computational domain by computing the trajectory of $n_s$ new parcels, each representing a total of $N N_s/n_s$ particles, where $N$ is the number of droplets in the impinging parcel. A value for $n_p$ of at least 10 was found to give a good compromise between accuracy and computational cost. The splashing parcel velocities are sampled from a normal probability density function [17]. As the wall interaction model presented depends on the boundary normal at the impingement point, some unwanted behaviour was noticed for the particles splashing against a wall. Due to the discrete description of the boundary, the front of the splashing droplets presented a dashed-like distribution (Figure 1). A solution to this problem was obtained by using a spline to locally represent the boundary. When computing the interaction model, the normal used is that of the splined boundary, which allows to obtain a more realistic behaviour for the splashing droplets.

To compute the particle trajectories, a computer code was implemented to integrate the equation of motion (1) for each particle in the simulation. The equations (1) are written in terms of quantities defined in the gas phase and therefore the carrier flow solution needs to be interpolated at the particle position. To do so, at each particle time step, each droplet must be mapped to the cell of the mesh containing the particle position, as described in Section 3. The knowledge of the particle owner cells is then used to interpolate the Eulerian solution at the cell nodes to the Lagrangian position of the particle, which is used to compute the forces acting on the droplet. A fifth order explicit Runge-Kutta scheme [18] is then used to find the position and velocity at the next time step. The embedded fourth order formula is used to compute the integration truncation error and adjust the time step accordingly. The process is repeated until all particles have left the computational domain or the next Eulerian time step is reached. In the latter case, the new updated carrier fluid solution is loaded and the process is repeated until the final simulation time is reached. The unsteadiness of the gas phase is treated as step-wise
constant in time, so that inside every Eulerian time step the cloud of droplet is coupled
to a steady carrier flow solution.

A parallel algorithm was implemented using the MPI standard. Each process simulates
a sub-cloud of droplets. Due to the nature of one-way coupled particle laden flows,
communication and synchronisation between processors is reduced to a minimum and
each sub-cloud can evolve independently. Processes communicate only at the end of the
simulation to compute the mass impinged on the walls, or to output the cloud to file. To
assess code performance and scalability, a simulation on a cloud of one million particles
was performed on an increasingly number of processor. A cluster of 16 nodes, each
node containing two Intel Xeon X5650 2.67 GHz (6 core units, totalling 192 cores) was
used. In Figure 2 the speed up factor for the total simulation time and for the mapping,
interpolation, and integration blocks is shown. The latter group represent the part of the
code that can be executed in parallel; as such it presents an almost linear scaling and
at the maximum number of processors used (84) the speed up factor is just 8% short of
the ideal scaling. The full simulation time instead includes operations that execute in
serial and therefore cannot benefit from the parallel implementation. The relative weight
of these overhead costs increases as the number of processors is increased, thus slowing
down the scaling. Nevertheless the speed up factor kept increasing for the number of
processor tested; the total simulation time on 84 processors resulted in a speed up factor
28% lower than that of the ideal scaling.

3 Tracking algorithm

The mapping of each particle position to a given cell is at the center of a particle
tracking code. It’s needed to interpolate the Eulerian solution at the particle position,
and to detect if a droplet has left the domain or impacted a boundary. A known vicinity algorithm [19] is used in the code to perform the mapping. Known vicinity algorithms make use of the knowledge of the particle owner cell before being displaced to find the new owner at the next position. Starting from the initial position in the mesh the particle is searched following a certain path that is defined by the algorithm. Each known vicinity algorithm must therefore define two different operations: the Particle In Cell test (PIC), which determines whether the particle is inside the current cell, and the definition of the search direction. The literature reports many examples of both the PIC and search direction being computed through the use of the cells shape functions [19] or via the definition of geometric tests [20]. This work follows the latter approach and defines an extended PIC that also accounts for the search direction. The algorithm follows the particle along its trajectory, computing the intersections with all faces of all cells it crosses during the time step. The extended PIC takes as input two positions $p_0$ and $p_1$, and the cell to check. One of the two positions in input ($p_1$) is always the particle next position $x_{p}^{n+1}$ that hast to be tracked, while the other can vary. A ray $r$ stemming from $p_0$ and directed towards $p_1$ is created, and the distance $d$ between the two points computed. Then the ray is intersected with the faces of the cell until a valid intersection is found and the intersection distance $d_I$ is computed. If this distance is greater than or equal to $d$ then the particle is in the current cell. This extended test is equivalent to the original PIC if point $p_0$ is taken as the cell centroid. If instead it is set equal to the position of the particle at the earlier time step $x_p^n$ then the ray represents the particle trajectory. When $d_I < d$ the particle is not in the current cell. In this case the PIC returns the face $f$ intersected and the search direction is therefore defined, by moving to the other cell sharing the same face. This way impact with the boundaries are easily detected from the knowledge of boundary faces. The extended PIC the algorithm mapping position $x_{p}^{n+1}$ to cell $C_{n+1}$ does the following:

1. mark the current cell $C_n$ as the cell to be checked $C^k$
2. compute PIC ($x^n_p, x_{p}^{n+1}, C^k$). If the particle is in the current cell assign $C_{n+1}^{n+1} = C^k$ and exit the procedure.
3. get the exit face form the output of the PIC and assign the neighbouring element to $C^k$. Return to 2

The computation of a valid intersection depends on the type of faces considered. In two dimensions faces are always segments as the elements considered are linear. In 3D we consider only the most common elements used by finite volume solvers: tetrahedra, pyramids, wedges, hexahedra. All this elements have planar (triangular) faces or quadrilateral faces that in this work are parametrized as non-planar bilinear patches. For planar 2D or 3D faces, the distance between $p_0$ and the intersection point is computed as

$$d_I = \frac{(p_f - p_0) \cdot n}{t \cdot n}$$
where $p_f$ is a point on the face, $n$ the outward pointing normal, and $t$ is the direction of the ray $(p_1 - p_0)$. As noted in [20], the above distance is computed only if the sign of the denominator is positive thus saving some computations. The intersection is valid if the point belongs to the face and not just to the plane or line on which it lays. In two dimensions for a face defined between nodes $f_0$ and $f_1$, the intersection is valid if $(r_s + d_I t - f_0) \cdot (r_s + d_I t - f_1) \leq 0$, where $r_s$ and $t$ are the starting point and the tangent of the ray representing the particle trajectory, and $d_I$ the intersection distance. For triangular faces, the intersection is valid if, for each edge of the face, the scalar product between the normal of the edge and the vector from the edge midpoint to the intersection point is negative or equal to zero. The normal of the edge $n$ is defined in the plane of the face and points outward. The condition therefore reads:

$$(r_s + d_I t - e_{i0} + e_{i1}) \cdot n_i \leq 0 \quad i = 1 : 3$$

where $e_{i0}$ and $e_{i1}$ are the coordinates of the vertices of the $i$ edge of the face. A bilinear patch can be parametrized as $r(u, v) = uva + ub + vc + d \quad u, v \in [0, 1]$ where $a = r_{00} - r_{10} + r_{11} - r_{01}, b = r_{10} - r_{00}, c = r_{01} - r_{00}, d = r_{00}$ and $r_{ij}$ are the vertices of the non-planar face. By substituting the ray $r(u, v)$, the intersection distance is obtained as

$$d_I = (uv\hat{a} + ub\hat{b} + vc\hat{c} + d - r_s) \cdot t \quad (6)$$

Multiplying the above equation by $t$ and subtracting the result, one obtains $uv\hat{a} + ub\hat{b} + vc\hat{c} + d - \hat{r}_s = 0$ where $(\cdot)$ represents the vector component normal to the direction of the ray, namely $(\cdot) = (\cdot) \cdot t$. A two by two square system is finally obtained by subtracting the third row to the other two, which can be solved for $u$ and $v$ by substitution. The resulting equation is a second order one and can yield up to two solutions. For a solution to be valid, both $u$ and $v$ must lie in the interval $[0, 1]$. If two valid solutions are found, and the further intersection distance is smaller than $d_I$, then the face can be discarded, as the trajectory would exit and then re-enter the same cell.

The above algorithm provides a robust way of tracking particles in 3D unstructured meshes. It is based on the existing literature on geometry based known vicinity algorithms and proposes to fix some shortcomings that were highlighted in earlier studies. The checking of a valid interface allows to track particles even in concave cells, whereas the sole computation of the intersection distance, although less computationally expensive, led to algorithms working only on convex elements [20]. The use of the bilinear patch to represent non planar faces allows a robust treatment of quadrilateral faces. In geometry based algorithms particles were being lost due to the use of the planar PIC equations to treat slightly non-planar faces. Many authors proposed to split those faces in two triangles in order to fix the problem. It was noted [21] that splitting non-planar faces can result in gaps being created if the splitting on one side of the face is not the same as that used on the other, and particles can be lost in that space. By representing the
actual non-planar faces none of the above problems were found. Another shortcoming of geometry based search algorithms is due to the finite precision of floating point numbers. When comparing two values, the errors arising from the finite precision of floating point numbers can yield the wrong result if the numbers are close enough. This can lead the algorithm to mistake a non valid intersection with a valid one or the other way around. Some authors [20] propose to use a tolerance when comparing two floating point values to account for these errors. In this work a different approach is used. The computations that are prone to floating point errors (i.e. selecting the trajectory exit face) are encapsulated in a routine (the extended PIC that will be presented later). A fatal floating point error is detected if, at the successive tracking step, no intersections can be computed. In such a case the computation is repeated with increased precision until the exact solution is recovered. The multiple precision floating point type provided by the MPFR library [22] is used for such computations.

4 Code assessment

The code developed was used to replicate the collection efficiencies obtained during an experimental campaign conducted by Papadakis et al [3] and aimed at providing the first extensive impingement database for Supercooled Large Droplets (SLD) as well as for smaller droplets. The authors of [3] measured the collection efficiency on a NACA 23012 airfoil. Catch efficiency was obtained for the clean geometry as well as for the iced geometries resulting from the LEWICE computation of 5, 10, 15, 22.5 and 45 minutes glaze ice shapes. The tests were conducted at the NASA Glenn Icing Research Tunnel (IRT) and the results obtained were compared with those computed numerically with the LEWICE code. The experiments were conducted at a total air temperature of 283 - 294 K and an air speed of 78 m/s, corresponding to a Reynolds number of approximately 5.25 million per meter. The profile used had a chord of 91.44 cm; collection efficiencies were measured for MVDs of 20, 52, 111, 154, and 236 micrometers.

The carrier fluid solution was obtained by solving the RANS equations with the CFD code SU2. The Spalart-Allmaras model was used to model the turbulent viscosity. The values for the collection efficiency were obtained by simulating a cloud of 20 000 droplets impinging the airfoil and their diameters were set equal to the MVDs of droplet distribution used in the experimental campaign. The wall impingement model of LEWICE [5] was implemented in the code in order to compare the results of the one presented earlier. Figure 3 shows the computed catch efficiency for two values of MVD (52 and 236 µm). The computation with the LEWICE model yields a good prediction of both impingement limits and maximum catch efficiency while the original model, although it retrieves the same values near the limits, strongly underestimates the efficiency near the nose of the profile. This is possibly due to the mass loss coefficient of the model being a function of only the Cossali parameter and not the incidence angle. In the LEWICE model splashing is inhibited for near normal impact thus explaining the large difference in the prediction between the two models. The same computation was performed on the
iced geometries reported in [3]. In Figure 4 are reported the results for the same values of MVD of the clean profile. As in the clean case, near the impingement limits both models yield accurate results for the collection efficiency. On the iced part, the LEWICE model, due to the correlation used for the mass loss coefficient, overestimates the catch efficiency by as much as 50% for the 52µm case. Instead the model presented earlier yields results much closer to the experimental data.

5 Conclusions

A particle tracking algorithm was presented to solve the particle trajectories of the supercooled cloud droplets for in-flight ice accretion simulations. A one-way coupling description of the particle laden flow is assumed because of the relatively small concentration of droplets within the clouds. State-of-the-art models for the aerodynamic forces acting on the particles are implemented. Considered wall interaction mechanics mechanics include sticking, splashing, rebounding and spreading particles and benefits from a detailed description of the boundary geometry. A robust particle tracking algorithm is implemented, which make use of arbitrary precision algebra to determine the intersection of the particle trajectories with the grid edges and nodes. Numerical simulations of a typical ice accretion problem confirmed the validity of the present approach.

REFERENCES


Figure 4: Values for the collection efficiency on a naca 23012 profile after an exposure time of 10 minutes. Left MVD 52 $\mu$m. Right MVD 236 $\mu$m.


CFD SIMULATION OF EVAPORATING ELECTRICALLY CHARGED SPRAYS IN FOOD CHILLING WAREHOUSES – COUPLED PROBLEMS 2019

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Key words: CFD, Charged Sprays, Food Chilling, Evaporation

Abstract. A potential novel application for electrically charged (water) spray is to improve cooling efficiency and reduce moisture loss in food chilling warehouses. In this paper we work toward a numerical (CFD) model that can be used to investigate the viability of this application. We build a simplified model which considers the spray droplets as inert particles and compare simulation results with data from literature. This model is then extended to include the effects of evaporation, which plays an important role in cooling and heat transfer.

1 INTRODUCTION

Electrostatic charging of spray droplets and particles is a well known method for improving the transfer efficiency of spraying systems. Electrostatic spraying systems are therefore good technological solutions when the spray material is expensive, or overspray is highly undesirable, and are used commonly in spray painting and agricultural pesticide application[1]. The present research aims to investigate a new application for charged sprays: chilling warehouses in food industry. Spraying water in a chilling warehouse has two purposes; it counteracts the drying effect of cold air on warm products, and provides additional evaporative cooling effort. High transfer efficiencies are required in this application, because excess moisture will condense and freeze in the evaporators. This makes it a potentially interesting application for charged sprays.

In this paper we work towards a Computational Fluid Dynamics simulation of a charged-spray-assisted chilling warehouse. The use of computer simulations to investigate this application is an obvious choice, given the costs involved with refitting entire production lines. It is however not straightforward, given the wide range of involved physical processes that need to be modelled efficiently and accurately.
Numerical simulation of charged sprays is not new in general. The scope of such simulations is however often limited based on the application case. In works on spray painting the spray droplets are often treated as inert particles, disregarding the effects of evaporation and heat transfer\cite{2, 3, 4}. Arumugham-Achari et al.\cite{5} provide a good framework for a model that includes evaporation, but focuses on a small-scale use case and does not consider droplet charging. Several works on electrostatic precipitators \cite{6, 7} do cover particle charging, but not discharging or evaporation. In the cooling application all these physical phenomena are relevant. This is why we aim to build a simulation that includes all these physical models, and can solve large scale problems.

The first step toward the complete model is a simulation that can simulate charged, inert particles, which is validated against results from literature. We choose to replicate the simulation and measurements by Domnick et al.\cite{2} to validate the model. Hence, the geometry and conditions that we simulated have been adapted from their work.

2 THEORY

The CFD model for the validation case needs to consider three “phases”. These are the gas, the droplets, and the electric field. The droplet phase interacts bi-directionally with the airflow and the electric field, but the airflow and the electric field are not directly connected. The governing equations for these phases, and how the interactions are modelled are described below.

2.1 Gas

The gas is assumed to be incompressible and isothermal, and is therefore governed by the continuity equation and the Navier-Stokes equations. Since the droplet phase will be exchanging momentum with the gas phase through drag, a reaction term must be added to the momentum equations. This reaction is implemented in the form of a volumetric force, i.e. a momentum source. The resulting formulation for the momentum equations is shown in equation (1).

\[
\rho \left( \frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} \right) = -\nabla p + \mu \nabla^2 \vec{u} + \vec{f}_d
\] (1)

Here \( \vec{f}_d \) is the volumetric drag force, positive in the direction of the force acting on the gas phase.

2.2 Droplets

The droplets are, in the validation case, treated as inert particles. The motion of any single droplet is the result of the sum of forces acting upon it, according with Newton’s
laws. In this case three forces are considered; drag, gravity and electrostatic force. The acceleration of a droplet/particle can be formulated as in equation (2).

$$\frac{d\vec{u}_p}{dt} = \frac{3 \rho C_D}{4 \rho_p d_p} |\vec{u} - \vec{u}_p| (\vec{u} - \vec{u}_p) + \frac{\vec{g}(\rho_p - \rho)}{\rho_p} + \frac{6 q_p \vec{E}}{\pi d_p^3 \rho_p}$$

(2)

Here $C_D$ denotes the drag coefficient of the droplet, $\vec{E}$ denotes the local electric field and $q_p$ the droplet charge.

2.3 Electric field

Although not typically considered to be a fluid “phase”, the electric field can be treated as such. The electric field is assumed to be static, and can therefore be written as the gradient of an electric potential: $\vec{E} = -\vec{\nabla} \Phi$. The electric potential satisfies Poisson’s equation, see equation (3).

$$\vec{\nabla} \cdot \vec{E} = -\nabla^2 \Phi = \frac{\rho_q}{\epsilon_0}$$

(3)

Here $\rho_q$ denotes the local volumetric charge density and $\epsilon_0$ the permittivity of vacuum.

2.4 Coupling

The gas flow and electric field equations treat the solution as a continuum, while the droplets are treated as (point-)particles with discrete properties. Coupling these requires the use of control volumes, i.e., a computational grid. The strength and direction of the momentum source $\vec{f}_d$ in equation (1) is determined by taking the sum of the drag forces experienced by all particles inside the control volume, and dividing by the volume. Similarly, the charge density $\rho_q$ in equation (3) is the sum of the droplet charges $q_p$ in the grid cell divided by the volume.

3 NUMERICAL METHOD

For this simulation we have chosen to use the commercial Ansys Fluent code (version 18) as the CFD solver. The models necessary to compute the electrostatic potential and electrostatic force are implemented using so-called “User Defined Functions” (UDFs).

The validation problem is a steady state case, which means a RANS approach can be used for modelling the fluid flow. The droplets are modelled using a Lagrangian approach, which facilitates the implementation of evaporation modelling. A Lagrangian approach does not allow for true steady state modelling, so instead a quasi-steady approach is taken. Each tracked parcel represent a mass flow rather than a discrete mass of particles, and the parcel locations are represented by trajectory lines instead of points. Due to the disperse nature of the spray and electrostatic repulsion between droplets, droplet collision
and coalescence can be neglected, and are not modelled.

3.1 Solver sequence

Figure 1: The process flow of the solver

Figure 1 illustrates the process flow of the solver. After initialisation the Eulerian solver is run, calculating the gas flow and the electric field. Then, droplets are injected and their trajectories are calculated, using the flow data from the previous step. Based on the droplet trajectories the volumetric source fields, representing the drag force acting on the fluid and the electric charge density, are updated. If the solution is converged the solver is stopped, otherwise intermediate data is recorded and the steps are repeated.

3.2 Continuous phase model

To obtain a steady state solution for a turbulent flow we solve the Reynolds-averaged Navier-Stokes equations. The k-ε turbulence model is used to close the model, as done in many preceding works[2, 3, 5].

3.3 Particle tracking

The droplets are modelled using a quasi-steady Lagrangian approach. This means that parcels of droplets are injected in between fluid flow iterations, and their trajectories are integrated until they impact the target or leave the domain through an outlet. Each of the calculated trajectories represents a “continuous” flow of particles of a specific diameter and charge. The amount of particles per trajectory is represented as a so-called strength, or mass flow per second.

To account for electrostatic repulsion between droplets a two-way interaction with the electric field model is used. The electric field applies a force to the droplets, while the charge of the droplets acts as the source term seen in equation (3), influencing the
electric field. Because the electric field and droplet trajectories are calculated in turns the solution can become unstable. Each set of droplet trajectories will repel the next iteration of droplet trajectories to the opposite side of the domain. To prevent this under-relaxation is used when the volumetric space charge is updated.

### 3.4 Electric field

The governing equation for the electric potential is the Poisson equation, see equation (3). We implement this as a Eulerian “phase” which is transported exclusively though diffusion. The diffusion coefficient is $\epsilon_0$, and the charge-density acts as a source term. Two types of boundary conditions are used. For grounded or electrified surfaces a Dirichlet condition is used, and the surface potential is set to the applied voltage. For insulated surfaces a Neumann condition is used, and the normal derivative of the potential is set to zero.

### 4 CASE SETUP

The validation case is a simulation of a rotary bell sprayer, of a type typically used in automotive industry. The geometry, boundary conditions and parameters have been adapted from Domnick et al.\cite{2,8}. The sprayer is oriented vertically downward, and positioned 230 mm above a 1x1 m flat plate that serves as the target. The computational domain is box with sides of 2 m and a height of 0.7 m, enclosing the geometry as shown in figure 2.

#### 4.1 Mesh

![Figure 2: Cros section of the used mesh](image)

An unstructured mesh with approximately 10 million elements was used for the validation simulation. The global element size is 10 mm, with refinement and inflation layers near the sprayer and target surface.
4.2 Boundary conditions

The top and bottom of the bounding box are treated as an inlet and an outlet respectively, creating a 0.3 m/s downwash around the sprayer. The sides of the bounding box are treated as symmetry conditions. All solid surfaces are treated as no-slip walls for the gas flow. Droplets impacting any solid surface are removed from the domain, while the total massflow of droplets is recorded in each surface element.

For the electric field, the target plate and the sprayer bell are treated as grounded and electrified respectively, with a constant electric potential. All other surfaces are considered to be insulated, i.e. the normal derivative of the potential being zero.

4.3 Sprayer and droplets

Primary and secondary breakup of the liquid near the sprayer is not modelled. Instead droplets are injected 1 mm outside the bell edge, equally distributed around the circumference with a ± 0.5 mm vertical stagger. A total of around 300000 droplet streams are tracked, with 22 different droplet sizes. The sprayer parameters are given in table 1, the used droplet size distribution is shown in figure 3.

<table>
<thead>
<tr>
<th>Table 1: Sprayer parameters</th>
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<tbody>
<tr>
<td>Bell diameter</td>
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<tr>
<td>Bell speed</td>
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<tr>
<td>Liquid flow rate</td>
</tr>
<tr>
<td>Sprayer voltage</td>
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<tr>
<td>Droplet charge</td>
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<tr>
<td>Droplet density</td>
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<td>Droplet surface tension</td>
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The droplet charge is based on the Rayleigh stability limit, $Q_R$, defined as equation (4).

$$Q_R = 8\pi \sqrt{\epsilon_0 \sigma r_p^3}$$

*Figure 3: Size distribution of injected droplets*
5 RESULTS

5.1 Validation simulation

Figure 4 shows a snapshot from the simulation results. The droplet trajectories are coloured according to mass, the electric potential is plotted on the symmetry plane and the target surface shows the accretion rate. This figure illustrates the complexity of the problem, as the droplet trajectories are wildly different depending on their size and charge. At small sizes, droplets are driven mostly by drag, at intermediate sizes by electrostatic force, and at large sizes inertia dominates their behaviour.

The figure also shows a slightly asymmetric and irregular spray deposition pattern. This we attribute to a minor instability remaining in the simulation, and the fact that only a limited amount of particle trajectories can be calculated. To remedy this, the simulation was left to run for a total of 1000 cycles, the results of which were averaged, resulting in a smooth deposition pattern.

To compare our results with those obtained by Domnick et al. the spray deposition rate was sampled along the middle of the target plate. The results are displayed in figures 5a (present simulation) and 5b (Domnick’s, experimental and numerical). In our results two lines are plotted, representing sampling along both horizontal axes.

The experimental results adapted from Domnick et al. were obtained by measuring the paint layer thickness obtained after an unspecified period of spraying. This makes quantitative comparison impossible, so only the overall profiles shapes may be compared. Doing so, several similarities and differences are apparent. In both cases the spray deposition tapers to near zero at the edges of the target plate, and has a local minimum at the centre. In our case the spray pattern forms an additional “ring”, with a local minimum around...
200 mm from the sprayer axis. Not all boundary conditions could be retrieved from Domnick’s work, which we expect is a reason for the observed mismatch.

![Figure 5: Comparison of simulation results with literature](image)

In general the simulation results match the experimental data, thus the model is extended to include the effects of evaporation.

### 5.2 Evaporation

To investigate the effects of including evaporation a new test case, which is more representative for our application, is constructed. It consists of cylinder placed inside a cubic box, with a cone-shaped spray aimed at the centre. Figure 6 shows a snapshot from a simulation of this case. An evaporation model based on Ranz and Marshall is used. A free ion transport model is not used, meaning that the charge of evaporated droplets is completely removed from the domain.

When evaporation is included the general behaviour of the spray and the deposition pattern on the target do not change significantly. However, the total amount of fluid transferred to the target becomes highly dependent on the initial temperature and relative humidity. In addition, the results are highly sensitive to the droplet charge. In some cases with high charge and/or high spray mass flow the electric potential in the domain locally exceeds the sprayer voltage.

### 6 CONCLUSIONS

We succeeded in building a numerical model of an electrically charged spray using the Ansys Fluent (version 18) solver. With this model a stable solution could be found for several test cases. To validate the model we attempted to replicate the results obtained by Domnick et al. Our results did qualitatively agree with experimental data, although
some differences were observed. We suspect these mostly come from the fact that some information regarding the geometry and operating conditions of the experimental setup was unavailable to us. Thus, despite the differences we conclude that our model produces accurate results, but foresee further validation efforts.

The present model has been expanded to include the effects of evaporation, which are necessary to model the application of charged sprays in a chilling warehouse. Initial simulations with evaporation modelling show promise, and the expected cooling effects are observed. Nevertheless, more work is necessary to include the exchange of charge between droplets and the continuous phase.

NOMENCLATURE

\[ \epsilon_0 \quad \text{Permittivity of the vacuum} = 8.85 \times 10^{-12} \text{[F/m]} \]
\[ \mu \quad \text{Gas dynamic viscosity [Pa.s]} \]
\[ \Phi \quad \text{Electric potential [V]} \]
\[ \rho \quad \text{Gas density [kg/m}^3\text{]} \]
\[ \rho_p \quad \text{Droplet density [kg/m}^3\text{]} \]
\[ \rho_q \quad \text{Charge density [C/m}^3\text{]} \]
\[ \sigma \quad \text{Droplet surface tension [N/m]} \]
\[ \vec{E} \quad \text{Electric field [V/m]} \]
\[ \vec{g} \quad \text{Gravity vector [m/s}^2\text{]} \]
\[ \vec{u} \quad \text{Gas velocity vector [m/s]} \]
\[ \vec{u}_p \quad \text{Droplet velocity vector [m/s]} \]

Figure 6: Evaporating spray, droplet trajectories coloured by diameter, target cylinder coloured by temperature
\( C_D \)  
Droplet drag coefficient [-]

\( d_p \)  
Droplet diameter [m]

\( f_d \)  
Volumetric force applied by droplets on the airflow [N/m³]

\( p \)  
Pressure [Pa]

\( q_p \)  
Droplet electric charge [C]

\( Q_R \)  
Rayleigh stability limit for charged droplets [C]

\( r_p \)  
Droplet radius [m]

\( t \)  
Time coordinate [s]

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**REFERENCES**


CORROSION OF A THIN-WALLED SPHERICAL SHELL UNDER TIME DEPENDENT INTERNAL PRESSURE

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Abstract.
Elastic thin-walled closed spherical shell is considered exposing to mechanochemical corrosion under constant external pressure and internal pressure decreasing with time. It is important that the equivalent stresses are chosen to be dependent not only on difference of internal and external pressures but on both internal and external pressure values themselves. We are investigating the dependencies of a vessel lifetime on the rate of pressure decrease, under the assumption that corrosion rate depends linearly on stress.

1 INTRODUCTION

Thin-walled elastic spherical shells are typical structural component, they are often used as a part of high-pressure vessels. During operation pressure vessels may be under mechanical loads and in aggressive environment. Aggressive environment causes corrosion damage, which, being intensified by stresses in the body, becomes more destructive [1]. Corrosion may cause local defects, for example pittings, cracks, caverns, or may lead to uniform thinning of the structure, i.e. general corrosion. Localized corrosion results in stress concentration around defects, to estimate stresses around local imperfections, finite element method is often used [2], however, there are some analytical assessments [3, 4, 6]. General corrosion accelerated by mechanical stresses is called mechanochemical corrosion. Experiments have shown that for metals, the rate of mechanochemical corrosion is often linearly dependent on stress at the corresponding points of the surface [7, 8].

Mechanochemical corrosion of thin-wall spherical and cylindrical shells under pressure was considered in [9, 10], where the stresses are assumed to follow Laplace’s law. According to Laplace’s law, stresses are the same on both shell’s surfaces and does not take into account the inner and outer pressures, only their difference. However, for pressurized vessels under machenochemical corrosion the use of the law of P.-S. Laplace may under- or overestimate the service life because only pressure difference affects corrosion rate, and...
error grows as the inner and outer pressures increase. In [11] an analytical solution for thin pressurized sphere exposed to double-sided corrosion was presented taking into account the effect of hydrostatic pressure and the difference of hoop stresses on the inner and outer surfaces. Thin corroded sphere exposed to nonuniform heating considered in [12]. Several papers devoted to mechanochemical corrosion problems of thick shells [5, 13].

However, solutions mentioned in [8, 10] deal with constant internal and external pressures, whereas another challenging problem is the case of pressure that changes with time. Such problem arises in different areas of engineering, for example, the pressure in oil well declines with time. Pressure decline in a well is often driven by few factors, one of such factors is reservoir pressure depletion.

In the present paper a linearly elastic thin-walled closed spherical shell is considered exposing to mechanochemical corrosion under constant external pressure and internal pressure decreasing with time. The dependencies of the vessel lifetime on the rate of pressure decrease is investigated.

2 PROBLEM FORMULATION

Consider a thin-walled spherical shell subjected to pressure and mechanochemical corrosion. It is supposed that sphere’s material is linearly elastic. Let the internal pressure \( p_{in} \) linearly decline with time \( t \) while the external pressure \( p_{out} \) remains constant:

\[
p_{in} = p_r - at, \quad p_{out} = p_R = \text{const},
\]

in this paper we consider the situations when the parameter \( a \) is positive: \( a > 0 \).

Consider two cases of corrosion damage: internal and external mechanochemical corrosion. Corrosion is understood here as a uniform dissolution along the entire surface such that surface remains spherical with no localized attack. When the shell is subjected to internal corrosion, the inner radius increases with time due to dissolution: \( r = r(t) \), while the outer radius \( R \) remains constant: \( R = \text{const} \), the rate of internal corrosion is denoted by \( v_r \). In case of external corrosion the inner radius of the sphere remains constant: \( r = \text{const} \), while the outer radius of the sphere is decreasing with time: \( R = R(t) \), the corrosion rate is denoted by \( v_R \). Let us denote inner and outer shell’s radii at initial time \( t_0 = 0 \) by \( r(0) = r_0 \) and \( R(0) = R_0 \).

Corrosion rates \( v_r \) and \( v_R \) are supposed to be linearly dependent on the stress at the corresponding surface [7, 8, 14]:

\[
v_r = \frac{dr}{dt} = a_r + m_r \sigma(r),
\]

\[
v_R = -\frac{dR}{dt} = a_R + m_R \sigma(R).
\]

Here, \( a_r, m_r, a_R, m_R \) are experimentally determined constants, which are dependent on sphere’s material and environment; \( \sigma(r) \) and \( \sigma(R) \) are the maximum (in absolute value)
principal stresses on the corresponding surface of the shell, and

$$\text{sign } m_r = \text{sign } \sigma(r), \quad \text{sign } m_R = \text{sign } \sigma(R).$$

The problem is to find the circumferential stress, shell’s thickness and to assess its lifetime.

3 PROBLEM SOLUTION

3.1 Equivalent Stress

The stresses defined by the law of P.-S. Laplace do not reflect the effect of the hydrostatic pressure $p = \min \{p_{in}, p_{out}\}$, but depend on only the difference $p_{in} - p_{out}$. However, for high pressure vessels subjected to mechanochemical corrosion, the use of the law of P.-S. Laplace may lead to a large error [11].

Article [11] presents the refined expressions for stress in a thin-walled pressurized sphere under corrosion which provide results more accurate than the solutions based on Laplace’s law, and at the same time, have a simple form (in contrast to the solutions based on Lamé’s formulas [13]). According to [11] the stress values on the sphere’s surfaces determined by the formulas

$$\sigma(r) = \frac{\Delta pr_c}{2h} - \frac{p_{in} + 3p_{out}}{4}, \quad (4)$$

$$\sigma(R) = \frac{\Delta pr_c}{2h} - \frac{3p_{in} + p_{out}}{4}, \quad (5)$$

where $\Delta p$ is the difference between inner and outer pressures: $\Delta p = p_{in} - p_{out}$, $h$ is a thickness of the shell, $r_c$ is the mid-surface radius which is supposed to be constant: $r_c = (R_0 + r_0)/2 = \text{const}$. Note that, in general case mid-surface radius of the corroded shell changes with time. However, it is shown in [11] that the change in the mid-surface radius during the corrosion process (even for one-sided corrosion) can be neglected, so the assumption $r_c = \text{const}$ is justified.

Substituting (1) in Eqs. (4) and (5) yields

$$\sigma(r) = \frac{(p_r - at - p_R)r_c}{2h} - \frac{p_r - at + 3p_R}{4}, \quad (6)$$

$$\sigma(R) = \frac{(p_r - at - p_R)r_c}{2h} - \frac{3p_r - 3at + p_R}{4}. \quad (7)$$

3.2 Internal Corrosion

When the sphere is subjected to internal mechanochemical corrosion, the inner radius increases with time due to corrosion: $r = r(t)$, while the outer radius $R$ remains constant: $R = R_0 = \text{const}$. The shell thickness $h$ at any time is defined as
\[ h = h(t) = R_0 - r(t). \]  

Substituting Eqs. (6) and (8) into Eq. (2) gives the basic differential equation

\[ \frac{dr}{dt} = a_r + m_r \left( \frac{(p_r - at - p_R)r_c}{2(R_0 - r(t))} - \frac{p_r - at + 3p_R}{4} \right). \]  

The initial condition of Eq. (9) to be satisfied at time \( t_0 = 0 \) is \( r(0) = r_0 \).

Solution of Eq. (9) provides the corresponding values of inner radius \( r \) and time \( t \). For every values of \( r \) and \( t \), the shell thickness can be found from (8) and stresses \( \sigma_r \) and \( \sigma_R \) can be calculated by Eqs. (6) and (7).

3.3 External Corrosion

In the case of external mechanochemical corrosion the outer radius decreases with time: \( R = R(t) \), while the inner radius \( r \) remains constant: \( r = r_0 = \text{const} \). Thus the shell thickness \( h \) at any time is

\[ h = h(t) = R(t) - r_0. \]  

Substituting Eqs. (7) and (10) into Eq. (3) yields

\[ \frac{dR}{dt} = -a_R - m_R \left( \frac{(p_r - at - p_R)r_c}{2(R(t) - r_0)} - \frac{3p_r - 3at + p_R}{4} \right). \]  

The initial condition to be satisfied at time \( t_0 = 0 \) is \( R(0) = R_0 \).

Solution of Eq. (11) gives the corresponding values of outer radius \( R \) and time \( t \). Shell thickness for a given \( R \) and \( t \) can be found from (10). Since \( R, t, \) and \( h \) are found, stresses \( \sigma_r \) and \( \sigma_R \) can be calculated by Eqs. (6) and (7).

3.4 Lifetime Estimation

Let us define the lifetime of the shell as a minimum time \( t^* \) at which the equivalent stress in the shell reaches a given limit \( \sigma^* \). The value \( \sigma^* \) supposed to be a strength limit or any other critical stress (taking into account safety factors) depending on the operating conditions [15, 16]. Note that this model is not applicable to local corrosion which can be caused by stress concentration in the vicinity of surface or near-surface defects [17, 18, 19, 21, 22, 20].

Note that, here we consider only the situations where \( p_{in} > p_{out} \), i.e. \( p_r - at > p_R \). For such cases the equivalent stress on inner shell’s surface is greater than the outer stress: \( \sigma(r) > \sigma(R) \). Thus, the shell’s lifetime \( t^* \) is a solution of equation \( \sigma(r) = \sigma^* \).
4 CALCULATION RESULTS

An example of the effect of the initial internal pressure on the maximum stress and the radii of the corroded shell is shown in figures 1 and 2. A spherical shell is considered with the initial radii $R_0 = 82[l_c]$ and $r_0 = 78[l_c]$ subjected to internal pressure $p_{in} = p_r - at$ and external pressure $p_R = 0$. Different values of initial internal pressure are used: $p_r = 8[p_c]$ (red curves), $p_r = 12[p_c]$ (green curves), and $p_r = 16[p_c]$ (yellow curves), $p_c$ is a certain unit of stress; pressure decline parameter $a = 0.1[p_c/t_c]$. Here and below, $p_c$, $t_c$ and $l_c$ is a certain unit of stress, time and length.

In figure 1 the dependencies of $\sigma(r)$ on $t$ (a) and $r$ on $t$ (b) are demonstrated for internal corrosion of the sphere. Corrosion rate parameters are $a_r = 0.16[l_c/t_c]$ and $m_r = 0.0008[l_c/(t_c p_c)]$.

Figure 2 shows the dependencies of $\sigma(r)$ on $t$ (a) and $R$ on $t$ (b) in case of external corrosion. Corrosion rate parameters are $a_R = 0.16[l_c/t_c]$ and $m_R = 0.0008[l_c/(t_c p_c)]$.

From figures 1 (a) and 2 (a) it is seen that for a fixed value $a$, the greater the initial value of $p_{in}$ is, the greater $\sigma(r)$ is, and the earlier a certain stress value is reached. Figure 1 (b) demonstrates that the inner radius increases with time due to corrosion, and the greater the initial value of $p_{in}$ is, the faster $r$ increases. Figure 2 (b) illustrates that the outer radius of the shell decreases with time, and the greater $p_r$ is, the faster $R$ decreases. Thus, in both cases of internal and external corrosion, an increase in the initial value of $p_r$ accelerates the process of dissolution.

Figures 3 and 4 illustrate the effect of parameter $a$ on the maximum stress and the radii of the sphere exposed to internal (fig. 3) and external (fig. 4) corrosion.
In figure 3 the dependencies of $\sigma(r)$ on $t$ (a) and $r$ on $t$ (b) are shown. Figure 4 shows the dependencies of $\sigma(r)$ on $t$ (a) and $R$ on $t$ (b). Curves in figures 3 and 4 are built for pressures $p_r = 30[p_c]$, $p_R = 0$ and different values of parameter $a$: $a = 4.5$, $a = 3$, $a = 1.5$, and $a = 0$. All other parameters are the same as in figures 1 and 2.

Figures 3 (a) and 4 (a) show that the stress in the shell grows slower for greater $a$, and can even diminishes at sufficiently high values of $a$. From figures 3 (b) and 3 (b) it is seen that the sphere’s thickness reduces faster as $a$ decreases. Thus, the larger $a$ is, the greater the lifetime is.

5 CONCLUSIONS

- A linearly elastic thin-walled closed spherical shell exposing to mechanochemical corrosion under constant external pressure and internal pressure decreasing with time is considered. Corrosion rates are assumed to be linearly depend on stress.

- It is confirmed that the greater the initial value of internal pressure $p_r$ is, the faster the corrosion process.

- The stress in the shell grows slower at a higher rate of the decrease of internal pressure. At sufficiently high rate of the decrease of internal pressure the stress in the shell may decline with time.

6 ACKNOWLEDGMENTS

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a) Dependencies of $\sigma(r)$ on $t$

b) Dependencies of $r$ on $t$

**Figure 3**: Internal corrosion. Effect of various values of $a$

**REFERENCES**


O. S. Sedova, O. O. Iakushkin and A. B. Vakaeva

Figure 4: External corrosion. Effect of various values of $a$


DYNAMICS OF A SYSTEM OF COUPLED NONLINEAR OSCILLATORS WITH PARTIAL ENERGY DISSIPATION

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Key words: Tuned mass damper, Nonlinear vibration absorber, Bistable system, Lyapunov characteristic exponents, damping rate.

Abstract. We study the dynamics of the 3-DoF system with bistable nonlinear energy sink absorber, connected to the primary 2-DoF system. With the assumption that the mass of the absorber is small enough we study the local behaviour of the system in the neighbourhood of the stationary points. Under condition that parameters of the mechanical system are uncertain, the analytical approximations of eigenvalues of the linearized system are presented. These approximations are used to determine the characteristics of absorber (damping coefficient and negative linear stiffness component), which guarantee the optimal damping rate of the responses of the main system to perturbations. The theoretical results are compared with numerical experiments. The dependence between linear and nonlinear stiffnesses of the absorber is discussed.

1 INTRODUCTION

Problems associated with undesirable vibrations are encountered in many applied tasks in mechanical engineering, construction, aerospace engineering, biomechanics, etc. For various reasons, a structure may encounter sources of excitation, which are not predicted for the project. To increase reliability, design engineers seek a simple, low-cost, and efficient solution. In many cases, the dynamic vibration absorbers (DVA) are used that meet these requirements. Dynamic vibration absorbers or tuned mass dampers are small
elements locally attached to the structure, designed to dissipate the excessive vibration energy.

One of the important goals of vibration control is to create a frequency zone in which resonance (or a spectral gap around an inconvenient frequency) cannot occur, by connecting a vibration absorber. In this case, usually DVA parameters are determined in accordance with the eigenvector of the unstable oscillation mode, which ensures the spatial distribution of the oscillation energy within one oscillation mode. The disadvantage of such a single-mode approach is that it does not take into account the influence of adjacent oscillation modes, which may become important in some circumstances.

In order to solve the problem with a narrow band TMD, remaining within the framework of passive interference suppression, with using only one device, many researchers studied the effect of additional nonlinearities in the absorber [1 – 10], seeking to allow a resonator to resonate at more than one frequency. This led to the development of the concept of nonlinear energy sink (NES), which we can represent schematically in the form of a small mass, connected with the primary system by essential nonlinearity. On today, a number of NES constructions have been proposed, such as cubic nonlinearity [11], a vibro-impact device [12, 13], an eccentric rotator [14], and a tuned pendulum [15]. Also, more recently, a bistable NES (BNES) has been proposed, consisting of a small mass connected with the primary system by a spring with both cubic nonlinear and negative linear components [16, 17].

2 DESCRIPTION OF THE SYSTEM AND STABILITY ANALYSIS

We consider the 3-Degrees-of-Freedom mechanical system which is schematically presented on fig.1. It consists of two masses connected to each other and to fixed supports by springs (linear) and a bistable absorber connected to one of them.

The motion equations of the mechanical system considered are

$$
\begin{align*}
    m_1 \ddot{x}_1 + c(\dot{x}_1 - \dot{x}_a) + k_1 x_1 + k_2 (x_1 - x_2) - k_{a1}^\text{lin}(x_1 - x_a) + k_{a1}^\text{nonlin}(x_1 - x_a)^3 &= 0 \\
    m_2 \ddot{x}_2 + k_2 (x_2 - x_1) + k_3 x_2 &= 0 \\
    m_a \ddot{x}_a + c(\dot{x}_a - \dot{x}_1) + k_{a1}^\text{lin}(x_1 - x_a) - k_{a1}^\text{nonlin}(x_1 - x_a)^3 &= 0
\end{align*}
$$

(1)

Here $x_1$ and $x_2$ refer to the displacements of the primary 2-DoF system, while $x_a$ refers to the displacement of the bistable absorber; $m_1, m_2$ ($m_2 \leq m_1$) are masses of the bodies, and $k_j (j = 1, 2, 3)$ – the stiffnesses of the springs; $c, k_{a1}^\text{lin}, k_{a1}^\text{nonlin}$ are the absorber damping coefficient, negative linear spring coefficient and cubic (positive) spring coefficient respectively. The overdots denote the differentiation on time. It is supposed that parameters of main system are given, parameters of absorber are tunable, and the mass of the absorber $m_a$ is much less then $m_1$.

It is easy to see that the ODE system (1) has three stationary points: the origin (unstable one) and two points $(0, 0, \pm \sqrt{k_{a1}^\text{lin}/k_{a1}^\text{nonlin}})$ on the axis $Ox_a$. Let us introduce the perturbation

$$
x_a = \sqrt{k_{a1}^\text{lin}/k_{a1}^\text{nonlin}} + \bar{x}_a,
$$

Here
Figure 1: Three-degree-of-freedom system consisting of two coupled linear oscillators and a bistable absorber connected to one of them

and dimensionless parameters and time with formulas

$$\beta = \frac{m_2}{m_1}, \mu = \frac{m_a}{m_1}, \lambda_1 = \frac{k_1}{m_1}, \lambda_2 = \frac{k_2}{m_2}, \lambda_3 = \frac{k_3}{m_2},$$

$$\left(\omega^2\right)_{1,2} = \frac{1}{2} (p \pm \sqrt{p^2 - 4q}), \ p = \lambda_1 + (1 + \beta)\lambda_2 + \lambda_3, \ q = \lambda_1(\lambda_2 + \lambda_3) + \beta\lambda_2\lambda_3,$$  \hspace{0.5cm} (2)

$$h = \frac{c}{m_2\omega_2}, \ \tau = \frac{2k_{lin}}{m_2\omega_2}, \ \tau = \omega_2 t.$$  \hspace{0.5cm} (4)

Here $\omega_1, \omega_2$ are the natural frequencies of the main system.

The linearized system in the vicinities of stationary points is associated with the following $\lambda-$ matrix

$$\begin{pmatrix} \omega_2^2\lambda^2 + \lambda_1 + \beta\lambda_2 & -\beta\lambda_2 & -\mu\omega_2^2(h\lambda + \lambda) \\ -\lambda_2 & \omega_2^2\lambda^2 + \lambda_2 + \lambda_3 & 0 \\ -\mu\omega_2^2(h\lambda + \lambda) & 0 & \omega_2^2(\lambda^2 + h\lambda + \lambda) \end{pmatrix}. \hspace{0.5cm} (3)$$

Accordingly, the characteristic polynomial is as follows

$$f(\lambda) = \omega_2^4[\lambda^6 + h\omega_2^2(1 + \mu)\lambda^5 + \omega_2^2(\lambda_1 + \lambda_2(1 + \beta) + \lambda_3 + \lambda(1 + \mu))\lambda^4 +$$

$$+ h\omega_2^4[\lambda_1 + \lambda_2(1 + \beta + \mu)]\lambda^3 + \omega_2^2(\lambda_1(\lambda_2 + \lambda_3) + \beta\lambda_2\lambda_3 + \lambda(\lambda_1 + \lambda_2(1 + \beta + \mu) +$$

$$+ \lambda_3(1 + \mu))]\lambda^2 + h(\lambda_1\lambda_2 + \lambda_1\lambda_3 + \beta\lambda_2\lambda_3)\lambda + \lambda(\lambda_1\lambda_2 + \lambda_1\lambda_3 + \beta\lambda_2\lambda_3). \hspace{0.5cm} (4)$$

For any set of parameters of the system considered all coefficients of the polynomial $f(\lambda)$ are strictly positive, as well as determinants

$$\Delta_3 = \mu h^2[\lambda_1^2 + \beta\lambda_2^2(1 + \beta + \mu) + 2\beta\lambda_1\lambda_2],$$

$$\Delta_5 = \mu^2 h^3\beta(\lambda_2^2\lambda_1 + \lambda_1\lambda_3 + \beta\lambda_2\lambda_3)^2. \hspace{0.5cm} (5)$$

Then, according to Lienard – Chipart criterion [18], all eigenvalues of linearized system have negative real parts, i.e. two non-origin stationary points are stable focuses (spirals).
3 ESTIMATION OF EIGENVALUES AND TUNING THE ABSORBER

Now we shall count $\mu$ as small parameter. In origin case $\mu = 0$ the polynomial $f(\lambda)$ has six different roots:

$$\pm \iota, \pm \iota \frac{\omega_1}{\omega_2}, \frac{1}{2}(h \pm \sqrt{h^2 - 4\kappa}).$$

Consequently the eigenvalues of linearized system are analytical functions on $\mu$ and may be presented as taylor expansions

$$\lambda_j = \lambda_{j0} + \mu \lambda_{j1} + \mu^2 \lambda_{j2} + \cdots, j = 1, 6 \quad (6)$$

and the coefficients $\lambda_{js}$ are calculated sequentially by substitution expression (6) in (4). Taking into account that the corresponding expressions in general case are very bulky, in present paper we limit ourselves with "canonical" case: $m_2 = m_1, k_3 = k_2 = k_1$. Hence, $\beta = 1, \omega_1 = \sqrt{3} \omega_2$. Thus we have

$$\lambda_{11} = -\frac{1}{4} h + \iota h^2 + \frac{\kappa^2 - \kappa}{\kappa^2}, \lambda_{31} = -\frac{\sqrt{3}}{4} \frac{3\sqrt{3} h + \iota(3h^2 + \kappa^2 - 3\kappa)}{3h^2 + (3 - \kappa)^2},$$

$$Re\lambda_{12} = \frac{h}{8} \frac{h^4 + h^2(3\kappa^2 - 3\kappa - 1) + \kappa(2\kappa^3 - 3\kappa^2 + 1)}{[2h^2 + (\kappa - 1)^2]^3}, \cdots \quad (7)$$

The damping rate of the oscillations of the system is governed by maximal Lyapunov exponent value. In rather small vicinity of stationary point this value is close to the $maxRe\lambda_j$ ($j = 1, 6$), i.e. in first approximation the biggest of values $Re\lambda_{11}, Re\lambda_{31}$ is responsible for it.

Thus, for tuning the absorber we suggest the minimization of function $z(h, \kappa) = max(Re\lambda_{11}, Re\lambda_{31})$. There are two possibilities here:

A) The surface $z_1(h, \kappa) = [h^2 + (\kappa - 1)^2]^{-1}$ intersects the surface $z_2(h, \kappa) = 9[3h^2 + (3 - \kappa)^2]^{-1}$;

B) there is no intersection.

Case A) leads to relation

$$h^2 = \frac{2}{3} \kappa(3 - 2\kappa). \quad (8)$$

Now, if the value of $z$ is maximized on the set (8), then any other point of the both surfaces is situated below and gives the bigger value to $Re\lambda$. Substituting $h$ from (8) to $z_1$ (or $z_2$, no matter) we have the function of one argument

$$\psi(\kappa) = \frac{\kappa(3 - 2\kappa)}{(3 - \kappa^2)^2} \quad (\kappa > \frac{3}{2}).$$
Figure 2: The intersection of the surfaces $z_1(h, \kappa)$ and $z_2(h, \kappa)$

Its derivative is equal to zero as

$$9 - 12\kappa + 9\kappa^2 - 4\kappa^3 = 0.$$ 

The roots of the last equation are $\approx 1.2797; 0.4852 \pm 1.2341i$, and the real one gives the maximal value for $\psi(\kappa)$. Consequently, $h \approx 0.6131$, $Re\lambda_{11} \approx -0.3375\mu$.

The case B) is characterized by condition $\kappa \geq 1.5$, and $Re\lambda_{11} > Re\lambda_{31}$. For any value of $h$ the function $z_1(h, \kappa)$ is decreasing on argument $\kappa$, and the least possible value of $\kappa$ is the choice, and $h = \kappa - 1$. Then $\kappa = 1.5$, $h = 0.5$, and $Re\lambda_{11} = -0.25\mu$. Definitely, this value is worse comparatively with $-0.3375\mu$, so the choice of case A) is optimal.

Remark. It should be noted that the next terms of expansion of $Re\lambda$ are positive and decrease slightly the initial value. For instance, with $\mu = 0.04$, $\kappa = 1.2797$, $h = 0.6131$ the calculated value of $max Re\lambda$ is $-0.0135$. At the same time the roots of $f(\lambda)$ are:

$$-0.01371 \pm 1.7365i, -0.01263 \pm 0.9828i, -0.2925 \pm 1.1101i.$$ 

So, there is about 7 percent error. This fact must be taking into account while tuning the absorber. The calculated values of $h$ and $\kappa$ may be taken as the initial point, and numerical scrolling the neighborhood of this point will lead to the best effect.

4 Numerical simulations and discussion

We have simulated the motion of the system by integrating the equations (1) (in dimensionless parameters) with small enough initial values for primary system $-x_1(0), x_2(0), x_1'(0), x_2'(0)$ (prime means the differentiation on time $\tau$). Generally, the results are consistent with theoretical expectations, however few things should be noted. One of them is the influence of nonlinear stiffness of the absorber on the responses of the system. Numerical experiments show that its value must be small enough to prevent the mitigation of oscillations (see also [19]). With this condition the typical view of phase trajectories is illustrated on fig.3 ($\mu = 0.04, h = 0.7, \kappa = 1.4, k_{nonlin} = 0.004$). Displacements of the primary masses are bounded (fig.3a), and slowly on $\tau$ tend to zero (fig. 3b). Initial perturbation of absorber is not so important - it goes to the vicinity of stationary point very quickly (fig. 3c).
Figure 3: Displacements of the masses of main system and time histories, $\kappa = 1.4$

Figure 4: Projection of phase trajectory, $\kappa = 1.2$

The variation of dimensionless damping coefficient $h$ on interval $[0.5, 1]$ is not very important, while small values (below 0.2) as well as big (more then 1.3) have negative effect on system’s behaviour.

The influence of parameter $\kappa$ on system’s dynamics is also remarkable. The calculated value is equal to 1.2797 (1.414 in [19]). The decreasing of this value leads to the following results. The "mediocre" decrease has the dual effect: the responses of the main system becomes weaker (compare with fig.3a), but the amplitude of oscillations decreases very slowly (fig.4b, 4c). The further decrease leads to growth of the responses (and, probably, to chaotic motion). The initial values for all figures were taken identical, so the "spindle" form of trajectory on fig.5 is in discord with its counterparts on fig.3 and fig.4.
REFERENCES


MECHANICAL CHARACTERISTICS FOR CONCRETE AS A PERMEABLE MATERIAL BASED ON COUPLED PROBLEM WITH SOLID, LIQUID AND GAS PHASES

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Key words: Two Phase Material, Liquid Migration, Surface Tension, Cavitation.

Abstract. It is well known that the static and dynamic strength of cement based material are influenced by the water content, moreover its value is greatly dependent on the surface tension of the liquid. However, the mechanism for the effect of the surface tension of liquid on the solid strength has not been investigated yet. In the beginning, the cavitation phenomenon is incorporated to the developed model which is assumed to be a two phase porous material of solid and liquid and then the effect of the erosion of bubbles on the solid phase is estimated and compared with the experimental results.

1 INTRODUCTION

It is noted that the static or dynamic strength of the cement based materials such as the compressive, tensile and flexural strength are influenced by the water content and then it is reported that the gradual decrease of these behavior occur with the increase of water content [1][2][3][4]. Benedicks[3] and Hori[5] pointed out that the microcracks easily occur and propagate for the wetting specimens since the surface energy of solid phase decrease for the surface energy of liquid phase due to the presence of liquid. Therefore, it may be seen that the strength varies by the liquid type, namely the decrease of the strength of cement based materials occur with the increase of the surface tension of liquid [3][5][7][8]. However, the decrease of the strength simply is defined as an index such as the interface energy between the solid and liquid phase and therefore, its mechanism does not have been investigated yet.

On the other hands, Oshita et al.[6] pointed out that the water migration are expected to significantly affect the mechanical characteristics and then the positive pressure such as a disjoining pressure occurring in the elastic region causes the microcracks and the negative pressure occurring in the plastic region causes the crush between the solid phases due to the experimental and analytical procedures.

In this study, an extended mathematical model that incorporated the cavitation phenomenon in the model developed by authors[6] which is assumed to be a two phase porous material of solid and liquid is developed to investigate in microlevel the detailed mechanism such that the liquids with the different surface energy and its content influences on the decrease of the strength.
2 MECHANICAL BEHAVIOR DUE TO PRESENCE OF LIQUID

2.1 Influence of water content on strength

The representative research referring the effect of water content in concrete on the various strength is shown in figure 1. Figure 1 shows the relationship between the strength and water content[2].

![Figure 1](attachment:figure1.png)

(a) Compressive Strength (b) Splitting Strength

Figure 1: Effect of water content.

It can be seen that the compressive and tensile strength gradually decreases with the increase of the water content and therefore its value with drying is the most high. Okajima[2] expressed the dependency of water content on the tensile strength by modified the Griffith theorem taken into the reduction of the surface energy of solid by the adsorption of vapors account, as shown in following equation. However, its model does not show an agreement with the experiments since the stress concentration in the tip of cracks and microcracks are taken the Griffith theorem itself into account.

\[
\sigma_t = \frac{2E(\gamma_S - \Delta\gamma)}{\pi C}
\]  

where \(\sigma_t\) is the tensile strength, \(E\) is a young's modulus, \(C\) is half length of crack, \(\gamma_S\) is a surface energy of solid and \(\Delta\gamma\) is a interfacial energy between the solid and liquid which is a function of the relative humidity shown as Gibbs equation.

2.2 Influence of surface tension of liquid on strength

The representative research referring the strength characteristics of the mortar in which the pore are completely saturated the various liquids with the different surface tension is shown in figure 2. Figure 2 shows the relationship between the strength and the surface tension of the
liquid.

It can be seen that the decrease of each strength linearly occur with the increase of the surface tension except for the ethanol and methanol. It may be said that such strength behavior dependent on the surface tension of the liquid are caused by that the microcracks easily occur and propagate due to the reduction of the surface energy of the solid for the surface energy of liquid [5]. Namely, the strength seems to be proportional to the interface energy between the solid and liquid as shown in the following equations.

\[ \gamma_{sl} = \gamma_s - \gamma_l \rightarrow \sigma \propto \gamma_s - \gamma_l \]  

where \( \gamma_{sl} \), \( \gamma_s \) and \( \gamma_l \) are interface energy between solid and liquid, surface energy of solid and liquid, respectively. \( \sigma \) is the strength.

However, Matsushita[8] pointed out that the effect of the surface tension of the liquid on the strength behavior is different due to the water cement ratio (W/C) of the mortar and concrete material and then its effect becomes higher with the increase of W/C. This fact is that the strength behavior is dependent on the surface tension of the liquid, but not directly the interface energy between the solid and liquid. Therefore, the mechanism related the surface tension of the liquid to the occurrence and progress of cracks and the reduction of the strength are remained to be not clear. There is no doubt that the strength characteristics of the porous material such as the mortar and concrete are influenced by the surface tension of the liquid.

Figure 2: Effect of surface tension of liquid.

3 COUPLED ANALYTICAL MODEL WITH LIQUID AND SOLID PHASE

3.1 Modelling of concrete by saturated porous two phase material

In the analysis which is a coupled model In the analysis which is a coupled model with liquid and solid phase of concrete structure (called as Analysis 1) developed by authors[7], concrete is regarded as a porous material which is composed of aggregate, cement paste and water. Aggregate is considered as perfectly elastic material while cement paste is assumed to behave as an elasto-plastic permeable material.
(a) Formulation of equilibrium equation

With the presence of pore water pressure \( p \), the relation of effective stress \( \{\sigma'\} \) and total stress \( \{\sigma\} \) will become

\[
\{\sigma'\} = \{\sigma\} - \{m\}p
\]

(3)

where the sign of tensile stress is taken as positive and \( \{m\} = \{1 \ 1 \ 1 \ 0 \ 0 \ 0\}^T \).

The incremental effective stress-strain relation for concrete can be written as

\[
d\{\sigma'\} = [D^{ep}_s]\left[d\{\varepsilon'\} - d\{\varepsilon^{pr}\} - d\{\varepsilon^h\} - d\{\varepsilon^{pu}\}\right]
\]

(4)

where \([D^{ep}_s]\) is the elasto-plastic stiffness matrix of concrete where voids are not saturated with water, and \(d\{\varepsilon^{pr}\}\) is the incremental strain of solid phase resulted from the incremental pore water pressure \(dp\). Elasto-plastic stiffness of concrete can be written with the use of average elasto-plastic stiffness matrix of solid phase \([D^{ep}_s]\) and porosity \(\xi\) as follows.

\[
[D^{ep}_s] = (1 - \xi)[D^{ep}_s]
\]

(5)

\[
d\{\varepsilon^{pr}\} = -[D^{ep}_s]^{-1}\{m\}dp
\]

(6)

Then by using the principle of virtual work and appropriate shape function, the equilibrium equation can be written in differential form as

\[
K_T \frac{d\{\bar{u}\}}{dt} - L \frac{d\{\bar{p}\}}{dt} - \frac{d\{\bar{f}\}}{dt} = 0
\]

(7)

where matrices \(K_T\) and \(L\) are the tangential stiffness and effect of both pore water pressure and volume change of solid phase, respectively. The vector \(\{f\}\) denotes the effect of external force on displacement. These notations can be defined as follows.

\[
K_T = (1 - \bar{\xi}) \int_B^T D^{ep}_s B \ d\Omega \quad L = \bar{\xi} \int_B^T \{m\} \bar{N} \ d\Omega
\]

(8)

\[
\{\bar{f}\} = \int_B^T \{b\} \ d\Omega + \int_{\Gamma} N^T \{t\} \ d\Gamma
\]

where \(N\) and \(\bar{N}\) are the shape functions for displacement, pore water pressure, while \(B\) is the strain-displacement matrix.

(b) Formulation of Flow Continuity Equation

Water head \( h \) can be written as

\[
h = z + \frac{p}{\gamma}
\]

(9)

where \(z\) is the vertical coordinate of the point which is positive for upward direction, \(\gamma\) is the specific gravity of fluid. From the mass conservation law, the volume change in a unit volume \(\Delta V\) is equal to the difference of the amount of inflow \(q\) and outflow from this volume, which can be written as
\[ \Delta V = q - \nabla^T \{ v \} \quad (10) \]

where \( v \) is the flow velocity, which is considered to follow Darcy's law. The factors which contribute to the volume change can be summarized as follows.

- Due to total strain change
- Due to the change of volume of particles caused by changes of hydrostatic pressure
- Due to the change of fluid volume
- Due to the change of particle size by effective stresses

Substituting these factors into Eq. (10) and applying the Galerkin's method, Eq. (10) becomes in differential form as

\[ H\{ \bar{p} \} + S \frac{d\{ \bar{p} \}}{dt} + L^T \frac{d\{ \bar{u} \}}{dt} - \{ f_p \} = 0 \quad (11) \]

where

\[
H = \int_\Omega (\nabla \nabla)^T k \nabla \nabla d\Omega \\
S = \int_\Omega \nabla^T s \nabla d\Omega \\
L^T = \int_\Omega \nabla^T \{ m \} \nabla d\Omega \\
\{ f_p \} = \int_\Omega \nabla^T q d\Omega - \int_\Omega (\nabla \nabla)^T k \nabla \gamma d\Omega \\
s = \frac{\xi}{k_f}, \quad k' = \frac{k}{\gamma}
\]

(c) Formulation of Coupled Equations

The coupled equations which satisfy the force equilibrium and continuity condition can be written in the next matrix form.

\[
\begin{bmatrix} 0 & 0 \\ 0 & -[H] \end{bmatrix} \begin{bmatrix} \{ \sigma \} \\ \{ \overline{\sigma} \} \end{bmatrix} + \begin{bmatrix} [K_f] & -[L] \\ -[L]^T & -[S] \end{bmatrix} \begin{bmatrix} \frac{d\{ \bar{u} \}}{dt} \\ \frac{d\{ \bar{p} \}}{dt} \end{bmatrix} = \begin{bmatrix} \frac{d\{ f \}}{dt} \\ \{ f_p \} \end{bmatrix} \quad (13)
\]

In Eq. (13), if the initial conditions are known, it can be solved for both the displacement and the pore water pressure. The same equation can be transformed to the following form.

\[
\begin{bmatrix} [K_f] & -[L] \\ -[L]^T & -\Delta t [H] - [S] \end{bmatrix} \begin{bmatrix} \{ \Delta \bar{u} \} \\ \{ \Delta \overline{\sigma} \} \end{bmatrix} = \Delta t \begin{bmatrix} \frac{d\{ f \}}{dt} \\ \{ f_p \} \end{bmatrix} - \begin{bmatrix} [0] & [0] \\ [0] & [-H] \end{bmatrix} \begin{bmatrix} \{ \Delta \bar{u} \}_i \\ \{ \Delta \overline{\sigma} \}_i \end{bmatrix} \quad (14)
\]

where \( \{ \Delta \bar{u} \}_i \), \( \{ \Delta \overline{\sigma} \}_i \) are the nodal displacement and the nodal pore water pressure at the previous step.
Since, in the analysis, incompressibility of solid by pore pressure is assumed, porosity $\xi$ and the incremental strain of solid phase resulted from the incremental pore $d\{\varepsilon^p\}$ are ignored in the above equations.

### 3.2 Analytical estimation of compressive strength

In this section, the effect of the pore water pressure occurring in pore structure on the uniaxial compressive strength of concrete is discussed analytically. The analysis are performed for the perfectly drying state and perfectly saturated state with water. Figure 3 shows the relationship between the concrete stress and strain, figure (a) and (b) shows the average stress and the inside of concrete stress, respectively. In figure(a), the result of the drying concrete and saturated concrete are shown with solid line and dotted line, respectively. In figure(b), the stress at the center and surface neighborhood of the concrete are shown with solid and dotted line. Figure 4 shows the relationship between the pore water pressure and strain. In this figure, the result of the saturated concrete at the center and surface neighborhood of concrete are shown with solid and dotted line, respectively. Young’s modulus of the concrete in the elastic region used in the analysis is 1700MPa. In the plastic region, the initial cohesion is taken as a half of compressive strength and the final internal friction is taken as 27° for the failure surface. The permeability of liquid is $1.67 \times 10^{-8}\text{cm/s}$. The boundary conditions of the flow analysis are that the pore pressure at the surface of the concrete is equal to the atmospheric pressure.

As shown in figure 3(a), it may be seen that the compressive strength of the drying state is higher around 20% than that of saturated state. In the elastic region, there seems no difference of concrete stress between the both, but in the plastic region, the concrete stress of the drying state becomes gradually higher than that of the saturated state. On the other hands, as shown in figure 4, the positive pore pressure occurs and becomes the maximum value at the elastic limit of concrete. After yielding, the negative incremental pore pressure occurs due to the plastic expansion of the concrete and then the sudden decrease occur due to the progress of microcracks, finally becomes the slightly negative value. Concerning with the difference of the pore pressure behavior by the position, the maximum and minimum value at the center of the concrete is higher than that of surface, because the water migration cannot easily occur inside the concrete. Therefore, the effect of the pore pressure on the concrete stress becomes greater as the inside of concrete and then the value of the concrete stress becomes smaller. Namely, the positive pore pressure distributing a part of the external load is released and then the released stress transfer to the solid phase. As the result, the concrete stress reduces due to the occurrence and progress of microcracks caused by the increase of the compressive stress among the solid phase. These phenomenon gradually progress with the increase of the load and finally the concrete stress reaches the maximum value due to the occurrence of the negative pore pressure and then the failure occurs.
4 EXPANSION OF CAVITATION FLOW MODEL

4.1 Surface tension and cavitation

Once the pressure of the liquid becomes below the saturated vapor pressure, the bubbles as the nucleus such as an air, particles etc. occur in the liquid due to the evaporation caused by the boiling phenomenon, namely the cavitation phenomenon occurs. The pressure inside the bubbles have the value that only a value based on the Young-Laplace equation as follows has a bigger than the pressure of the liquid and the Young-Laplace equation shows that the difference between the pressure inside the bubble and of the liquid is dependent on the surface tension of the liquid and the diameter of the bubble. Therefore, the pressure inside the bubble becomes larger with the decrease of the diameter and the increase of the surface tension of the liquid. On the other hand, when the evaporation of the liquid gradually occurs toward the...
bubbles, the pressure inside the bubble becomes smaller with the gradual increase of the
diameter of bubble. Finally, the bubbles collide with and cling to the wall surface of the solid
by the liquid migration and after the surrounding liquid collapses the bubbles, the microcracks
occur on the solid surface due to the shock wave, namely the erosion occurs.

\[ p_G - p_L = \frac{2\gamma}{r_G} \]  

(15)

where \( p_G \), \( p_L \) are the pressure of bubble and liquid, respectively, \( r_G \) is a diameter of a
bubble, \( \gamma \) is a surface tension of the liquid.

The representative structures in which the cavitation is a very important problem such as
the fatigue fracture, the loss of the energy are the fluid machine such as the pomp, impeller,
vane wheel, screw etc. In the cement based materials, it may be seen that the cavitation
phenomenon easily occur under the circumstances that the pressure of the liquid becomes
below the saturated vapor pressure because there are much air, micro particles such as a dust,
unreacting cement etc. inside the pore which is able to becomes a nucleus and the bubbles are
easy to adsorb and cling to the rough wall surface of the micro porous structure.

The analytical method to estimate the cavitation erosion is a mainly surface tracking or
capturing model and a bubble flow method. The former is to estimate the bubble flow by
tracing and capturing the interface between the liquid and vapor considering the phase
changing for one or some bubbles. The latter is to estimate the liquid flow included the bubble
by one flow model which considers one density and one velocity (called as homogeneous
flow model) or two flows model which considers two densities, two velocities and
constitutive equation (called as bubble flow model). In this study, the bubble flow model is
introduced to Analysis 1 (called as Analysis 2). This model is a coupled procedure which
satisfy the bubble motion equation such as a Rayleigh-Plesset equation, the bubble number
density conservation and the bubble flow conservation for momentum, is applied to the liquid
flow in micro porous pore of the cement based material.

Rayleigh-Plesset equation, which describes a volumetric motion and an erosion behavior,
is expressed as following equation.

\[ \frac{\partial^2 r_G}{\partial t^2} + \frac{3}{2} \left( \frac{\partial r_G}{\partial t} \right)^2 = \frac{p_G - p_L}{\rho_L} + \frac{1}{4} \left( v_{Li} - v_G \right) \left( v_{Li} - v_G \right) t \]  

(16)

where \( v_G \), \( v_L \) are a velocity of the bubble and liquid, respectively, \( \rho_L \) is a density of the
liquid, \( t \) is a time, a subscription \( i \) is a direction and the pressure inside a bubble \( p_G \) can be
expressed as follows.

\[ p_G = p_B + p_V - \frac{2\gamma}{r_G} - 4\mu \frac{1}{r_G} \frac{\partial r_G}{\partial t} \]  

(17)

where \( p_B \) is a pressure of incondensable gas, \( p_V \) is a saturated vapor pressure and \( \mu \) is a
coefficient of viscosity.

Void ratio \( f_G \) can be expressed as follows by assuming a bubble to be a sphere.

\[ f_G = \frac{4}{3} \pi r_G^3 n_G \]  

(18)

where \( n_G \) is a bubble number density.
Then the density of the liquid included the bubbles $\rho$ is can be written as follows by assuming the bubble density to be zero.

$$\rho = (1 - f_G)\rho_L$$  \hspace{1cm} (19)

where $\rho_L$ is a liquid density.

The coefficient of the viscosity is expressed as follows.

$$\mu = (1 - f_G)\mu_L + f_G\mu_G$$  \hspace{1cm} (20)

where $\mu_L$, $\mu_G$ are a coefficient of the liquid and bubble viscosity, respectively.

This research is located the fundamental one which estimate the effect of cavitation erosion in micro pores of the cement based materials on the strength. Therefore, in this study, the following assumptions are introduced in analysis.

Bubble is compressibility and liquid is incompressibility.

All bubbles are assumed to be sphere, incorporation and separation does not occur.

Bubble is saturated with the air and vapor phase does not change and materials does not transfer at the liquid-vapor interface.

Bubble density is small to be able to ignored compared with liquid density.

There is no difference between liquid and bubble velocity.

Ignore the coefficient of viscosity of liquid and bubble.

### 4.2 Compressive strength due to surface tension

In this section, the effect of the cavitation erosion on the strength is discussed in detail due to the comparison between the results of Analysis 1 in section 3.1 and Analysis 2 shown in section 4.1.

<table>
<thead>
<tr>
<th>Table 1: Liquid property</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liquid</td>
</tr>
<tr>
<td>Surface Tension (dyn/cm)</td>
</tr>
<tr>
<td>Saturated Vapor Pressure at 20°C (kPa)</td>
</tr>
</tbody>
</table>
Analyses are performed in the state such that the mortar are perfectly dried, in which pore are perfectly saturated with water and aniline. The surface tension and saturated vapor pressure for the water and aniline are quite different as shown in Tab.1. Young’s modulus of the mortar used in analysis is 25GPa. In the plastic region, the initial cohesion is taken as a half of compressive strength and the final internal friction is taken as 27° for the failure surface. The permeability is $1.67 \times 10^{-8}$ cm/s. The volumetric elastic modulus of the water and aniline are 2.2 MPa and 1.1 MPa, respectively. The boundary conditions of the flow analysis are that the pore pressure at the surface of the concrete is equal to the atmospheric pressure.

Figure 5 shows the relationship between the compressive strength ratio and the surface tension of the liquid and the compressive strength ratio is defined as the strength of the mortar immersed in the liquid normalized by that of drying mortar. In this figure, the experimental results are marked with circles and the analytical result of Analysis 1 and Analysis 2 are marked with square and triangle respectively.

As shown in figure 5, Analysis 2 shows a good agreement with the experimental results for both the liquid of water and aniline. On the other hand, Analysis 1 shows a good agreement with the experiment for the aniline having a relatively small surface tension, but for the water having a large surface tension, Analysis 1 shows a quietly different from the experiments. Namely, for the liquid with a larger surface tension, it may be seen that the strength is influenced by not only the pore pressure, but also the surface tension. This seems to be caused by the difference between the pressure inside and outside the bubble is relatively larger.

5 CONCLUSIONS

In this study, an extended mathematical model which is introduced the cavitation phenomenon into the coupled model of solid and liquid phase is developed to investigate the detailed mechanism for the effect of the surface tension of liquid on the solid strength. It is concluded by the comparison between the experimental and analytical results that the strength is influenced by not only the pore pressure occurring in liquid phase, but also the cavitation erosion in micro pore of the porous materials.
REFERENCES

NUMERICAL INVESTIGATION ON ANTI-ICING PERFORMANCE OF HEATING SURFACE FOR NACA0012 AIRFOIL

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Key words: Ice Accretion, Anti-Icing Method, Airfoil, Heating Surface, Super-Cooled Water Droplet.

Abstract. Ice accretion is a phenomenon that super-cooled water droplets impinge and accrete on wall surfaces. It is known that icing can cause severe accidents. To prevent the icing, an electro-thermal heater is recently adopted as the de- and anti-icing device for wings. In the present study, we conducted icing simulations of a two-dimensional NACA0012 airfoil with an electro-thermal heater on the leading-edge surface to optimize the heating area. The attack angle and the heating area were changed from 0 to 4 degrees and from 0 to 2.0% chord length, respectively. Through the simulations, we found that the lift coefficient was significantly improved by the heating, the drag coefficient generally decreased with increasing the heating area, and at the attack angle of 0 degree and the heating area of 1.0% chord length, the drag coefficient exceptionally became worse because of the residual ice shape with horns.

1 INTRODUCTION

Icing is a phenomenon that super-cooled water droplets collide on a solid surface and it forms an ice layer on the surface. The icing problem occurs for many industrial apparatuses such as power lines, buildings, cars, ships, aircraft wings, jet engines and so on. For aircraft wings, the icing makes ice layer and roughness on the surface and they lead a drastic decrease of aerodynamic performance. Therefore, the icing is one of the reasons to cause a fatal accident of aircraft. To prevent the accident, the prediction of icing and the development of de- and anti-icing techniques are very important from the viewpoints of aircraft safety. As the de- and anti-icing techniques, bleed air, anti-freezing liquid and an electric heater have been proposed and implemented for aircraft. Because of the easy setting and the low environmental burden, the electric heater has recently been adopted in current aircraft. We can find a number of technical papers on icing in the literature. For example, Al-Khalil et al. [1] performed experimental and numerical studies of icing on the wing with the electric heater. They reported the effect of the different heating temperatures of the electric heater. Bu et al. [2] conducted the icing simulation...
of a wing with considering heat flux from the wing surface. Reid et al. [3] performed the numerical simulation of an electric-thermal de-icing system, and they reported the temporal variation of surface temperature for the de-icing process. However, the research focusing on the heating area of the electric heater has not been conducted yet.

Taking into account these backgrounds, in the present study, we perform two-dimensional icing simulations of NACA0012 airfoil to investigate the effect of the heating area on the aerodynamic performance. Through this study, the influences of heating area on the residual ice formation, the drag and the lift of the airfoil and energy consumption are clarified.

2 NUMERICAL PROCEDURE

The numerical simulation consists of four steps: (1) generation of computational grids; (2) computation of flow field; (3) computation of droplet trajectories and collection efficiency; (4) thermodynamics computation. According to them, we can obtain ice shape on the airfoil. In the following, the details of each numerical procedure are briefly explained.

The computational target is a NACA0012 airfoil. The computational grid is shown in Fig. 1. The overlap grid is employed. The main is used to simulate the whole flow field around the airfoil, and as shown in Fig. 1, the sub grid has high resolution to correctly obtain the ice shape around the leading edge and the boundary layer on the airfoil. The total number of grid points is about 26,000. The convergence of the ice shape by the grid points has preliminarily been confirmed through the grid independent study.

The flow around the airfoil is assumed to be two-dimensional, compressible, and fully turbulent. The governing equations are the continuity, Navier-Stokes, energy equations and transport equations of the turbulent kinetic energy $k$ and its dissipation rate $\epsilon$. The Kato-Launder $k-\epsilon$ turbulent model [4] is employed to suppress the over-production of turbulence around the leading edge region.

The droplet trajectory is computed based on the Lagrangian approach. Since the size of droplet and the concentration are small enough, a one-way coupling method is employed. That is, the droplet motion is affected from the flow field, whereas the droplet does not affect the flow field. The motion equation of a droplet is a simplified BBO equation as

$$\frac{dU_d}{dt} = \frac{3}{4} C_D \frac{\rho_g}{\rho_d} \frac{1}{d_d^4} \frac{d}{d} \mathbf{U}_r |\mathbf{U}_r|. \quad (1)$$

Here, $\mathbf{U}_d$ is the velocity of a droplet and $\mathbf{U}_r$ is the relative velocity between the flow and the droplet. $\rho_g$ and $\rho_d$ are the density of the gas (i.e. air) and the droplet respectively, $d_d$ is the diameter of the droplet, and $C_D$ is the drag coefficient. Since we suppose that the droplet does not deform and rotate, as the drag coefficient of a sphere, Schiler model [5] is used, which is defined as

$$C_D = \frac{24 \left( 1 + 0.15 \text{Re}^{0.687} \right)}{\text{Re}} \quad (2)$$

where Re is the droplet Reynolds number based on the droplet diameter, the relative velocity, density of the fluid $\rho_f$, and viscosity of the fluid $\mu_f$. 

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In the thermodynamics computation, since the time scales of the flow field and the icing are significantly different, we use the weak coupling method. The Extended Messinger Model [6] (referred as EMM, hereafter) is adopted as the icing model. The EMM is based on the mass and energy conservation law of the ice and water and the equation for phase change at the interface between the ice and the water. Although the EMM is widely used in icing simulations, the surface heating and the temperature of run-back water are not considered. Thus, in the present study, we improve the EMM to reproduce them as follows. First, the heat flux is computed by the temperature of the colliding droplet. Second, the temperature and thickness of the ice or water film are computed. If the temperature is over 0 degree Celsius, the adhered droplet is treated as a water film.

![Figure 1](image_url) Computational domain and grid. Left and right figures represent the entire computational domain and the enlarged view of sub-grid around airfoil, respectively. Main and sub grids are colored in red and blue, respectively.

The computational conditions are tabulated in Table 1, which are set in accordance with the experimental study performed by Olsen et al. [6]. In the present study, the anti-icing simulation of the NACA airfoil is carried out and therefore the surface of the airfoil is partially heated. At the heated region, the constant temperature is fixed, and at the other region, the adiabatic condition is imposed. The three different angle of attack and heating-region cases are examined as tabulated in Table 2. The heater temperature is set to be 5.0 °C for all cases with heating.

<table>
<thead>
<tr>
<th>Table 1: Computational conditions</th>
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</thead>
<tbody>
<tr>
<td>Static Temperature [°C]</td>
</tr>
<tr>
<td>Accretion Time [sec.]</td>
</tr>
<tr>
<td>Inflow Velocity [m/s]</td>
</tr>
<tr>
<td>MVD (Median Volume Diameter) [µm]</td>
</tr>
<tr>
<td>LWC (Liquid Water Content) [g/m³]</td>
</tr>
<tr>
<td>Chord Length [m]</td>
</tr>
<tr>
<td>Attack Angle [deg.]</td>
</tr>
<tr>
<td>Ambient Pressure [kPa]</td>
</tr>
<tr>
<td>Exposure Time [s]</td>
</tr>
</tbody>
</table>
Table 2: Parameters of test cases

<table>
<thead>
<tr>
<th>Case</th>
<th>A00</th>
<th>A01</th>
<th>A02</th>
<th>A20</th>
<th>A21</th>
<th>A22</th>
<th>A40</th>
<th>A41</th>
<th>A42</th>
</tr>
</thead>
<tbody>
<tr>
<td>Attack Angle [deg]</td>
<td>0.0</td>
<td>2.0</td>
<td>4.0</td>
<td>0.0</td>
<td>1.0</td>
<td>2.0</td>
<td>0.0</td>
<td>1.0</td>
<td>2.0</td>
</tr>
<tr>
<td>Heating Area $x/c$ [%]</td>
<td>0.0</td>
<td>1.0</td>
<td>2.0</td>
<td>0.0</td>
<td>1.0</td>
<td>2.0</td>
<td>0.0</td>
<td>1.0</td>
<td>2.0</td>
</tr>
</tbody>
</table>

Figure 2 Streamline and ice shape of the airfoil. White regions represent adhered ice shape, and the color of the streamlines denotes the flow speed.

3 RESULT AND DISCUSSION

Figure 2 shows the accreted ice shapes and streamlines for cases consisting of clean, A20, A21, and A22. The color of the streamlines denotes the flow speed. In Fig. 2 (b), the large ice is formed around the leading edge, and recirculation regions appear behind the ice. Owing to add the heater, as shown in Fig. 2 (c) and (d), the ice at the leading edge of the wing vanished, though the small ice remains at the downstream of heater. However, the recirculation regions disappear in applying the heater. Obviously, ice formation strongly depends on the heating area and the attack angle.

Figure 3 indicates lift coefficient $C_l$ and normalized drag to represent the aerodynamic performance. Without heating, $C_l$ increase non-linearly with the increase of the attack angle. By applying the heater, $C_l$ drastically recovers and increases almost linearly with the increase of the attack angle. Therefore, the heater works well to prevent a lift loss even in applying 2.0% chord length. On the other hand, the drag distributes more complexly. Interestingly, in case that the attack angle is 0.0 degree, the drag increases by setting the 1.0% heater in comparison to the without heating case. Then, the drag decreases by applying the 2.0% heater. In the cases
that the attack angle is 2.0 degrees, the drag decreases with expanding heating area. However, in case that the attack angle is 4.0 degrees, the drag increases with expanding heating area. Clearly, the drag distribution changes irregularly by the heating area.

Figure 4 shows the heating power ratio normalized by the thrust power. The heating power ratio decreases by increasing the attack angle and heating area. It is confirmed that the heating ratio is less than 0.4%, therefore, the heating power is extremely lower than the trust power.

Figure 3: Lift coefficient (left) and drag change from the clean airfoil (right). The drag is normalized by the drag for clean airfoil at the same attack angle.

Figure 4: Heating power ratio against thrust power.
4 CONCLUDING REMARKS

The icing simulation of a NACA0012 airfoil is performed to investigate the effect of the surface heating area on the icing and the aerodynamic performance. The Extended Messinger model for the thermodynamics calculation is modified to simulate the heated surface. As a result, the findings obtained in this study are as follows.

➢ Ice formation strongly depends on the heating area and the attack angle of the airfoil.
➢ In the unheated case, the large ice forms around the leading edge and induces the flow separation behind the ice. It results in the increase of the fluid drag.
➢ The heater applied at the leading edge prevents the ice formation, and it significantly improves the aerodynamics performance, i.e., increase of lift coefficient.
➢ For the case that attack angle is 0.0 degree, the drag coefficient increases at the case of 1.0% heating area, while it decreases at the case of 2.0% heating area.
➢ The heating power is very small comparing the thrust power.

REFERENCES

INTERFACIAL STRESSES IN BIMATERIAL COMPOSITES
WITH NANOSIZED INTERFACE RELIEF

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Key words: Bimaterial Composites, Nanomaterials, Interfacial Stress, 2-D Problem, Boundary Perturbation Method, Finite Element Method

Abstract. The paper compares analytical and numerical solutions for two-dimensional solid mechanics problems of elastic bimaterial composites with a nanosized interface relief that arises on a boundary between two bulk layers and on an interface of a nearly circular inclusion. It is supposed that the uniform stress state takes place at infinity. Here, we use Gurtin–Murdoch model in which interphase domains are represented as negligibly thin layers ideally adhering to the bulk phases. Static boundary conditions at the interface are formulated according to the generalized Laplace–Young law. To solve corresponding boundary value we use first-order boundary perturbation method based on Goursat–Kolosov complex potentials. To examine the perturbation results, we use a finite element calculations.

1 INTRODUCTION

At the macrolevel, the effect of surface/interface energy for a stressed solid is ignored as it is small compared to the bulk energy [1]. However, the surface/interface effects become significant for nanoscale materials and structures due to the high surface-to-volume ratio. Stress fields in the vicinity of nanosized structures can appreciably depend on the surface energy and surface stresses, which was first proposed by Gibbs [2]. As a result, the surface/interface stresses are directly related to the size effect, that means the material properties of a specimen depend on its size. To explain the surface phenomena, Gurtin and Murdoch developed the surface elasticity theory [3, 4] which is based on the concept of the surface strain energy and surface stress. The continuum surface/interface stress model assumes that solid consists of bulk and surface phases which are perfectly bonded and have different elastic properties. This theory was confirmed by molecular dynamics
simulations [5]. In numerous papers, a finite element modeling was presented to explore the effects of surface/interface stresses in nanoscale structures (see, for example, [6, 7]). In summary, the consideration of these models helps to understand the unusual elastic properties of nanomaterials.

In the work [8], boundary perturbation method (BPM) was used to solve the problem of an elastic infinity plane with a nearly circular inclusion at the macrolevel. The influence of surface stress on an elastic materials containing the nanosized topological defects at external boundary and at internal void boundary was investigated in [9]. Special features of the surface layer behavior in a stressed material particularly is that an initially smooth surface becomes rough under a number of natural phenomena: heat, light, short-wavelength electromagnetic radiation, radioactive emissions, chemicals, mechanical stress, etc. [10]–[14].

Based on the approaches developed in [8, 9, 15], we study the effect of interfacial stresses on stress-strain state of elastic bimaterial with a smooth undulated interface. We consider the 2-D solid mechanics problems of elastic bimaterial composites with a nanometer interface relief that arises between two different bulk layers (the first problem) and between a nearly circular inclusion and a matrix (the second problem). It is supposed that the uniform stress state takes place at infinity. Here, we use Gurtin–Murdoch model [3, 4] in which interphase domains are represented as negligibly thin layers ideally adhering to the bulk phases. Static boundary conditions at the interface are formulated according to the generalized Laplace–Young law [16]. To solve corresponding boundary value we use first-order boundary perturbation method based on Goursat–Kolosov complex potentials. As a result, we come to the hypersingular integral equations in the unknown interfacial stress for any-order approximation of the perturbation procedure. The numerical results are given for a first-order approximation. To examine the perturbation results, we use finite element method (FEM).

2 FORMULATION OF THE PROBLEM

The first problem is following: we consider an elastic isotropic bimaterial with slightly perturbated interface under the uniaxial tension (Fig. 1). It is assumed that the interface profile is defined by the periodic function (1). The interface domain has an elastic properties which differ from the bulk ones. Following Gurtin–Murdoch model of surface elasticity [3, 4], this domain is represented as a negligibly thin layer \( \Gamma \) adhering to the bulk phases \( B_1 \) and \( B_2 \) without slipping:

\[
\Gamma = \{ z : z = x_1 - i \varepsilon_1 a \cos (b x_1) \}, \quad b = \frac{2 \pi}{a}, \quad \varepsilon_1 = \frac{A}{a} \ll 1
\]

\[
B_1 = \{ z : x_2 < \varepsilon_1 a \cos (b x_1) \}, \quad B_2 = \{ z : x_2 > \varepsilon_1 a \cos (b x_1) \},
\]

where \( a \) is the wavelength of perturbation, \( b \) is the wavenumber and \( \varepsilon_1 \) is the small parameter.
The second problem describes an elastic plane with a nearly circular nanoinclusion (Fig. 2). In this case the interface between the matrix and inclusion $\Gamma$ is defined by the relation:

$$\Gamma = \{ z : z \equiv \zeta = r (1 + \varepsilon_2 \cos 2\theta) e^{i\theta} \}, \quad (2)$$

where $\varepsilon_2$ is the small parameter which is equal to the maximum deviation of the interface from the circular one of radius $r$, $\varepsilon_2 > 0$, $\varepsilon_2 \ll 1$. 

Figure 2: Interface profile of the nanoinclusion described by the cosine function (firm line) for $r = 1$ nm and $\varepsilon_2 = 0, 1$. 

**Figure 1:** A model of bimaterial with curved interface under uniaxial tension.
In equations (1) and (2), \( z = x_1 + ix_2 \) is the complex variable (\( i \) is the imaginary unit). The elastic properties of each domain \( B_k, \Omega_k, k = 1, 2 \), are determined by the Poisson’s ratio \( \nu_k \) and shear modulus \( \mu_k \).

We assume that the discontinuity of the displacement on the interface \( \Gamma \) between two domains is absent and the stress jump \( \Delta \sigma^k (k = 1, 2) \) is determined by the interfacial stress \( \tau \) according to the generalized Laplace–Young law [9, 15]. The contact conditions can be written in the form

\[
\Delta \sigma_n(\zeta) = \sigma_n^+ - \sigma_n^- = \frac{\tau}{R} - i \frac{1}{h} \frac{d\tau}{d\theta} \equiv t^s(\zeta), \quad \Delta u(\zeta) = u^+ - u^-. \tag{3}
\]

Stresses \( \sigma_{ij} \) (\( i, j = 1, 2 \)) and the rotational angle \( \omega \) of a material particle are specified at infinity as

\[
\lim_{z \to \infty} \sigma_{ij} = \sigma_{ij}^\infty, \quad \lim_{z \to \infty} \omega = 0.
\]

Here, \( \sigma_n = \sigma_{nn} + i\sigma_{nt} \), \( \sigma_{nm}, \sigma_{nt} \) are the components of stress vector \( \sigma_n \) at the area with the normal \( n \) in the local Cartesian coordinates \( n, t \); \( u = u_1 + iu_2 \), \( u_1, u_2 \) are the displacements along axes of the global Cartesian coordinates \( x_1, x_2 \); \( \tau \) is the interfacial stress. In equation (3), \( \sigma_n^+ = \lim_{z \to \zeta \in \Gamma} \sigma_n(z), u^+ = \lim_{z \to \zeta \in \Gamma} u(z), h \) is the metric coefficient [17] and \( R \) is the curvature radius of the boundary. The superscript “−” corresponds to \( z \in B_1 \) for the first problem and \( z \in \Omega_1 \) for the second problem; “+” to \( z \in B_2 \) and \( z \in \Omega_2 \), correspondently.

According to [3, 4], constitutive relations of surface and bulk elasticity theory, in the case of the plane strain, are defined as

\[
\tau = (\lambda_s + 2\mu_s)\varepsilon_{tt}^s, \quad \sigma_{nt} = 2\mu\varepsilon_{nt}, \tag{4}
\]

\[
\sigma_{nn} = (\lambda + 2\mu)\varepsilon_{nn} + \lambda\varepsilon_{tt}, \quad \sigma_{tt} = (\lambda + 2\mu)\varepsilon_{tt} + \lambda\varepsilon_{nn}. \tag{5}
\]

In equations (4) and (5), \( \sigma_{ij} \) is the stress tensor component, \( \varepsilon_{tt}^s \) and \( \varepsilon_{ij} \) are the components of the surface and bulk strain tensors, \( \lambda, \mu \) (\( \lambda_s, \mu_s \)) are Lame constants of the bulk (surface) material.

From the continuity condition of the displacement, passing from two domains to the interface \( \Gamma \), we obtain the inseparability condition of the surface and the bulk (see [9, 15, 18]), expressed in terms of hoop strains:

\[
\lim_{z \to \zeta} \varepsilon_{tt}^k(z) = \varepsilon_{tt}^\infty(z), \quad k = 1, 2.
\]
3 INTEGRAL EQUATION OF N-ORDER APPROXIMATION

According to [15, 19], the relation of the stresses and the displacements with complex potentials \( \Phi_k(z) \) and \( \Psi_k(z) \) can be written as

\[
G(z, \eta_k) = \eta_k \Phi_k(z) + \overline{\Phi_k(z)} + \left[ z \overline{\Phi_k(z)} + \Psi_k(z) \right] \frac{d\bar{z}}{dz},
\]

where \( z \) is the point anywhere in the domains.

It is important to note that

\[
G(z, \eta_k) = \begin{cases} 
\sigma_n, & \eta_k = 1, \\
-2\mu_k \frac{du}{dz}, & \eta_k = -\kappa_k,
\end{cases}
\]

where \( \kappa_k = (3 - \nu_k)/(1 + \nu_k) \) for the plane stress state and \( \kappa_k = 3 - 4\nu_k \) for the plane strain; \( d\bar{z} = |dz| e^{i\alpha}, \frac{d\bar{z}}{dz} = \alpha \) is the angle between the direction \( \mathbf{t} \) of the area and the \( x_1 \) axis. Functions \( \Phi_k(z) \) and \( \Psi_k(z) \) are holomorphic in the corresponding domains \( B_k \) for the first problem and \( \Omega_k \) for the second problem.

Following the BPM [8, 9, 15], the complex potentials \( \Phi_k(z) \), \( \Psi_k(z) \) and the interfacial stress \( \tau \) are sought in terms of power series in a small parameter \( \varepsilon_k, k = 1, 2 \). The problem is reduced to the solution of two independent Riemann – Hilbert’s boundary problems [8]. With the help of Goursat – Kolosov complex potentials, Muskhelishvili’s representations [20], the BPM and simplified Gurtin – Murdoch surface elasticity theory, the solution of the first type of the problem leads to the successive solution of hypersingular integral equation in the unknown functions \( \tau_n, n = 0, 1, \ldots [9] \)

\[
\tau_n'(x_1) - \frac{M(\kappa + 1)}{2\pi} \int_{-\infty}^{\infty} \frac{\tau_n'(t)}{(t - x_1)^2} dt = F_n(x_1), \tag{6}
\]

and the solution of the second type of the problem leads to the similar equation

\[
[2a - M(\kappa - 1)] \tau_n(\eta) + \frac{M(\kappa + 1)}{2\pi i} \int_{|\xi|=1} \frac{(\xi + \eta^2/\xi)\tau_n(\xi)}{(\xi - \eta)^2} d\xi = G_n(\eta), \quad |\eta| = 1, \tag{7}
\]

where \( M = (\lambda_s + 2\mu_s)/2\mu; \ \kappa = (\lambda + 3\mu)/(\lambda + \mu) \); functions \( F_n, G_n \) depend on all previous solutions.

4 NUMERICAL RESULTS

The elastic properties are defined by Lame constants \( \lambda_1 = 58, 17 \) GPa, \( \mu_1 = 26, 13 \) GPa for the bulk domains \( B_1 \) and \( \Omega_1 \) and \( M = M_1 = 0, 117 \) nm when \( \lambda_s = 6, 851 \) N/m and \( \mu_s = -0, 376 \) N/m for the interface domain [5, 21]. In this study, we assume elastic
properties of the bulk domain $B_2$ ($\Omega_2$) are related with those for $B_1$ ($\Omega_1$) as follows: $m = \mu_2/\mu_1 = 1/3$, where $m$ is stiffness ratio. Poisson’s ratio $\nu_1 = \nu_2 = 0.34$.

We have verified our numerical results taken from the above first-order approximation by comparing with those of finite element calculations within ANSYS program. The finite element models for two types of considered problems are shown in Fig. 3 and Fig. 4. Following [6], the bulk and the interface layers are considered as different phases with different elastic properties. The model is built of high-order 2-D 6-node triangular elements ”plane183” with an intensively-refined mesh near the interface region that allows us to approximate the interface between two phases with high accuracy. The interface region is meshing by 1-D 2-node elements ”link180” with unitary cross-section area.

![Finite element models of elastic bimaterial composites](image)

**Figure 3**: Finite element models of elastic bimaterial composites with the nanometer interface relief that arises between two different bulk phases (one perturbation (a)) and between the nearly circular inclusion and the matrix (quarter of solid (b)) when $\varepsilon_1 = \varepsilon_2 = 0, 1$.

Owing to the periodicity of the interface profile for the first problem, it is enough to consider only 5 perturbation periods in the numerical calculation (Fig. 3a). On the symmetry plane ($x = 0$) the displacement $u_x$ is assumed to be zero. The right boundary of the domain $B_1$ is subjected to a constant load $\sigma_1$. Since we assume that the upper half-plane $B_2$ and lower half-plane $B_1$ are coherent, the load $\sigma_2 = \sigma_1 m$ is applied on the right boundary of the domain $B_2$. The interface is considered as domain with elastic properties which differ from those for both bulk phases $B_1$ and $B_2$. Using FEM and BPM we studied effect of interfacial stress on the stress-strain state of the bimaterial composite. Fig. 5a reveals the stress concentration factor (SCF) $S_1^a = \sigma_{1t}/\sigma_1$ as a function of perturbation wavelength $a$ for $\varepsilon_1 = 0, 1$ and $m = 1/3$. The dotted line is plotted for $M = M_1$ using the first-order approximation of BPM. FEM calculations of SCF $S_1^a$ for different wavelength...
Figure 4: The stress state of the considered problems when $\varepsilon_1 = \varepsilon_2 = 0, 1$.

$a$ and $M = M_1$ are marked by crosses. It is shown that both solutions come to constant values with increase of $a$. Dashed line correspond to the classical solution ($M = 0$) in the case surface elasticity is neglected.

For the second problem, we investigate the stress field plane containing the nearly circular nanoinclusion with the interface relief described by the function $f(\theta) = \cos 2\theta$ (Fig. 2). Using simplified Gurtin–Murdoch surface elasticity theory and BPM [15], the solution for this problem is reduced to the singular integro-differential equation for any-order approximation (7). For the inclusion described by the cosine function when $\varepsilon_2 = 0, 1$ and $r = 2$ nm, in the first-order approximation SCF $S_{1a}^2 = \sigma_{tt}^1 / \sigma_{tt}^\infty$ is equal 1.77 and $S_{2a}^2 = \sigma_{tt}^2 / \sigma_{tt}^\infty$ is equal 0.72, here $\sigma_{tt}^k$ is hoop stress in the matrix ($k = 1$) and in the inclusion ($k = 2$). Fig. 5b reveals the SCF $S_{ka}^k$, $k = 1, 2$ ($\theta = 0$) along the boundary of almost circular nanoinclusion for the matrix $k = 1$ (blue lines) and for the inclusion $k = 2$ (red lines) upon the radius $r$ in the case of the uniaxial tension $\sigma_{tt}^\infty$ along axis $x_2$, i.e., for $\sigma_{tt}^1 = \sigma_{tt}^\infty = 0, \sigma_{tt}^\infty > 0$ when $\varepsilon_2 = 0, 1$ and $m = 1/3$. The dotted lines are plotted for $M = M_1$ using the first-order approximation of BPM. FEM calculations of SCF $S_{hn}^k$, $k = 1, 2$ when $M = M_1$ are marked by crosses. The stress field near the nanoinclusion under the uniaxial tension is shown in Fig. 4b. Dashed lines also correspond to the classical solution when $M = 0$.

5 CONCLUSIONS

We have analyzed the mathematical models of the nanopatterned interphases region of two coherently bonded elastic solids and an elastic body with a nearly circular nanoinclusion. In particular:
• Analytical solutions of considered problems in any-order approximation of BPM is obtained. The effect of interfacial stress on stress-strain state of bimaterial composites near the interface is investigated using first-order approximation. As it was shown, with the increase of the wavelength perturbation $a$ and the radius $r$ of the basic circular inclusion, the maximum hoop stresses at the interface tends to the classical solution when the interfacial stress is not considered. However, with the decrease of the wavelength perturbation $a$ and the radius $r$, the SCF decreases indefinitely when $M = M_1$. This fact illustrates the size effect as a dependence of the stress state on the size of the interface boundary topological defects.

• To verify the obtained analytical solutions, the considered problems were also solved using FEM. Analytical results for smooth undulated surface when $\varepsilon_1 = \varepsilon_2 = 0, 1$ are in a good agreement with FEM calculations. The relative differences between solutions obtained by the describes approaches less than 10% for the first problem and does not exceed 16% for the second problem. Moreover, this results confirmed the previous studies. By increasing the size parameters of the interface boundaries, we came to the solutions obtained in the studies [8, 18], where interface elastic properties was neglected. However, as the small parameter increases, the relative difference between FEM and first-order BPM solutions increase [22, 23]. As a result, it’s important to take into account the nonlinear terms of the perturbation solution.

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REFERENCES


AN ENERGY-MOMENTUM CONSISTENT TIME INTEGRATION SCHEME BASED ON A MIXED FRAMEWORK FOR NON-LINEAR ELECTRO-ELASTODYNAMICS

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Abstract. The objective of the present work is the introduction of new mixed variational principles for EM time integrators in electromechanics, hence bridging the gap between the previous work presented by the authors in References [11] and [1], opening up the possibility to a variety of new Finite Element implementations.

1 Introduction

Dielectric elastomers represent an important family of Electro Active Polymers (EAPs) which are well-known for their outstanding actuation capabilities and low stiffness properties, which makes them ideal for their use as soft robots. Very recently, the authors in [11] proposed a new energy-momentum (EM in the sequel) preserving time integrator [15, 9, 14] for reversible electro-elastodynamics building upon [6]. As shown in [11], the new EM time integrator proved to be very robust and accurate for the long-term simulation of EAPs. The consistent implicit EM time integration scheme developed inherits the conservation laws of total energy,
linear momentum, angular momentum and electric charge. Specially relevant for
the work carried out in this work is the recent work by Betsch et al. [1], where
a new consistent EM time integration scheme has been developed in the context
of polyconvex elasticity. In comparison to previously proposed discrete derivative
expressions (see e.g. [9]), the new stress formula in [1, 6] assumes a remarkably
simple form. A key factor for that simplification is the use of a tensor cross product
pioneered by the Boer [4] and employed for the first time by Bonet et al. [2] in the
case of nonlinear electromechanics [8, 13, 12]. Building upon the work presented
in [11] and [1], the objective of this paper is to develop a new EM time integrator
in the context of electro-elastodynamics based on a mixed variational formulation.
The resulting new formulation opens up several possibilities in terms of its spatial
discretisation and subsequent computational finite element implementation.

2 Nonlinear continuum electromechanics

A brief introduction into nonlinear continuum electromechanics and the relevant
governing equations will be presented in this section.

2.1 Kinematics: motion and deformation

Let us consider the motion of an EAP with reference configuration \( B_0 \in \mathbb{R}^3 \)
and its boundary \( \partial B_0 \) with unit outward normal \( N \). During its motion, the EAP
occupies a deformed configuration \( B \in \mathbb{R}^3 \) with boundary \( \partial B \) and unit outward
normal \( n \). The motion of the EAP is defined by the mapping \( \phi(X, t) \), which
links a material particle from the reference configuration \( X \in B_0 \) to the deformed
configuration \( x \in B \) according to \( x = \phi(X, t) \). Associated with \( \phi(X, t) \) it is
possible to define the deformation gradient tensor \( F_\phi \) [3] as

\[
F_\phi = \nabla_0 \phi(X, t); \quad F_{\phi i I} = \frac{\partial \phi_i}{\partial X_I}.
\]

The deformation gradient tensor \( F_\phi \)\(^1\) relates a fibre of differential length from
the material configuration \( dX \) to the deformed configuration \( dx = F_\phi dX \). In addition, differential area vector and volume elements in the reference configuration,
\( dA \) (colinear with \( N \)) and \( dV \) respectively, are mapped to the deformed configuration
\( da \) (colinear with \( n \)) and \( dv \), respectively, by means of the co-factor or adjoint
tensor \( H_\phi \) as \( da = H_\phi dA \) and the Jacobian \( J_\phi \) as \( dv = J_\phi dV \), respectively. Both
\( H_\phi \) and \( J_\phi \) can be related to \( F_\phi \) as

\[
H_\phi = (\det F_\phi) F_\phi^{-T}; \quad J_\phi = \det F_\phi.
\]

\(^1\)Subscript \( \phi \) is included throughout the paper in order to emphasise the geometrically exact
deformation term.
Equivalent expressions to those in (2) can be obtained by making use of the tensor cross product operation introduced by de Boer [4] and defined as

\[ H_\phi = \frac{1}{2} F_\phi \times F_\phi; \quad H_{\phi iI} = \frac{1}{2} \mathcal{E}_{ijk} \mathcal{E}_{IJK} F_{\phi jJ} F_{\phi kK}; \] (3a)

\[ J_\phi = \frac{1}{3} H_\phi : F_\phi; \quad J_\phi = \frac{1}{3} H_{\phi iI} F_{\phi iI}, \] (3b)

where \( \mathcal{E}_{ijk} \) (or \( \mathcal{E}_{IJK} \)) symbolises the third order alternating tensor components and the use of repeated indices implies summation, unless otherwise stated.

### 2.2 Governing equations in nonlinear electromechanics: conservation of linear momentum and angular momentum

The local form of the balance of linear momentum [10] can be written as

\[
\rho_0 \dot{v} - \text{DIV} (F_\phi S) - f_0 = 0; \quad \text{in } B_0; \\
(F_\phi S) \cdot N = t_0; \quad \text{on } \partial_t B_0; \\
\phi = \bar{\phi}; \quad \text{on } \partial_\phi B_0; \\
\phi(t = 0) = \phi_0; \quad \text{in } B_0; \\
v(t = 0) = v_0; \quad \text{in } B_0,
\] (4)

where \( \rho_0 : B_0 \to \mathbb{R}^+ \) represents the mass density of the EAP in the reference configuration, \( v \) the velocity field and \( \bullet \) denotes differentiation with respect to time. \( f_0 \) represents a body force per unit undeformed volume \( B_0 \) and \( t_0 \), the traction force per unit undeformed area applied on \( \partial_t B_0 \subset \partial B_0 \), where \( \partial_t B_0 \cup \partial_\phi B_0 = \partial B_0 \) and \( \partial_t B_0 \cap \partial_\phi B_0 = \emptyset \). Furthermore, \( \phi_0 \) and \( v_0 \) denote the initial configuration and velocity, respectively. Finally, \( S \) represents the second Piola-Kirchhoff stress tensor and the local balance of angular momentum leads to the well-known tensor condition \( S = S^T \). Note that \( S \) depends on the displacement and the electrical field and is comprised of unsymmetrical mechanical and an electrical contributions.

### 2.3 Governing equations in non-linear electromechanics: Gauss’s and Faraday’s laws

In the absence of magnetic and time dependent effects, Maxwell equations reduce to Gauss’s and Faraday’s laws. The local form of the Gauss’ law can be written in a Lagrangian setting as

\[
\text{DIV} D_0 - \rho_0^e = 0; \quad \text{in } B_0; \\
D_0 \cdot N = -\omega_0^e; \quad \text{on } \partial_\omega B_0,
\] (5)

\(^2\)Lower case indices \( \{i, j, k\} \) will be used to represent the spatial configuration whereas capital case indices \( \{I, J, K\} \) will be used to represent the material description.
where $D_0$ is the Lagrangian electric displacement vector, $\rho_0^e$ represents an electric volume charge per unit of undeformed volume $B_0$ and $\omega_0^e$, an electric surface charge per unit of undeformed area $\partial_\omega B_0 \subset \partial B_0$. Alternatively, the spatial electric displacement vector $D$ can be obtained through the area push forward relationship

$$D_0 = H_T^\phi D, \ [5].$$

The local form of the static Faraday’s law can be written in a Lagrangian setting as

$$E_0 = -\nabla_0 \varphi; \quad \text{in } B_0;$$

$$\varphi = \bar{\varphi}; \quad \text{on } \partial_\varphi B_0,$$

where $E_0$ is the Lagrangian electric field vector and $\varphi$, the scalar electric potential. In (6), $\partial_\varphi B_0$ represents the part of the boundary $\partial B_0$ where essential electric potential boundary conditions are applied, where $\partial_\omega B_0 \cup \partial_\varphi B_0 = \partial B_0$ and $\partial_\omega B_0 \cap \partial_\varphi B_0 = \emptyset$. The spatial electric field vector $E$ can be obtained through the standard fibre transformation $E_0 = F_T^\phi E \ [5]$.

### 3 Electro-Elastodynamics

The objective of this section is to present the variational formulation that will be used in order to develop an EM time integration scheme in Section 4.

#### 3.1 Extension to electro-elastodynamics

A point of departure is the following ten field action integral

$$L_{\tilde{W}}(\mathbf{v}, \phi, \varphi, D_0, \mathbf{D}, \Lambda) = \int_{t_0}^t \left( \int_{B_0} \left( \dot{\phi} - \frac{1}{2} \mathbf{v} \cdot \mathbf{v} \right) \cdot \rho_0 v \, dV - \Pi_{\tilde{W}}(\phi, \varphi, D_0, \mathbf{D}, \Lambda) \right) \, dt;$$

$$\Pi_{\tilde{W}}(\phi, \varphi, D_0, \mathbf{D}, \Lambda) = \int_{B_0} \tilde{W} (\mathbf{C}, \mathbf{G}, \mathbf{C}, D_0) \, dV + \int_{B_0} D_0 \cdot \nabla_0 \varphi \, dV$$

$$+ \int_{B_0} \Lambda C : (\mathbf{C} \varphi - \mathbf{C}) \, dV + \int_{B_0} \Lambda G : \left( \frac{1}{2} \mathbf{C} \times \mathbf{C} - \mathbf{C} \right) \, dV$$

$$+ \int_{B_0} \Lambda C \left( \frac{1}{3} \mathbf{C} : \mathbf{G} - \mathbf{C} \right) \, dV - \Pi_{\text{ext}}^m (\phi) - \Pi_{\text{ext}}^e (\varphi), \quad (7)$$

where $t_0$ and $t$ represent any two instances of time with $t > t_0$. Moreover, we introduce the sets $\mathbf{D} = \{ \mathbf{C}, \mathbf{G}, \mathbf{C} \}$ and $\Lambda = \{ \Lambda C, \Lambda G, \Lambda C \}$. Note that $\tilde{W}$ denotes the internal energy expressed in terms of the extended symmetric mechanical kinematic set $\{ \mathbf{C}_\phi, \mathbf{G}_\phi, \mathbf{C}_\phi \}$, defined as

$$\mathbf{C}_\phi = F_T^\phi \mathbf{F}_\phi; \quad \mathbf{G}_\phi = \frac{1}{2} \mathbf{C}_\phi \times \mathbf{C}_\phi = H_T^\phi \mathbf{H}_\phi; \quad \mathbf{C}_\phi = \frac{1}{3} \mathbf{G}_\phi : \mathbf{C}_\phi = J_{\phi}^2. \quad (8)$$

and $D_0$. See [8] and the references therein for details concerning material stability of reversible electro-elastology problems. Furthermore, in (7) the external

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contributions $\Pi_{\text{ext}}^m$ and $\Pi_{\text{ext}}^e$ are defined as

$$\Pi_{\text{ext}}^m (\phi) = \int_{B_0} f_0 \cdot \phi \, dV + \int_{\partial_\phi B_0} t_0 \cdot \phi \, dA; \quad \Pi_{\text{ext}}^e (\varphi) = - \int_{B_0} \rho_0^e \varphi \, dV - \int_{\partial_\omega B_0} \omega_0^e \varphi \, dA.$$  \hspace{1cm} (9)

Moreover, in (7) $\{v, \phi, \varphi, D_0, D, \Lambda\} \in \mathcal{V}^\phi \times \mathcal{V}^\varphi \times \mathcal{V}^D \times \mathcal{V}^{D_0} \times \mathcal{V}^D \times \mathcal{V}^D$, with $\mathcal{V}^D = \mathcal{V}^C \times \mathcal{V}^G \times \mathcal{V}^C$, where

$$\mathcal{V}^\phi = \{ \phi : B_0 \to \mathbb{R}^3; \ \phi \in H^1 (B_0) \mid J_\phi > 0, \ \phi = \bar{\phi} \ \text{on} \ \partial_\phi B_0 \};$$

$$\mathcal{V}^\varphi = \{ \varphi : B_0 \to \mathbb{R}; \ \varphi \in H^1 (B_0) \mid \varphi = \bar{\varphi} \ \text{on} \ \partial_\varphi B_0 \};$$

$$\mathcal{V}^{D_0} = \{ D_0 : B_0 \to \mathbb{R}^3; \ (D_0)_I \in L_2 (B_0) \};$$

$$\mathcal{V}^G = \{ G : B_0 \to \mathbb{R}; \ G_{1J} \in L_2 (B_0) \};$$

$$\mathcal{V}^C = \{ C : B_0 \to \mathbb{R}; \ C \in L_2 (B_0) \},$$

where $H^1$ denotes the Sobolev functional space of square integrable functions and derivatives, $L_2$, the space of square integrable functions and $\mathbb{S}$, the space of symmetric second order tensors. By means of Hamilton’s principle, the stationary conditions of $\bar{W}$ in (7) with respect to variations $\{\delta v, \delta \phi, \delta \varphi, \delta D_0\}$ are

$$\mathcal{W}_v = \int_{B_0} (v - \dot{\phi}) \cdot \rho_0 \delta v \, dV = 0;$$

$$\mathcal{W}_{\phi} = \int_{B_0} \rho_0 \dot{\phi} \cdot \delta \phi \, dV + \int_{B_0} \Lambda_C : D C_\phi [\delta \phi] \, dV - \int_{B_0} f_0 \cdot \delta \phi \, dV - \int_{\partial_\phi B_0} t_0 \cdot \delta \phi \, dA = 0; \hspace{1cm} (11)$$

$$\mathcal{W}_\varphi = \int_{B_0} D_0 \cdot \nabla_0 \delta \varphi \, dV + \int_{B_0} \rho_0 \delta \varphi \, dV + \int_{\partial_\omega B_0} \omega_0^e \delta \varphi \, dA = 0;$$

$$\mathcal{W}_{D_0} = \int_{B_0} \delta D_0 \cdot (\partial_\omega \bar{W} + \nabla_0 \varphi) \, dV = 0,$$

with the admissible variations defined as $\{\delta v, \delta \phi, \delta \varphi, \delta D_0\} \in \mathcal{V}^\phi_0 \times \mathcal{V}^\varphi_0 \times \mathcal{V}^{D_0}$, being

$$\mathcal{V}^\phi_0 = \{ \phi : B_0 \to \mathbb{R}^3; \ \phi \in H^1 (B_0) \mid \phi = 0 \ \text{on} \ \partial_\phi B_0 \};$$

$$\mathcal{V}^\varphi_0 = \{ \varphi : B_0 \to \mathbb{R}; \ \varphi \in H^1 (B_0) \mid \varphi = 0 \ \text{on} \ \partial_\varphi B_0 \}. \hspace{1cm} (12)$$

Note that integration by parts with respect to time has been used on the inertia term of (11)$_b$. Equation (11)$_a$ represents the weak form for the relationship between the velocity field $v$ and the time derivative of the mapping $\phi$ and equation (11)$_b$, the balance of linear momentum (4). Notice that in (11)$_b$, the Lagrange multiplier $\Lambda_C$ coincides in a weak sense with half of the second Piola-Kirchhoff stress tensor $S$. Eventually, equations (11)$_c$ and (11)$_d$ represent the weak forms of the Gauss
(5) and Faraday (6) laws, respectively. The stationary conditions of $L_{\tilde{W}}$ (7) with respect to variations $\delta \mathbf{D}$ yield,

$$W_C = \int_{B_0} \delta \mathbf{C} : \left( \partial_{\mathbf{C}} \tilde{W} - \Lambda_C + \Lambda_G \times \mathbf{C} + \frac{1}{3} \Lambda_C \mathbf{G} \right) dV = 0;$$

$$W_G = \int_{B_0} \delta \mathbf{G} : \left( \partial_{\mathbf{G}} \tilde{W} - \Lambda_G + \frac{1}{3} \Lambda_C \mathbf{C} \right) dV = 0;$$

$$W_C = \int_{B_0} \delta \mathbf{C} \left( \partial_{\mathbf{C}} \tilde{W} - \Lambda_C \right) dV = 0,$$

with $\{\delta \mathbf{C}, \delta \mathbf{G}, \delta \mathbf{C}\} \in \mathbb{V}_C \times \mathbb{V}_G \in \mathbb{V}_C$. Notice that equation (13) represents the weak form of the constitutive equations. Finally, the stationary conditions of $L_{\tilde{W}}$ (7) with respect to $\delta \mathbf{A}$ are

$$W_{\Lambda_C} = \int_{B_0} \delta \Lambda_C : (\mathbf{C}_\phi - \mathbf{C}) dV = 0;$$

$$W_{\Lambda_G} = \int_{B_0} \delta \Lambda_G : \left( \frac{1}{2} \mathbf{C} \times \mathbf{C} - \mathbf{G} \right) dV = 0;$$

$$W_{\Lambda_C} = \int_{B_0} \delta \Lambda_C \left( \frac{1}{3} \mathbf{C} : \mathbf{G} - \mathbf{C} \right) dV = 0,$$

with $\{\delta \mathbf{C}, \delta \mathbf{G}, \delta \mathbf{C}\} \in \mathbb{V}_C \times \mathbb{V}_G \in \mathbb{V}_C$. It is worth emphasising that equation (14) represents the weak form of the kinematic constraints. This particular choice of kinematic constraints, taken from the EM time integrator presented by Betsch et. al. [1] in the context of elastodynamics, is crucial for the design of the EM time integration scheme in Section 4.

4 Energy-Momentum integration scheme for electro-elastodynamics

The objective of this section is to propose an EM preserving time discretisation scheme for the set of weak forms given in (11), (13) and (14). Let us consider a sequence of time steps $\{t_1, t_2, ..., t_n, t_{n+1}\}$, where $t_{n+1}$ denotes the endpoint of the current time step. From the stationary conditions in (11), the following implicit one-step time integrator is proposed

$$(W_v)_{\text{algo}} = \int_{B_0} \left( v_{n+1/2} - \frac{\Delta \phi}{\Delta t} \right) \cdot \rho_0 \delta v dV = 0;$$

$$(W_\phi)_{\text{algo}} = \int_{B_0} \rho_0 \frac{\Delta v}{\Delta t} \cdot \delta \phi dV + \int_{B_0} \Lambda_C : (DC_\phi[\delta \phi])_{\text{algo}} dV - \int_{B_0} f_{n+1/2} \cdot \delta \phi dV - \int_{\partial t B_0} t_{n+1/2} \cdot \delta \phi dA = 0,$$

with $(W_v)_{\text{algo}}$ and $(W_\phi)_{\text{algo}}$.
and

\[
(W_\varphi)_{\text{algo}} = \int_{B_0} D_0^{n+1/2} \cdot \nabla_0 \delta \varphi \, dV + \int_{B_0} \rho_0^{n+1/2} \delta \varphi \, dV + \int_{\partial_0 \Omega_0} \omega_0^{n+1/2} \delta \varphi \, dA = 0; \\
(W_D)_0 \text{ algo} = \int_{B_0} \delta D_0 \cdot \left( D_0 \tilde{W} + \nabla_0 \varphi_n^{n+1/2} \right) \, dV = 0. \tag{16}
\]

Note that \((W_v)_{\text{algo}}\), \((W_\phi)_{\text{algo}}, (W_\varphi)_{\text{algo}}\) and \((W_D)_0\)_{\text{algo}} in (15)-(16) represent the algorithmic or time discrete versions of the stationary conditions in (11) and 
\((\bullet)_{n+1/2} = \frac{1}{2} ((\bullet)_{n+1} + (\bullet)_n)\) and \(\Delta (\bullet) = (\bullet)_{n+1} - (\bullet)_n\). Furthermore the Lagrange multipliers \(\Lambda_0(\bullet)\) are constant throughout the timestep, such that \(\Lambda_0(\bullet) := \Lambda_0(\bullet)_{n+1}\). In equation (15)\(_b\), where the algorithmic or time discrete directional derivative \((DC_\phi[\delta \phi])_{\text{algo}}\) is defined as

\[
(DC_\phi[\delta \phi])_{\text{algo}} = \left( (\nabla_0 \delta \phi)^T F_{\phi_n^{n+1/2}} + F_{\phi_n^{n+1/2}}^T \nabla_0 \delta \phi \right). \tag{17}
\]

In addition, following [1], the algorithmic counterparts of the stationary conditions \(W_C, W_G, W_\varphi\) in (13) are

\[
(W_C)_{\text{algo}} = \int_{B_0} \delta C : \left( D_C \tilde{W} - \Lambda_C + \Lambda_G \times C_n^{n+1/2} + \frac{1}{3} \Lambda_C G_n^{n+1/2} \right) \, dV = 0; \\
(W_G)_{\text{algo}} = \int_{B_0} \delta G : \left( D_G \tilde{W} - \Lambda_G + \frac{1}{3} \Lambda_C C_n^{n+1/2} \right) \, dV = 0; \tag{18}
\]

\[
(W_C)_{\text{algo}} = \int_{B_0} \delta C \left( D_C \tilde{W} - \Lambda_C \right) \, dV = 0.
\]

Finally, following [1], the algorithmic counterpart of the stationary conditions \(W_{\lambda C}, W_{\lambda G}\) and \(W_{\lambda C}\) (14) are

\[
(W_{\lambda C})_{\text{algo}} = \int_{B_0} \delta \Lambda_C : \left( C_{\phi_n^{n+1}} - C_{n+1} \right) \, dV = 0; \\
(W_{\lambda G})_{\text{algo}} = \int_{B_0} \delta \Lambda_G : \left( \frac{1}{2} C_{n+1} \times C_{n+1} - G_{n+1} \right) \, dV = 0; \tag{19}
\]

\[
(W_{\lambda C})_{\text{algo}} = \int_{B_0} \delta \Lambda_C \left( \frac{1}{3} C_{n+1} : G_{n+1} - C_{n+1} \right) \, dV = 0.
\]

In (15)-(16) and (18), \(\{D_C \tilde{W}, D_G \tilde{W}, D_C \tilde{W}, D_D \tilde{W}\}\) represent the discrete derivatives [9, 11, 6] of the internal energy \(\tilde{W}\) with respect to \(\{C, G, C, D_0\}\), respectively. In particular \(\{D_C \tilde{W}, D_G \tilde{W}, D_C \tilde{W}, D_D \tilde{W}\}\) are the algorithmic or time discrete counterparts of \(\{\partial_C \tilde{W}, \partial_G \tilde{W}, \partial_C \tilde{W}, \partial_D \tilde{W}\}\), respectively. The expressions for the
discrete derivatives $D_C\tilde{W}$, $D_G\tilde{W}$, $D_C\tilde{W}$ and $D_D\tilde{W}$ in [11] comply also with the required conservation properties of the new time integrator in equations (15)-(16), (18) and (19). See [7] for details on the discrete derivatives and the consistent approximation of the balance laws for this time integrator.

5 Finite Element implementation

As standard in finite elements, the domain $B_0$ described in Section 2.1 and representing the EAP is sub-divided into a finite set of non-overlapping elements $e \in \Xi$ such that

$$B_0 \approx B_0^h = \bigcup_{e \in \Xi} B_0^e.$$  \hfill (20)

The unknown fields $\{v, \phi, \varphi, D_0, \mathcal{D}, \Lambda_D\}$ in the semi-discrete weak forms $\{W_v, W_\phi, W_\varphi, W_{D_0}\}$ in (15)-(16), $W_D$ in (18) and $W_{\Lambda_D}$ in (19) are discretised employing the following functional spaces $\mathbb{V}^{\phi^h} \times \mathbb{V}^{\varphi^h} \times \mathbb{V}^{\phi^h} \times \mathbb{V}^{D_0^h} \times \mathbb{V}^{D^h} \times \mathbb{V}^{D^h}$, with $\mathbb{V}^{D^h} = \{\mathbb{V}^{C^h}, \mathbb{V}^{G^h}, \mathbb{V}^{C^h}\}$ defined as

$$\mathbb{V}^{\phi^h} = \{\phi \in \mathbb{V}^\phi; \phi^h|_{B_0^e} = \sum_{a=1}^{n_{\text{node}}^\phi} N_a^\phi \phi_a \mid \phi_a = \bar{\phi}^h \text{ on } \partial_e B_0^h\};$$

$$\mathbb{V}^{\varphi^h} = \{\varphi \in \mathbb{V}^\varphi; \varphi^h|_{B_0^e} = \sum_{a=1}^{n_{\text{node}}^\varphi} N_a^\varphi \varphi_a \mid \varphi_a = \bar{\varphi}^h \text{ on } \partial_e B_0^h\};$$

$$\mathbb{V}^{D_0^h} = \{D_0 \in \mathbb{V}^{D_0}; \ D_0^h|_{B_0^e} = \sum_{a=1}^{n_{D_0}^e} N_a^{D_0} D_0a\};$$

$$\mathbb{V}^{D^h} = \{\mathcal{D} \in \mathbb{V}^\mathcal{D}; \ D^h|_{B_0^e} = \sum_{a=1}^{n_{D}^e} N_a^\mathcal{D} \mathcal{D}_a\},$$

where for any field $\mathcal{Y} \in \{\phi, \varphi, D_0, \mathcal{D}, \Lambda_D\}$, $n_{\text{node}}^\mathcal{Y}$ denotes the number of nodes per element of the discretisation associated with the field $\mathcal{Y}$ and $N_a^\mathcal{Y} : B_0^e \to \mathbb{R}$, the $a^{\text{th}}$ shape function used for the interpolation of $\mathcal{Y}$. In addition, $a^\mathcal{Y}$ represents the value of the field $\mathcal{Y}$ at the $a^{\text{th}}$ node of a given finite element. Similarly, following a Bubnov-Galerkin approach, the functional spaces for the virtual variations $\{\delta \mathcal{V}, \delta \phi, \delta \varphi, \delta D_0, \delta \mathcal{D}, \delta \Lambda_D\} \in \mathbb{V}_0^{\phi^h} \times \mathbb{V}_0^{\phi^h} \times \mathbb{V}_0^{\phi^h} \times \mathbb{V}_0^{D_0^h} \times \mathbb{V}_0^{D^h} \times \mathbb{V}_0^{D^h}$ are defined as

$$\mathbb{V}_0^{\phi^h} = \{\forall \phi \in \mathbb{V}^{\phi^h}; \ \phi = 0 \text{ on } \partial_e B_0\}; \ \mathbb{V}_0^{\varphi^h} = \{\forall \varphi \in \mathbb{V}^{\varphi^h}; \ \varphi = 0 \text{ on } \partial_e B_0\}.$$

Even though the relation between the time derivative of $\phi$ and the velocity field $\mathbf{v}$ is considered in a weak manner (refer to the weak form $W_v$ in (15)), the consideration of equal functional spaces for both fields, namely $\phi \in \mathbb{V}^{\phi^h}$ and $\mathbf{v} \in \mathbb{V}^{\phi^h}$
enables to conclude that equation (15)_a holds strongly at the discrete level, namely

$$\Delta \phi \over \Delta t = v_{n+1/2}. \quad (23)$$

Finally, in order to reduce the computational cost of the proposed formulation, a piecewise discontinuous interpolation of the fields \{D_0, C, G, C, \Lambda_C, \Lambda_G, \Lambda_C\} is followed. A standard static condensation procedure [13, 2] is used to condense out the degrees of freedom of the fields \{D_0, C, G, C, \Lambda_C, \Lambda_G, \Lambda_C\}.

6 Numerical example

In the numerical examples the internal energy is split into a purely mechanical and a coupled electromechanical part: $\tilde{W}(C, G, C, D_0) = \tilde{W}_m(C, G, C) + \tilde{W}_{em}(C, D_0)$. Herein we focus on ideal dielectric elastomers modelled by

$$\tilde{W}_{em}(C, C, D_0) = \frac{1}{2\varepsilon_r \varepsilon_0 C^{1/2}} D_0 \cdot C D_0. \quad (24)$$

An isotropic behaviour is considered for the mechanical component $\tilde{W}_m$. Specifically, a Mooney-Rivlin strain energy functional is used, defined as

$$\tilde{W}_m^{MR}(C, G, C) = \frac{\mu_1}{2}(\text{tr} C - 3) + \frac{\mu_2}{2}(\text{tr} G - 3) - (\mu_1 + 2\mu_2) \ln C^{1/2} + \frac{\lambda}{2} \left( C^{1/2} - 1 \right)^2. \quad (25)$$

The material parameters are $\mu_1 = 5 \times 10^4$ Pa, $\mu_2 = 1 \times 10^5$ Pa, $\lambda = 5 \times 10^5$ Pa, $\varepsilon_0 = 8.854 \times 10^{-12}$ A$^2$ s$^4$ kg$^{-1}$ m$^{-3}$, $\varepsilon_r = 4$ with reference density of $\rho_0 = 1000$ kg m$^{-3}$. From a mechanically point of view the actuator is free in space, i.e. no mechanical Dirichlet conditions are imposed and the initial velocity is assumed to be $V_0 = \omega \times X$, with $\omega = [0, 0, 0.05]^T$ s$^{-1}$. On the blue electrode, a constant value of $\phi = 0$ V is applied. On the purple electrode a time dependent electrical surface charge $\omega_0^e$ is applied, where the time dependent function of $\omega_0^e$ is given by $\omega_0^e = 5 \times 10^{-3} \cdot \sin\left(\frac{0.5\pi}{0.48} t\right)$ for $t \leq 0.4$ s, $\omega_0^e = 5 \times 10^{-3}$ for $0.4$ s $< t \leq 3.0$ s, $\omega_0^e = 5 \times 10^{-3} \cdot \cos\left(\frac{0.5\pi}{0.48} (t - 3.0)\right)$ for $3.0$ s $< t \leq 3.4$ s and $\omega_0^e = 0$ for $t > 3.4$ s. The geometry and boundary conditions of the H-shaped actuator are depicted in Fig. 1.

Ten node quadratic/four node linear tetrahedron (tet 10/4) elements are used, where Quadratic continuous interpolation spaces $P^2$ and linear discontinuous interpolation spaces $P^1$ are employed such that \{\phi, \Phi\} $\in P^2$ and \{D_0, D, \Lambda\} $\in P^1$. A mesh comprised of 15013 tet 10/4 elements with a total of 95776

$^3$Notice that in the discrete setting, (15)_a transforms into a mass matrix multiplied by the discrete vector version of $\Delta \phi \over \Delta t - v_{n+1/2}$ equaling zero. For this to hold, given the positive definite nature of the mass matrix, the discrete vector version of $\Delta \phi \over \Delta t - v_{n+1/2}$ must be zero. Thus, equation (23) holds at the nodes of the discretisation and thus, at the quadrature points.
displacement and electrical potential unknowns is employed. Fig. 1 shows typical snapshots of the H-shaped actuator displaying the von Mises stress $\sigma_{vM}$ where extremely large deformations can be observed. Results are smooth and do not show any spurious pressure or electric field. Fig. 2 shows the evolution of the total Hamiltonian $H$ and Fig. 3 the evolution of the norm of the total angular momentum $J$ of the actuator for the proposed EM time integrator and the midpoint-rule. In addition, Fig. 2 shows that the midpoint-rule time integrator exhibits an energy blow-up and becomes unstable approximately in the interval $0.4 s < t < 1.8 s$. In contrast, the newly proposed EM time integrator perfectly conserves the energy after the loading phase. Also the discrete balance of angular momentum is perfectly preserved. The EM time integrator remains stable for the entire simulation time for the same fixed time step size of $\Delta t = 0.05 s$. Accordingly, the proposed scheme is more robust and stable than the midpoint-rule.

See [7] for more numerical investigations demonstrating the beneficial spatial convergence behavior of the mixed formulation.

7 Conclusions

A new consistent energy-momentum one-step time integrator scheme is presented in the context of nonlinear electro-elastodynamics. The proposed schemes shows the typical advantages for the structure-preserving discretization in time. Furthermore, the mixed formulation offers several options for the discretization in space.
Figure 2: Left: Time evolution of $H$ (left) and time evolution of $\Delta H$ (right).

Figure 3: Time evolution of $||J||$ (left) and time evolution of $\Delta ||J||$ (right).

REFERENCES


Application of Frontal Solution Method in Dam-Reservoir Problem

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Key words: Dam and Reservoir Interaction, Frontal Solution Method, Time Domain Analysis.

Abstract. Solution of the total equations of the phenomenon in time domain is the main target in the current study. The advantages of the method are high accuracy comparing with iterative methods, and possibility of handling the nonlinear affects. Deficiencies are due to high system requirement, the use of same formulation either Lagrangian or Eulerian which are suitable for the structure or reservoir respectively, and solving the variables with very different orders. The proposed method is to take advantage of frontal solution scheme. In this solution method some of the variables are gathered in a front, and solution is performed each time for successive fronts. The size of the front is different for each problem, but it is much less than total variables. Therefore, computational requirement is limited without losing accuracy. The hydrodynamic pressure variables are chosen to be located in front. Therefore some notable changes had to be made in formal scheme. In common version the choosing the variables and placing them in the front is done automatically. While in proposed application the hydrodynamic pressure variables are forced to be located in front. Other advantages are also achieved. Having the hydrodynamic pressure variables, the structure and reservoir are solved separately using their suitable formulations.

This paper studies two methods for analysis of the dam-reservoir system. The first method is based on using frontal method, while the other utilizes iterative schemes. A typical dam-reservoir system is performed by five different meshes. These analyses are compared from efficiency point of view. Frontal method requires less system requirement than iterative methods.

CPU time are calculated for two approaches. All the execution times are calculated on the same hardware to achieve an appropriate criterion for comparison purposes. Compared to iterative scheme, CPU time is decrease in frontal method. As the number of the elements are
increase, execution time is saved more in frontal method even up to 90 percent.

1 INTRODUCTION

The safety of the dams are really important for the people who lived downstream. The response of the concrete gravity dam depends on the lot of factors. For example the interaction of the dam with reservoir and foundation and even the behavior of the concrete have great influence on the response of the dam. The calculation of the hydrodynamic force which acts on the interface of dams as a result of earthquake is important for analysis of the dams.

Several approaches have been proposed to consider this effect. Most of the approaches are involved with an iterative schemes in time domain. Fellippa and Park [1] described staggered solution for coupled problems in detail. Staggered approach make us capable to reduce couple problem to subsystems therefor we only deal with symmetric equations for each subsystems [2]. However the stability of the method is conditional and must be care about convergence of the solution of the subsystems at each time step. So, in this approach we need iteration in each time step even in linear problems. And this procedure is time consuming.

Some approaches are direct. The direct method is exact. However this method need massive storage space. The modal method have been used to analyze the dam-reservoir problem [3]. Modal approach is very efficient in time but it can’t be used in nonlinear problems.

A lot of work have been done in frequency domain by Chopra and coadjutor on dam-reservoir-foundation interaction [4,5]. The concept of the frequency domain formulation are more difficult than the time domain formulation. And the main disadvantage of the frequency domain was that, it can’t be used in nonlinear problems.

The best method for solving the coupled equations, is simulation method. Simulation method in time domain, need massive storage space because of solving the all of equations including structure and fluid including far field variable for each time step. As well as, solving numerically the all variables including displacement and pressure which have different orders is really difficult.

Frontal method enable us to overcome these disadvantages [6]. The principal aim of this paper is to employ frontal solution for solving the dam-reservoir system [7,8]. The frontal method for solving the equations was presented by Irons for the first time[7].

By using frontal solution, all equations are assembled but only a selection of the degrees of freedom are solved. In the other words, by considering the interface pressure degree freedoms in the front, total model including the displacement of the structure and the pressure of the fluid are assembled by frontal method. Then only the interface degree freedoms front, which is pressure acting on the interface, are solved. After finding the values of the pressure which act on the interface of the dam, the structure can be analyzed due to seismatic force and dynamic pressure, and the fluid can be analyzed due to determined boundary conditions, separately. This schema have a lot of advantages: only the value of the pressure which acts on interface compute first and this value is the same as the value of which solved the entire equations. So there is no approximation. Also this schema can be used in nonlinear problems because none of the fields was eliminated or partitioned.
2 METHOD OF ANALYSIS

Dam’s equation of motion can be written as below:

\[
[M] \dddot{u} + [C] \ddot{u} + [K] u = -[M] \dddot{a}_g - [Q] p \tag{1}
\]

Where \([M]\), \([C]\) and \([K]\) are mass, damping and stiffness matrices of the dam structure body respectively. \(\dddot{a}_g\) is the ground acceleration. \(u\), \(\dot{u}\) and \(\ddot{u}\) are vectors of displacement, velocity and acceleration of structure body respectively.

The equation of motion for reservoir domain due to earthquake motion can be written as below:

\[
[G] \dddot{p} + [D] \ddot{p} + [H] p = F - \rho_f[Q]^T \dddot{u} + \dddot{a}_g \tag{2}
\]

Where \([G]\), \([D]\) and \([H]\) are assembled matrix of reservoir domain. \(F\) is load vector due to boundary condition of the fluid domain. \(p\) is the vector of hydrodynamic pressure, \(\dot{p}\) and \(\ddot{p}\) are vectors of first and second derivation of the hydrodynamic pressure.

The coupled equation of dam-reservoir can be written as below:

\[
\begin{bmatrix}
M & 0 & 0 \\
\rho_fQ^T & G & D \\
0 & 0 & H
\end{bmatrix}
\begin{bmatrix}
\dddot{u} \\
\dddot{p} \\
\dddot{p}
\end{bmatrix} +
\begin{bmatrix}
C & 0 & 0 \\
0 & K & H \\
0 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
\ddot{u} \\
\dot{p} \\
p
\end{bmatrix} =
\begin{bmatrix}
-M\dddot{a}_g \\
-\rho_f[Q]^T \dddot{u} \\
0
\end{bmatrix} \tag{3}
\]

Where \(Q\) is coupling matrix defined as below:

\[
[Q] = \int N_s n N_f^T ds \tag{4}
\]

where \(N_s\) and \(N_f\) are shape function of structure and fluid respectively.

By using step by step integration scheme of Newmark, the coupled equation of dam-reservoir can be written as below [6]:

\[
\begin{bmatrix}
\frac{4}{\Delta t^2} M + \frac{2}{\Delta t} C + K & -Q \\
-Q^T & -\frac{1}{\rho_f} G - \frac{\Delta t}{2\rho_f} D - \frac{\Delta t^2}{4\rho_f} H
\end{bmatrix}
\begin{bmatrix}
\begin{bmatrix}
\ddot{u}^{n+1} \\
\ddot{p}^{n+1}
\end{bmatrix} \\
\ddot{p}^{n+1}
\end{bmatrix} =
\begin{bmatrix}
F_s \\
F_f
\end{bmatrix} \tag{5}
\]

where:

\[
F_s = -M\dddot{a}_g + M\left(\frac{4}{\Delta t^2} u^n + \frac{4}{\Delta t} \dddot{u}^n + \dddot{u}^n\right) + C\left(\frac{2}{\Delta t} u^n + \dddot{u}^n\right)
\]

\[
F_f = \frac{\Delta t^2}{4} Q^T \dddot{a}_g + Q^T\left(\dot{u}^n + \Delta t \dddot{u}^n + \frac{\Delta t^2}{4} \dddot{u}^n\right) - G\left(\frac{1}{\rho_f} p^n + \frac{\Delta t}{\rho_f} \dddot{p}^n + \frac{\Delta t^2}{4\rho_f} \dddot{p}^n\right) + D\left(\frac{\Delta t^2}{4\rho_f} p^n + \frac{\Delta t^2}{4\rho_f} \dddot{p}^n\right) \tag{6}
\]
The interaction equations of dam and reservoir may be divided to liquid degrees of freedom, solid degrees of freedom and the interface degrees of freedom. It was shown that in frontal solution, the pressure variables on interface can be kept in front and can be solved without continuing the solution for the all equations. Then, the achieved results can be used as the boundary condition for solving the reservoir and as loading profile for solving the dam. In this way no iteration is needed, there is no loss of accuracy and each media can be solved by using its suitable formulation. The solution procedure is illustrated in Figure 1.

Figure 1: Frontal solution procedure for dam-reservoir problem

3 RESULTS

A computer program is developed based on the frontal solution method. Utilizing this solution, dynamic analysis of Dam with vertical upstream (Figure 2) is considered as a typical numerical example. Five types of mesh are used for analysis (Table 1).
A vertical dam with 180m height and reservoir have been subjected to ramp acceleration (Figure 3). For the concrete, unit weight and poisson’s ratio and modulus of elasticity were taken as 1113.86g/m³, 0.2 and 35GPa, respectively. For the water, unit weight and sound speed in the water were taken as 1000kg/m³ and 1440m/s, respectively.
The history of horizontal crest displacement and hydrodynamic pressure at bottom of the reservoir are presented in Figures 4 and Figures 5.

**Figure 4**: Crest displacement

**Figure 5**: Hydrodynamic pressure at bottom of the reservoir

For comparison purpose, the models were analyzed by using two different program, first program solved the equations by frontal method and second program solved the equations by iteration scheme. The results for mesh No.4 are presented in Figures 6 and Figures 7.
Figure 6: Crest displacement

Figure 7: Hydrodynamic pressure at bottom of the reservoir

Table 2 presents the calculation time of two solution scheme for five examples. As shows execution time is saved more in frontal solution even up to 90 percent.
Table 2: Execution time for each analysis (s)

<table>
<thead>
<tr>
<th>Mesh No.</th>
<th>Frontal method</th>
<th>Iterative method</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>20.00</td>
<td>27.36</td>
</tr>
<tr>
<td>2</td>
<td>23.39</td>
<td>34.98</td>
</tr>
<tr>
<td>3</td>
<td>217.42</td>
<td>2158.77</td>
</tr>
<tr>
<td>4</td>
<td>2028.52</td>
<td>45504.80</td>
</tr>
<tr>
<td>5</td>
<td>3699.98</td>
<td>*</td>
</tr>
</tbody>
</table>

4 CONCLUSIONS

- The frontal solution takes less calculation time than iterative method.
- As the number of the elements are increase, execution time is saved more in frontal method even up to 90 percent.
- The presented scheme is capable of considering the nonlinear phenomenon.
- The presented scheme does not has the geometrical and boundary condition limitation.

REFERENCES

COMPARISON OF VARIOUS COUPLING METHODS FOR 1D DIFFUSION EQUATIONS WITH A ANALYTICAL SOLUTION OF TWO PHASE STEFAN PROBLEM

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Key words: Stefan problem, coupling method, sea ice-ocean interaction

Abstract. We implemented loose and tight coupling methods to understand thermal diffusion between ocean and ice by means of a simplified one-dimensional model set-up proposed by Stefan. A Stefan problem is a prototypical two-phase model that can used to model, for example, melting and freezing of water due to the transfer of heat fluxes between the two phases. We discretized heat fluxes using low order derivatives for loose coupling and higher order derivatives for tight coupling while fluxes are computed at the (moving) interface. Compared to a known reference solution the tight coupling method exhibits a lower error when compared to the loose coupling discretization. However, further numerical tests are required to analyze these coupling methods.

1 Introduction

The interaction of sea ice with ocean and atmosphere through the exchange of heat, moisture and momentum is one of the most important interactions in climate models. Especially, in the polar regions, sea ice forms an interface between ocean and atmosphere. Thermal process such as downward radiation, turbulent heat flux from the atmosphere, the oceanic heat flux and dynamical processes such as wind stress, ocean ice stress and internal ice stress influence the sea ice distribution. This study mainly focuses on the sea ice thermodynamics, namely growth and melt through ice-ocean interaction. The relationship between sea ice melt and the heat supplied to the upper ocean from the atmosphere is explained in [6]. This study also suggests that during the ice melt season, the upper ocean and sea ice are thermodynamically strongly coupled. The growth and decay of sea ice affects the global thermohaline circulation and the intensity of oceanic deep convection [2].
The implementation of the sea ice component is a major issue during the development of any earth system model (ESM). In some ESMs, the ocean is coupled directly to the atmosphere over the sea ice, in which the ice model sends a sea ice fraction to the ocean and, in turn, the ocean sends information about new ice growth to the ice model. It is also common for ESMs to incorporate a subset of the sea ice thermodynamics into the atmosphere component where it is computed on the atmosphere grid with the atmosphere’s physics time step. The rest of the sea ice processes lies within the ocean component and are solved on the ocean grid with the ocean’s time step [5]. While there have been some major advances in the most complex sea ice models during the past decade, the processes of atmosphere-ice-ocean interaction are still only crudely understood and it is therefore not clear if they are realistically represented in the models. It is also very challenging to assess the quality of sea ice simulations in coupled climate models against the observed sea ice evolution.

Some of the differences between observations and models could be due to limited observations and inaccurate coupling methods between the ocean and sea ice models. In ESMs the sub-components of a climate model are coupled with each other at their boundaries through couplers. The main function of a coupler is to interpolate the coupling fields and provide input to the sub-components. However, it is still unclear if this coupling strategy provides a consistent framework for coupling components of climate models. Hence there is a need to understand the various coupling methods. Therefore, the motivation of the present study is to understand what we call loose and tight coupling methods (see below). We do this for thermodynamics, namely on melting and freezing of ice by exchanging temperatures and heat fluxes at the interface and compare the results with an analytical solution of the two phase Stefan problem. The spirit of this work lies in taking a different point of view: instead of coupling various subsystems of a complex system we look at the system as a whole and rather consider decoupling strategies into less complex model parts whose dynamics consistently reflect the dynamics of the whole system.

The Stefan problem was among the first mathematical models to study heat distribution in a phase changing medium [8]. Examples of Stefan problems include the melting of ice, solidification, fluid flow in porous media, and shock waves in gas dynamics. In this study, we consider the example of diffusion of heat in the melting of ice where the melting rate is based on the temperature gradients at the interface. This ad-hoc procedure is very simple, yet energy conserving. The Neumann method [3] is used to obtain an analytical solution for the two phase Stefan problem and is used as a reference to our study. For simplicity, the phase change temperature (interface temperature) between the two phases in our Stefan problem is assumed to be constant. More realistic models for the temperature at the ice-ocean interface are surveyed in [4].

Loose coupling was implemented in [1] to couple separate computations of one-dimensional thermal diffusion in liquid (ocean) and solid (ice) domains. In loose coupling, low order derivatives are used to discretize heat fluxes at the interface. However, the accuracy of the solution is dependant on the width of the subdomain overlap of the models [7]. In order to increase the overlap at the interface, we implemented a tight coupling in addition to loose coupling where we use higher order derivatives to compute fluxes at the interface. Here
we compare our solution of coupling methods to an analytical solution of two phase Stefan problem allowing for a rigorous comparison.

The organization of the paper is as follows. In Section 2, a two phase Stefan problem and its analytical solution are described. Section 3 describes the loose and tight coupling methods whereas Section 4 shows numerical tests. In Section 5 we discuss the results.

2 Model description of Two-phase Stefan Problem

A Stefan Problem is a specific type of a free boundary value problem for a partial differential equation for the distribution of heat in a phase changing medium. The Stefan problem is widely referenced in sciences where moving boundaries are considered. An example is the diffusion of heat in the melting of ice where melting causes the phase boundary of the ice to change position.

Consider a domain $\Omega = [0, X]$ in which the initial state of the material is assumed to be solid. We denote the temperature at the point $x$ at time $t$ by $u(x, t)$. A constant liquid temperature $u_l$ which is less than melting temperature $u_m$ is imposed at $x = 0$ resulting in an increase of temperature to reach the melting point causing liquid to appear in the domain. Let $s(t)$ be the point separating the two phases which determines the (initial) position of the interface. Movement of the interface is based on the temperature gradients of solid and liquid phase. The interface temperature is assumed to be constant, for simplicity. Two phase Stefan problem is mathematically expressed as heat conduction in liquid region

$$\frac{\partial u}{\partial t} = k_l \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < s(t), \quad t > 0 \quad (1)$$

and heat conduction in solid region

$$\frac{\partial u}{\partial t} = k_s \frac{\partial^2 u}{\partial x^2}, \quad x > s(t), \quad t > 0 \quad (2)$$

where $k_l > 0$ and $k_s > 0$ are constant but possibly different diffusion coefficients for each phase.

The temperature at the interface is given by

$$u(s(t), t) = u_m, \quad t > 0 \quad (3)$$

where $u_m$ is the melting temperature which is assumed to be constant in time. The position of the interface $s(t)$ is determined by the jump condition also called Stefan condition which satisfies the principle of conservation of energy:

$$\rho L \frac{ds}{dt} = k_s \frac{\partial u}{\partial x} - k_l \frac{\partial u}{\partial x}, \quad x = s(t), \quad t > 0 \quad (4)$$

where L and $\rho$ are latent heat and density respectively and are assumed to be constant. The initial condition is given by

$$u(x, 0) = u_s < u_m, \quad x > 0, \quad s(0) = 0 \quad (5)$$
where $u_s$ is the solid temperature which is also assumed to be constant. Boundary conditions are given by

$$u(0, t) = u_l > u_m, \quad t > 0$$

$$u(x, t) = u_s \quad t > 0$$

where $u_l$ is the liquid temperature which is also assumed to be constant.

2.1 An Analytical Solution

An analytical solution of the above two-phase Stefan problem was obtained by Neumann [3] in terms of a similarity variable $\xi$ given by

$$\xi = \frac{x}{2\sqrt{k_l}}.$$  \hfill (7)

The solution for the interface position can be written as

$$s(t) = 2\lambda \sqrt{k_l t}$$  \hfill (8)

the temperature in the liquid phase reads

$$u(x, t) = u_l - (u_l - u_m) \frac{\text{erf}(\frac{x}{2\sqrt{k_l}t})}{\text{erf}(\lambda)}$$  \hfill (9)

and the temperature in the solid phase as

$$u(x, t) = u_s + (u_m - u_s) \frac{\text{erfc}(\frac{x}{2\sqrt{k_s}t})}{\text{erfc}(v\lambda)}$$  \hfill (10)

where $\text{erf}(\xi)$ denotes the Gaussian error function and $\text{erfc}(\xi)$ denotes the complementary error function

$$\text{erf}(\xi) = \frac{2}{\sqrt{\pi}} \int_0^\xi \exp(-\theta^2) d\theta$$

$$\text{erfc}(\xi) = 1 - \text{erf}(\xi) = \frac{2}{\sqrt{\pi}} \int_\xi^\infty \exp(-\theta^2) d\theta$$  \hfill (11)

The basic properties of these functions are

$$\text{erf}(0) = 0, \quad \text{erf}(\infty) = 1,$$

$$\frac{d \text{erf}(\xi)}{d\xi} = \frac{2}{\sqrt{\pi}} \exp(-\xi^2) > 0, \quad \text{and}$$

$$\frac{d^2 \text{erf}(\xi)}{d\xi^2} = \frac{d}{d\xi} \frac{d \text{erf}(\xi)}{d\xi} = \frac{-4\xi}{\sqrt{\pi}} \exp(-\xi^2).$$

The parameter $\lambda$ in equations (8)-(10) is the solution to the transcendental equation

$$\lambda \sqrt{\pi} = \frac{S_{kl}}{\text{exp}(\lambda^2) \text{erf}(\lambda)} - \frac{S_{ls}}{v \text{exp}(v^2\lambda^2) \text{erfc}(v\lambda)}$$  \hfill (12)
where \( \text{St}_l = \frac{C_l(u_l-u_m)}{L} \) and \( \text{St}_s = \frac{C_s(u_m-u_s)}{L} \) are the Stefan number for the liquid and the solid, respectively. The parameters \( v = \sqrt{\frac{k_l}{k_s}} \), \( C_l \) and \( C_s \) are the heat capacities at constant pressure for liquid and solid, respectively, and are assumed to be constant.

### 3 Coupling methods

We consider the same heat equations as in (1) and (2), but the interface condition in these coupling methods are different from Stefan’s condition (4). For simplicity, the interface temperature in a Stefan problem is assumed to be constant. We, on the other hand, implement loose and tight coupling methods in which we compute the temperature at the interface by exchanging temperature values from liquid domain and heat fluxes from solid domain [1]. The solutions to our different coupling methods are compared to the analytical solution of the Stefan problem.

Figure 1(a) shows the initial condition of the model, where the material is solid and the interface is \( x = 0 \). Figure 1(b) represents the movement of the interface based on new interface temperature. The interface temperature is computed by exchanging temperature values from the solid domain for the computation of liquid domain, and heat fluxes for the computation of the liquid domain from the solid domain. If this interface temperature exceeds the melting point of ice, the interface temperature is set to that value and the excess energy is considered to melt the ice.

The heat equation for liquid and solid domains is same as (1) and (2). The coupling equation at the interface is

\[
\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left( k_s \frac{\partial u}{\partial x} - k_l \frac{\partial u}{\partial x} \right). \tag{13}
\]
In the following subsections, we elaborate on the implementation of loose and tight coupling methods.

3.1 Loose Coupling

The numerical algorithm for determining $u_{i}^{n+1}$ for the liquid is

$$\frac{(u_{i}^{n+1} - u_{i}^{n}) \Delta x}{\Delta t} = \frac{k_{l}}{\Delta x} (u_{i+1}^{n} - 2u_{i}^{n} + u_{i-1}^{n}), \quad (i \leq ib)$$

(14)

The corresponding numerical algorithm for determining $u_{i}^{n+1}$ for the solid is

$$\frac{(u_{i}^{n+1} - u_{i}^{n}) \Delta x}{\Delta t} = \frac{k_{s}}{\Delta x} (u_{i+1}^{n} - 2u_{i}^{n} + u_{i-1}^{n}), \quad (i \geq ib)$$

(15)

while the numerical algorithm to determine interface temperature $u_{ib}^{n+1}$ is

$$\frac{(u_{ib}^{n+1} - u_{ib}^{n}) \Delta x}{\Delta t} = -q_{w} - \frac{k_{l}}{\Delta x} (u_{ib}^{n} - u_{ib-1}^{n}), \quad (i = ib)$$

(16)

where $q_{w}$ is the heat flux specified at the interface, is given by

$$q_{w} = -\frac{k_{s}}{\Delta x} (u_{ib+1}^{n} - u_{ib}^{n}).$$

(17)

To summarize the communication between the two calculations for $i \leq ib$ and $i \geq ib$, at each time step there is an exchange of data, with the program performing the calculation for $i \leq ib$ supplying the temperature value of $u_{ib}^{n}$ to the other program performing the calculation for $i \geq ib$, while the program performing the calculation for $i \geq ib$ supplies heat flux $q_{w}$ to perform the calculation for $i \leq ib$.

If $u_{ib}^{n+1}$ exceeds the melting temperature $u_{m}$, the interface moves to the right of domain representing melting of solid. If $u_{ib}^{n+1}$ is less than the melting temperature, the interface moves to the left of domain, representing freezing of liquid.

3.2 Tight coupling

In order to achieve higher order accuracy, higher order approximations of the derivatives are used. We consider forward in time and centered difference in space for discretizing the heat equation. We use fourth order central difference approximations for first order derivatives to calculate the heat flux at the interface. These approximations use five point stencils in one dimension.

The numerical algorithm for determining $u_{i}^{n+1}$ for the liquid is

$$\frac{\Delta x}{\Delta t} (u_{i}^{n+1} - u_{i}^{n}) = \frac{k_{l}}{\Delta x} (u_{i+1}^{n} - 2u_{i}^{n} + u_{i-1}^{n}), \quad (i \leq ib)$$

(18)

while the corresponding numerical algorithm to determine $u_{i}^{n+1}$ for the solid is

$$\frac{\Delta x}{\Delta t} (u_{i}^{n+1} - u_{i}^{n}) = \frac{k_{s}}{\Delta x} (u_{i+1}^{n} - 2u_{i}^{n} + u_{i-1}^{n}), \quad (i \geq ib).$$

(19)
The numerical algorithm to determine interface temperature $u_{ib}^{n+1}$ is

$$\frac{\Delta x}{\Delta t}(u_{ib}^{n+1} - u_{ib}^n) = -q_w - \frac{k_l}{\Delta x}(u_{ib-2}^n/12 - 2u_{ib-1}^n/3 - 2u_{ib+1}^n/3 + u_{ib+2}^n/12), \quad (i = ib) \quad (20)$$

where $q_w$ denotes the heat flux specified at the interface given by

$$q_w = -\frac{k_s}{\Delta x}(u_{ib-2}^n/12 - 2u_{ib-1}^n/3 - 2u_{ib+1}^n/3 + u_{ib+2}^n/12)$$

If $u_{ib}^{n+1} \geq u_m$, the interface moves to the right of domain representing melting of solid. If $u_{ib}^{n+1} < u_m$, the interface moves to the left of domain, representing freezing of liquid. In the following section, we validate the results of loose and tight coupling methods to analytical solution of two phase Stefan problem.

4 Numerical tests

In order to investigate the relative error between the analytical solution and the coupling methods, we consider $L^2$-error norm, i.e., the root mean square error, for the temperature. Let $u_{analytical}$ be the analytical solution of the Stefan problem and $u_{coupling}$ be the solution for loose and tight coupling methods. The relative $L^2$-error norm at time $t^n$ for $nx$ (number of grid points) is given by

$$\text{Relative error} = \frac{\sum_{i=1}^{nx}|u_{i,\text{analytical}} - u_{i,\text{coupling}}|^2}{\sum_{i=1}^{nx}|u_{i,\text{analytical}}|^2} \quad (21)$$

Figure 3 shows the relative error for $L^2$ norm for temperature between the analytical solution of two phase Stefan problem and solution of loose and tight coupling methods.

5 Results and Discussion

Figure 1 shows that the initial state of the material is solid. We impose a liquid temperature $u_l$ which is greater than melting temperature $u_m$ at $x = 0$. This results in an increase of temperature from the side $x = 0$, and when the temperature reaches the melting point, the material starts melting into liquid. The interface separates the two phases, where there is an exchange of temperature values from the liquid domain and heat fluxes from the solid domain. In Stefan problem and coupling methods, the heat equations for liquid and solid, initial and boundary conditions are the same. But the equation at the interface for Stefan problem (Stefan condition) is different from coupling methods. In the Stefan problem, the interface temperature is fixed for simplicity and Stefan’s condition represents the movement of the interface based on the temperature gradients at the interface. However, assuming the fixed temperature at the interface is not realistic, and as a result, we compute the temperature at the interface in coupling methods.

We implemented loose and tight coupling methods to couple thermal diffusion equation for liquid and solid domains. The two domains are coupled by exchanging temperature values (Dirichlet type) and heat fluxes (Neumann type) at the interface. The heat equations
Figure 2: (a) Analytical solution of two phase Stefan problem, (b) solution of loose coupling, (c) solution of tight coupling at \( t \approx 1 \). The red line represents temperature and the blue line represents the position of the interface.
for liquid and solid domains in loose and tight coupling methods are discretized by forward in time and centered difference in space. For the calculation of fluxes at the interface, we considered low order derivatives for loose coupling and higher order derivatives for tight coupling. These coupling methods compute temperature at the interface at each time step, but the interface position does not change. We consider the analytical solution of two phase Stefan problem for comparison since it yields energy conserving and consistent solution. In order to move the interface position in coupling solutions to compare to the analytical solution, we consider index $ib$ to move to the right side of the domain by one grid point, representing melting if the interface temperature is greater than melting temperature. If the interface temperature is less than the melting temperature, we consider index $ib$ to move to left side of the domain by one grid point, representing freezing of liquid.

Figure 2a represents the analytical solution of two phase Stefan problem. Red lines represent the diffusion of temperature and the blue line represent the position of the interface. We observe that the position of interface is $x = 17.5$. Figure 2b represents the solution of loose coupling, and the interface position is at $x = 2.5$, while Figure 2c represents the solution of tight coupling and the interface is at $x = 10$. From the results, we observe that the interface in loose and tight coupling solutions moves to the right side of the domain representing melting of solid. We also observe that the solution with tight coupling looks closest to the analytical solution when compared to the solution of loose coupling. Furthermore, Figure 3 shows that the relative error for $L^2$-norm between the analytical solution of two phase Stefan problem and solution for tight coupling method shows less error when compared to the solution with loose coupling method. This may be due to the large overlap in tight coupling. However, this study requires further analysis for loose
and tight coupling methods and also needs realistic representation to move the interface in coupling methods.

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REFERENCES


GENERIC BASED THERMODYNAMICALLY CONSISTENT DISCRETISATION IN SPACE AND TIME FOR OPEN THERMOMECHANICAL SYSTEMS

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Abstract. In the present contribution structure-preserving numerical methods for finite strain thermoelastodynamics are proposed. The underlying variational formulation is based on the GENERIC formalism and makes possible the free choice of the thermodynamic state variable. The notion ‘GENERIC consistent space discretization’ is introduced which facilitates the design of Energy-Momentum-Entropy (EME) consistent schemes. In particular, three alternative EME schemes result from the present approach. These schemes are directly linked to the respective choice of the thermodynamic variable. A numerical example confirms the structure-preserving properties of the newly developed EME schemes, which exhibit superior numerical stability.

Since the pioneering work in [1], Energy-Momentum (EM) schemes established themselves in the field of nonlinear elastic solids and structures. Elastic solids and structures such as geometrically exact beams and shells fall into the framework of Hamiltonian systems with symmetry. EM schemes preserve main structural properties of the underlying reversible systems. In particular, by design, they correctly reproduce the balance laws for angular momentum and energy in the discrete setting. This way EM schemes often yield superior numerical stability and robustness. For more details on EM schemes, we refer the interested reader to [2, 3].

In the present work we aim at the extension of EM schemes to mechanical systems with dissipation. In particular, we focus on large-strain thermoelasticity. For that purpose, GENERIC (General Equation for Non-Equilibrium Reversible-Irreversible Coupling) provides an appealing framework since it recovers the Hamiltonian description in the absence of dissipative processes. In other words, GENERIC provides a natural extension of Hamiltonian mechanics to dissipative mechanical systems.

GENERIC was originally developed in the context of complex fluids (see [4] for a comprehensive account of the GENERIC framework) and later applied to solid mechanics, see [5, 6] and [7]. The GENERIC framework was first applied to computational solid mechanics in [8, 9] who coined the notion “thermodynamically consistent (TC) integrator”. Alternatively, [10] recently introduced ‘GENERIC integrators’ which can be regarded as extension of symplectic integrators for Hamiltonian systems to the realm of dissipative systems.
Another advantageous feature of the GENERIC framework is that it facilitates the use of different sets of independent state variables (see [4] and [7]). The entropy was initially preferred as thermodynamic state variable in GENERIC-based integrators (see [8, 9] and [11, 12]). The work by [7] has laid the theoretical foundation for the development of GENERIC-based integrators relying on the temperature as thermodynamic state variable, see [13], [14] and [15]. In particular, in [7] a special form of GENERIC is devised which makes possible the free choice of the thermodynamic state variable. Mielke’s procedure inspired further work on GENERIC-based integrators for finite-dimensional mechanical systems in [16] and finite-strain thermoelasticity in [17]. In particular, in [17] a GENERIC-based weak form is derived which makes possible the free choice of the thermodynamic state variable.

The GENERIC-based weak form in [17] provides the starting point for the development of Energy-Momentum-Entropy (EME) schemes (see [18] for more details). It was shown in [17] that the application of the standard mid-point rule already yields structure-preserving schemes. For example, choosing the internal energy density as thermodynamic state variable leads to an Energy-Momentum scheme. On the other hand, choosing the entropy density as thermodynamic state variable yields a Momentum-Entropy scheme. However, despite of their structure-preserving properties, all of the mid-point type schemes considered in [17] turned out to be prone to numerical instabilities. These observations led to the conjecture that only EME schemes will exhibit superior numerical stability for dissipative systems in the same way as do EM schemes for Hamiltonian systems.

Of course, the GENERIC framework is not a prerequisite for the development of structure-preserving numerical methods for non-isothermal solid mechanics. In the context of coupled thermomechanical problems alternative procedures have been proposed in [19], [20], [21] and [22].

As has been outlined above, the main goal of the present work is the development of EME schemes for large-strain thermoelasticity, starting from the GENERIC-based weak form developed in [17]. Correspondingly, Section 1 deals with large-strain thermoelasticity which includes the GENERIC-based weak form. In Section 2 the GENERIC-based weak form is discretized in space, resulting in a GENERIC-consistent space discretization. In Section 3, the semi-discrete system is further discretized in time leading to three alternative EME schemes. Section 4 contains a representative numerical example which confirms both the structure-preserving features and the enhanced numerical stability of the newly developed EME schemes when compared to the mid-point type schemes developed in [17]. Eventually, conclusions are drawn in Section 5.

1 Large-strain thermoelasticity

In this section we summarize the variational formulation of large-strain thermoelasticity with heat conduction which lies at the heart of the proposed discretization in space and time. This variational formulation has originally been developed in the context of the GENERIC framework (see [17] for more details).

1.1 Underlying variational formulation

We consider a continuum body with material points \( \mathbf{X} = X_i e_i \) in the reference configuration \( \mathcal{B} \subset \mathbb{R}^3 \), see Fig. 1. Here and in the sequel the summation convention applies to
repeated indices. Moreover, $e_i$ denote the canonical base vectors in $\mathbb{R}^3$.

**Figure 1:** Reference configuration $B$ with boundary $\partial B$ and current configuration $\varphi(B, t)$ at time $t$. External tractions $\bar{t} = P N$ act on the boundary of the current configuration. In addition to that, the heat flux across the current boundary is denoted by $\bar{q} = Q \cdot N$. Here, the vector $N$ denotes the unit outward normal field on the boundary $\partial B$ of the reference configuration.

Within the Lagrangian description of continuum mechanics the deformed configuration of the body at time $t$ is characterised by the deformation map $\varphi : B \times I \mapsto \mathbb{R}^3$, where $I = [0, T]$ is the time interval of interest. The velocity of the material point $X \in B$ located at $x = \varphi(X, t)$ is given by $v = \dot{\varphi}$, where a superposed dotes denotes the material time derivative. The deformation gradient is given by $F = \nabla \varphi$. In what follows the partial derivative with respect to the material coordinates will often be denoted by the nabla operator. Accordingly, the deformation gradient assumes the form

$$F = \nabla \varphi$$

(1)

Main ingredients of the GENERIC framework are the internal energy and the entropy. In addition to that, the choice of the thermodynamic variable plays an important role. Similar to [7], we allow for the free choice of the thermodynamic variable $\tau : B \times I \mapsto \mathbb{R}$ from among three options $\tau \in \{\theta, \eta, u\}$. These options are (i) the absolute temperature $\theta$, (ii) the entropy density $\eta$, and (iii) the internal energy density $u$. Depending on the choice of the thermodynamic variable, the absolute temperature can be written in the form (see also [4] and [7])

$$\theta = \theta'(C, \tau) = \frac{\partial_{\tau} u'(C, \tau)}{\partial_{\tau} \eta'(C, \tau)}$$

(2)

Here, the internal energy density and the entropy density, respectively, are given by

$$u = u'(C, \tau), \quad \eta = \eta'(C, \tau)$$

(3)

In this connection, a frame-indifferent constitutive formulation for thermoelastic materials is based on the right Cauchy-Green tensor $C = F^T F$. The GENERIC-based weak form
pertaining to large-strain thermoelasticity can be written in the form (see [17])

\[ 0 = \int_B w_\varphi \cdot (\varphi - \rho^{-1} p) \, dV \]
\[ 0 = \int_B \left( w_p \cdot (\dot{p} - b) + FS : \nabla w_p \right) \, dV - \int_{\partial_\varphi B} w_p \cdot \vec{t} \, dA \]
\[ 0 = \int_B \left( w_r \dot{\tau} + \nabla (\rho^{-1} p) : \left( \frac{w_r}{\partial_\eta' \eta} 2F \partial_C \eta' \right) - \nabla \left( \frac{w_r}{\partial_\tau' u} \right) \cdot Q \right) \, dV + \int_{\partial_Q B} \frac{w_r}{\partial_\tau' u} \vec{q} \, dA \]

where \( \rho : B \mapsto \mathbb{R}_+ \) is the mass density in the reference configuration. Moreover, \( p : B \times \mathcal{I} \mapsto \mathbb{R}^3 \) is the linear momentum density and \( b : B \mapsto \mathbb{R}^3 \) represent prescribed body forces which, for simplicity, are assumed to be dead loads. The second Piola-Kirchhoff stress tensor is given by

\[ S = S'(C, \tau) = 2 \left( \partial_C u' - \frac{\partial_\tau' u}{\partial_\eta' \eta} \partial_C \eta' \right) \]

Furthermore, the material heat flux vector assumes the form

\[ Q = Q'(C, \tau) = (\theta')^2 K' \nabla \left( \frac{\partial_\tau' u}{\partial_\eta' \eta} \right) \]

where \( K = K'(C, \tau) \) is the positive semi-definite material conductivity tensor. The weak form needs be supplemented with initial and boundary conditions, respectively. For that purpose, the boundary \( \partial B \) of the continuum body is decomposed into a displacement boundary \( \partial_\varphi B \), on which \( \varphi = \overline{\varphi} \) is prescribed, and a traction boundary \( \partial_\tau B \), on which the external traction \( \vec{t} \) is prescribed such that \( PN = \vec{t} \) (Fig. 2). In this connection, the standard relations \( \partial_\varphi B \cup \partial_\tau B = \partial B \) and \( \partial_\varphi B \cap \partial_\tau B = \emptyset \) hold. Similarly, for the thermal part we consider the subsets \( \partial_\tau B \) and \( \partial_\eta B \), with the properties \( \partial_\tau B \cup \partial_\eta B = \partial B \) and \( \partial_\tau B \cap \partial_\eta B = \emptyset \) (Fig. 3). The thermodynamic variable is prescribed on \( \partial_\tau B \), i.e. \( \tau = \overline{\tau} \), whereas the heat flux is prescribed on \( \partial_\eta B \), i.e. \( Q \cdot N = \overline{q} \).

The unknown fields are subject to initial conditions of the form \( \varphi(\cdot, 0) = X, p(\cdot, 0) = \rho v_0 \), and \( \tau(\cdot, 0) = \tau_0 \) in \( B \). Here, \( v_0 \) is a prescribed velocity field and \( \tau_0 \) is a prescribed field of the thermodynamic variable \( \tau \in \{ \theta, \eta, u \} \).

![Figure 2](image)

**Figure 2:** Mechanical part of the IBVP. Note that \( \vec{t} = PN \) denotes prescribed external Piola tractions acting on the current boundary expressed per unit area of the reference boundary \( \partial_\tau B \).
Figure 3: Thermal part of the IBVP. Note that \( \overline{q} = \mathbf{Q} \cdot \mathbf{N} \) is the prescribed rate of heat transfer across the current boundary expressed per unit area of the reference boundary \( \partial_q \mathcal{B} \).

2 Discretization in space

We next perform the discretization in space of the GENERIC-based weak form (4). To this end we apply the isoparametric finite element approach (see, for example, [23]), based on finite-dimensional approximations of the following quantities

\[
\varphi^h(X, t) = N^a(X) q_a(t), \quad v^h(X, t) = N^a(X) v_a(t) \tag{7}
\]

and

\[
\tau^h(X, t) = N^a(X) \tau_a(t) \tag{8}
\]

Here, the summation convention applies, where \( a = 1, \ldots, N \), and \( N \) denotes the total number of nodes in the finite element mesh. Moreover, \( N^a : B \rightarrow \mathbb{R} \) are the nodal shape functions and \( q_a(t), v_a(t) \in \mathbb{R}^3, \tau_a(t) \in \mathbb{R} \) are the respective nodal values at time \( t \).

Analogous approximations are used for the test functions \( w_\varphi, w_p \) and \( w_\tau \), denoted by \( w^h_\varphi, w^h_p \) and \( w^h_\tau \). Then weak form (4) leads to the following semi-discrete equations:

\[
0 = \int_B w^h_\varphi : (\varphi^h - v^h) \, dV
\]

\[
0 = \int_B \left( w^h_p : \left( \rho \dot{v}^h - \mathbf{b} \right) + \nabla w^h_p : \mathbf{F}^h \mathbf{S}^h \right) \, dV - \int_{\partial_q \mathcal{B}} w^h_p : \overline{\mathbf{t}} \, dA
\]

\[
0 = \int_B \left( \dot{w}^h + \nabla \tau^h : \left( \frac{2}{\Pi_h(\partial_T u^h)} \mathbf{F}^h \partial_C \eta^h \right) \right) \, dV
\]

\[- \int_B \nabla \left( \frac{w^h_r}{\Pi_h(\partial_T u^h)} \right) : \mathbf{Q}^h \, dV + \int_{\partial_q \mathcal{B}} \frac{w^h_r}{\Pi_h(\partial_T u^h)} \overline{\tau} \, dA \tag{9}
\]

where

\[
\mathbf{S}^h = 2 \left( \partial_C u^h - \Theta^h \partial_C \eta^h \right)
\]

\[
\mathbf{Q}^h = (\Theta^h)^2 \mathbf{K}^h \nabla \left( \frac{1}{\Theta^h} \right)
\]

\[
\Theta^h = \frac{\Pi_h(\partial_T u^h)}{\Pi_h(\partial_T \eta^h)} \tag{10}
\]
In this connection, \( u^h = u'(C^h, \tau^h) \), \( \eta^h = \eta'(C^h, \tau^h) \), and \( K^h = K'(C^h, \tau^h) \). The interpolation formulas in (7) give rise to

\[
\begin{align*}
F^h &= q_a \otimes \nabla N^a \\
C^h &= q_b \nabla N^a \otimes \nabla N^b
\end{align*}
\]

(11)

Moreover, \( \Pi_h(\partial_\tau u^h) \) denotes the \( L_2 \) projection of function \( \partial_\tau u^h \) into the finite-dimensional space spanned by the shape functions \( N^a \), \( a = 1, \ldots, N \). That is,

\[
\Pi_h(\partial_\tau u^h) = N^a(\partial_\tau u)_a
\]

(12)

where the nodal values \( (\partial_\tau u)_a \) are determined by

\[
\int_B N^a \left( \partial_\tau u^h - \Pi_h(\partial_\tau u^h) \right) dV = 0
\]

(13)

for \( a = 1, \ldots, N \). In particular, (13) together with (12) constitute a linear system of algebraic equations given by

\[
H^{ab}(\partial_\tau u)_b = \int_B N^a \partial_\tau u^h dV
\]

(14)

where \( H^{ab} \) denote the components of the positive definite Gram matrix \([H^{ab}]\) defined by

\[
H^{ab} = \int_B N^a N^b dV
\]

(15)

Analogous relationships hold for the projection of function \( \partial_\tau \eta^h \), \( \Pi_h(\partial_\tau \eta^h) \). It is worth mentioning that the projections \( \Pi_h(\partial_\tau u^h) \) and \( \Pi_h(\partial_\tau \eta^h) \) are only required if the functions \( \partial_\tau u^h \) and \( \partial_\tau \eta^h \) do not belong to the finite element space spanned by the shape functions \( N^a \). For example, in the temperature-based formulation (i.e. for \( \tau = \theta \)), \( \partial_\theta u^h = \partial_\theta \pi(C^h, \theta^h) \) corresponds to the specific heat at constant deformation. Thus, if this quantity is prescribed to be constant, the projection \( \Pi_h(\partial_\theta \pi) \) need not be performed. However, in general the temperature-based formulation requires both projections (i.e. \( \Pi_h(\partial_\theta \pi) \) and \( \Pi_h(\partial_\theta \eta) \)).

In contrast to that, the two alternative formulations based on the choice \( \tau \in \{ \eta, \sigma \} \) in general require only one projection. In particular, the formulation in terms of the internal energy density relies on \( \Pi_h(\partial_a \pi) \), whereas the entropy-based formulation relies on \( \Pi_h(\partial_a \eta) \). Originally, the projection has been introduced in the framework of the entropy-based formulation in [9] (see also [12]). The introduction of the above projections is essential for retaining consistency of the semi-discrete formulation and is therefore termed \( GENERIC\)-consistent space discretization, see [18] for more details.

### 3 Discretization in time

We aim at a second-order accurate, implicit time-stepping scheme which is capable of correctly reproducing the main balance laws outlined above. Due to its structure-preserving properties this type of integrator is called Energy-Momentum-Entropy (EME) scheme. To devise such a scheme, we essentially apply the mid-point rule in which the derivatives of the internal energy density and the entropy density, respectively, are replaced by appropriate discrete derivatives.
We focus on a representative time interval \([t_n, t_{n+1}]\) with corresponding time-step size \(\Delta t = t_{n+1} - t_n\). The discrete approximations at times \(t_n\) and \(t_{n+1}\) of a function \(f(t)\) will be denoted by \(f_n\) and \(f_{n+1}\), respectively. Assume that the nodal state variables at time \(t_n\), \(q_n\), \(v_n\), and \(\tau_n\) are given. The associated fields result from the nodal interpolation formulas (7) and are denoted by \(\varphi^h_n, v^h_n : \mathcal{B} \mapsto \mathbb{R}^3\) and \(\tau^h_n : \mathcal{B} \mapsto \mathbb{R}, \tau \in \{\theta, \eta, u\}\). We aim at the determination of the corresponding quantities at time \(t_{n+1}\) through the mid-point type discretization of the semi-discrete formulation (9) given by

\[
0 = \int_B w_n^h \cdot \left( \frac{\varphi^h_{n+1} - \varphi^h_n}{\Delta t} - \frac{v^h_n}{\Delta t} \right) dV
\]

\[
0 = \int_B \left( w_n^h \cdot \left( \frac{v^h_{n+1} - v^h_n}{\Delta t} - b \right) + \nabla w_n^h : F^h_{n+\frac{1}{2}} S^h_{alg} \right) dV - \int_{\partial_B} w_n^h \cdot \tau dA
\]

\[
0 = \int_B w^h_{\tau} \left( \frac{\tau^h_{n+1} - \tau^h_n}{\Delta t} + \nabla v^h_{n+\frac{1}{2}} : \left( \frac{2}{\Pi_h(D_{\tau} u^h)} F^h_{n+\frac{1}{2}} D_{\tau} \eta^h \right) \right) dV
- \int_B \nabla \left( \frac{w^h_{\tau}}{\Pi_h(D_{\tau} u^h)} \right) \cdot Q^h_{alg} dV + \int_{\partial_B} \frac{w^h_{\tau}}{\Pi_h(D_{\tau} u^h)} \tau dA
\]

where

\[
S^h_{alg} = 2 (D_C u^h - \Theta^h_{alg} D_C \eta^h)
\]

\[
Q^h_{alg} = (\Theta^h_{alg})^2 K'(C^h_{n+\frac{1}{2}}, \tau^h_{n+\frac{1}{2}}) \nabla \left( \frac{1}{\Theta^h_{alg}} \right)
\]

\[
\Theta^h_{alg} = \frac{\Pi_h(D_{\tau} u^h)}{\Pi_h(D_{\tau} \eta^h)}
\]

The above discretization in time relies on the use of discrete derivatives in the sense of Gonzalez [24]. In particular, the discrete derivatives are applied to the internal energy density and the entropy density, respectively. For example, in the case of the internal energy density, the discrete derivatives are denoted by \(D_{\tau} u^h\) and \(D_C u^h\), respectively. In particular, \(D_{\tau} u^h\) is defined by

\[
D_{\tau} u^h = \frac{1}{2} \left( du^h_C(\tau^h_n, \tau^h_{n+1}) + du^h_C(\tau^h_{n+1}, \tau^h_n) \right)
\]

where

\[
du^h_C(\tau^h_n, \tau^h_{n+1}) = \partial_{\tau} u'(C, \tau^h_n) + \frac{u'(C, \tau^h_{n+1}) - u'(C, \tau^h_n) - \partial_{\tau} u'(C, \tau^h_n) \Delta \tau}{(\Delta \tau)^2} \Delta \tau
\]

and \(\Delta \tau = \tau^h_{n+1} - \tau^h_n\). Furthermore, \(D_C u^h\) is defined by

\[
D_C u^h = \frac{1}{2} \left( du^h_C(C^h_n, C^h_{n+1}) + du^h_C(C^h_{n+1}, C^h_n) \right)
\]

where

\[
du^h_C(C^h_n, C^h_{n+1}) = \partial_C u'(C^h_{n+\frac{1}{2}}, \tau) + \frac{u'(C^h_{n+\frac{1}{2}}, \tau) - u'(C^h_n, \tau) - \partial_C u'(C^h_{n+\frac{1}{2}}, \tau) : \Delta C}{\Delta C : \Delta C} \Delta C
\]
and \( \Delta C = C_{n+1} - C_n \). It can be verified by a straightforward calculation that the discrete derivatives (18) and (19) satisfy the directionality condition

\[
D_C u^h : \left( C_{n+1}^h - C_n^h \right) + D_r u^h \left( \tau_{n+1}^h - \tau_n^h \right) = u'(C_{n+1}^h, \tau_{n+1}^h) - u'(C_n^h, \tau_n^h)
\] (20)

Analogous considerations apply to the discrete derivatives of the internal entropy density, \( D_\tau \eta^h \) and \( D_C \eta^h \), respectively. Moreover, the time-average of any quantity \( \langle \cdot \rangle \) is given by

\[
\frac{1}{2} \left( \langle \cdot \rangle_n + \langle \cdot \rangle_{n+1} \right)
\]

In particular, this implies

\[
C_{n+\frac{1}{2}} = \frac{1}{2} \left( C_n + C_{n+1} \right)
\] (21)

Note that in general \( C_{n+\frac{1}{2}} \neq F^T_{n+\frac{1}{2}} F_{n+\frac{1}{2}} \).

4 Numerical example

The numerical example deals with a rotating disc subjected to a prescribed heat flow over one quarter of the lateral boundary surface (Fig. 4), where the material model can be found in [17, 18]. The disc is discretized using 200 tri-linear finite elements leading to a total of 360 nodes. The prescribed heat flow vector as well as the initial velocity distribution over the disc, which results from a prescribed constant angular velocity \( \omega_0 \in \mathbb{R}^3 \), are given by

\[
v_0(X) = \omega_0 \times X, \quad \omega_0 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \bar{q} = -\frac{2000W}{\pi m^2} f(t), \quad f(t) = \begin{cases} \sin(2\pi t) & \text{for } 0 \leq t \leq 4 \\ 0 & \text{for } t > 4 \end{cases}
\]

![Figure 4: Rotating disc: Initial configuration (left), thermal boundary conditions (middle left), discrete disc (middle right), along with function \( f(t) \) for the prescribed heat flow over part of the boundary surface (right)](image)

The initial temperature of the disc is homogeneously distributed and equal to the reference temperature \( \theta_0 \). The heat flow is prescribed over one quarter of the lateral boundary surface (Fig. 4) during an initial period of time, \( t \in [0, 4] \) s. In Fig. 4 a plot of function \( f(t) \) can be found. The rest of the boundary of the disc is assumed to be thermally insulated (\( \bar{q} = 0 \)). After \( t = 4s \) the prescribed heat flow vanishes as well. A summary of the data used in the simulation of the rotating disc can be found in Table 1.
Table 1: Rotating disc: Data used in the simulations

<table>
<thead>
<tr>
<th>Material parameters</th>
<th>λ</th>
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<tr>
<td></td>
<td>µ</td>
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<td>Specific heat capacity</td>
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<td>Coupling coefficient</td>
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<td>Ref. temperature</td>
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<tr>
<td></td>
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<td>Thickness</td>
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<td>Simulation time</td>
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</tr>
<tr>
<td>Time step</td>
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<td>0.1 s</td>
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</tr>
</tbody>
</table>

Geometry of the rotating disc

During initial period \( t \in [0, 4] \) s the total energy of the system is expected to increase due to the prescribed heat flow into the system. After initial period the system is classified as closed and therefore the total energy of the system should stay constant. All \((EME)_τ\) integrators are capable to correctly reproduce the first law of thermodynamics (see Fig. 5) in contrast to the midpoint-based schemes, where only the formulation in the internal energy density was in accordance with the first law of thermodynamics, see [17].

The total entropy of the system is expected to increase due to the prescribed heat flow into the system during the initial period \( t \in [0, 4] \) s. As the system is closed after the initial period, the total entropy of the system should be a non-decreasing function, whereby the irreversibility is caused by heat conduction. All \((EME)_τ\) integrators correctly reproduce the second law of thermodynamics as can be observed from Fig. 6. Again this is in contrast to the mid-point-based schemes investigated in [17], where only the formulation in terms of the entropy density was shown to be consistent with the second law.
Eventually, the motion of the disc is illustrated in Fig. 7 with snapshots at successive points in time. In addition to that, the distribution of the temperature over the disc is shown.

**Figure 7:** Rotating disc: Snapshots of the motion at successive points in time $t \in \{0, 4, 8, 12, 16, 18, 24, 28\}$s, and corresponding temperature distribution, calculated with the (EME)$_\eta$ scheme and $\Delta t = 0.1$s

### 5 Conclusions

Starting from the GENERIC-based weak form (4) we have newly developed structure-preserving numerical methods for finite strain thermoelasticity with heat conduction. The proposed Energy-Momentum-Entropy (EME) schemes make possible the free choice of the thermodynamic state variable. In particular, one may choose from among three options which include the entropy density, the absolute temperature and the internal energy density. Each choice of the thermodynamic variable ($\tau \in \{\eta, \theta, u\}$) leads to a corresponding (EME)$_\tau$ scheme.

The underlying GENERIC-based weak form has proven to be especially well-suited for the design of structure-preserving schemes. Depending on the choice of the thermodynamic variable $\tau$, the application of the standard mid-point rule already leads to partially
structure-preserving schemes. For example, it was shown in [17] that the choice of the entropy density yields a Momentum-Entropy scheme, whereas the choice of the internal energy density yields an Energy-Momentum scheme. However, despite of their structure-preserving properties, all of the mid-point based schemes turned out to be prone to numerical instabilities (see [17]).

With regard to the discretization in space we have newly introduced the notion GENERIC-consistent space discretization. We have seen that the present discretization in space relying on standard Lagrangian shape functions necessitates the use of specific projections to reach a GENERIC-consistent space discretization.

It was shown that the present EME schemes lead to a significant improvement in the numerical stability when compared to mid-point type schemes. It would be of interest to extend the present approach to more involved coupled thermomechanical problems which also account for inelastic deformations.

References


HYBRID ANALYSIS FOR CONTINUA WITH SOLID AND LIQUID PROPERTIES IN INFINITE HIGH TUBES

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Key words: Functional, Principle, Granular Material, Infinite Tube, Coupled Problems.

Abstract. Many materials like sand, soil, cement, snow and grain, perform like solids or liquids depending on loads and boundary conditions. The proposed coupled solid-liquid analysis has the potential to deal conveniently with the severe nonlinearities that are associated with single state descriptions. Linear elastic behavior characterizes the solid part. Slowly moving incompressible viscous behavior characterizes the liquid part.

1 INTRODUCTION

Granular material in structural and geotechnical engineering generally is treated as a solid with special reference to large deformations. Transformation to a steadily moving state is not possible. If granular material is treated as a liquid with special properties, the hydrostatic pressure evolves in the static state which is not in agreement with the observed impact on structures [2]. The internally coupled solid-liquid analysis presented in this paper allows the complete transformation between static solid state and steady liquid state.

The interaction of static solid and steady incompressible liquid continua has been discussed for an infinite high tube in 2004 [3]. A detailed approximation has been proposed in 2006 [4]. In the present paper the liquid state is represented by pressure only. Dependent on loads and boundary conditions an inhomogeneous distribution of solid and liquid properties in space results from the relation of the first stress invariants. The velocities may be determined in a secondary analysis.

2 FUNCTIONAL AND PRINCIPLE

A functional is postulated for plane continua [1, 5, 7] with solid and liquid properties:

\[
\Pi = \frac{1}{2} \int_A \varepsilon^T \sigma_s dA - \int_A u^T \sigma_p dA - \int_{\partial A} u^T b d\gamma + \mu \int_{\partial A} u^{T} Q^T \sigma_d d\gamma + \int_{\partial A} u^{T} Q^T c d\gamma \tag{1}
\]

An elastic solid interacts with an incompressible liquid which is represented by a pressure field c.

\[
\sigma_s = E \varepsilon \tag{2}
\]

The composite stresses consist of elastic stresses and pressure:
The first integral of the functional represents the elastic energy. The area load \( p \) in the second integral consists of the specific weight \( \gamma \) and the horizontal force \( p_2 \) that interacts between solid and liquid (Figure 1). The red variables describe the solid part. The blue variables describe the liquid part.

The third integral refers to the part \( B_b \) of the boundary, which is subjected to the load \( b \). The boundary load consists of \( b_s \) acting on the solid part and \(-c\) acting on the liquid part.

\[
b = b_s - M^T c
\]

**Figure 1**: Displacements, pressure, loads and boundary conditions for the hybrid analysis of a silo

The last two integrals of the functional refer to the part \( B_m \) of the boundary, where slip is possible in the tangential direction. This part of the boundary is associated with a tangential force opposite to the direction of motion and results in a contribution to the internal virtual work. The lateral displacement is zero. Coulombs law determines the relation between stresses \( \sigma_S \) and load \( b_S \) for the solid part. Tension which would result in cavitation and the loss of bound is avoided for the liquid part by an appropriate relation between pressure \( c \) and load \( b_L \).

\[
b = b_s + b_L
\]
\[ b_0 = -\mu Q^T \sigma_b \]
\[ b_1 = -Q^T c \]
\[ u_n = 0 \quad \text{sign}(u_i) \]

Q Transformation matrix for interaction at the boundaries

At the remaining part \( B_u \) of the boundary the displacement \( u \) is zero.

\[ B = B_s + B_m + B_u \]   \hspace{1cm} (7)

The slip and stick parts of the boundary are determined a priori. The presented linearization requires a stationary motion at the walls. The validity of the a priori assumptions regarding boundaries and direction of motion are checked after the analysis and may lead to iteration.

The pressure field \( c \) becomes active if the displacement boundary conditions are not appropriate to maintain the equilibrium. Otherwise the pressure field vanishes, which results in a mere elastic analysis. The pressure \( c \) is assumed to be associated with an incompressible viscous slowly moving liquid that may be addressed in a secondary analysis.

\[ \Pi = \frac{1}{2} \int_{\Lambda} \varepsilon^T E \varepsilon \, d\Lambda - \int_{\Lambda} u^T p \, d\Lambda - \int_{B_s} u^T (b_s - M^T c) \, dB + \int_{B_m} u^T Q^T (\mu E \varepsilon + c) \, dB \]   \hspace{1cm} (8)

The functional covers the complete range from elastic static behavior to mere liquid behavior. It is restricted to applications without tension.

The variation of the displacements of the functional is set to zero. The pressure depends on the displacements for the prospective applications. It results the following hybrid principle:

\[ \int_{\Lambda} \delta \varepsilon^T E \varepsilon \, d\Lambda - \int_{\Lambda} \delta u^T p \, d\Lambda - \int_{B_s} \delta u^T (b_s - M^T c) \, dB + \int_{B_m} \delta u^T Q^T (\mu E \varepsilon + c) \, dB = 0 \]   \hspace{1cm} (9)

The derivations of the displacements determine the strains:

\[ \varepsilon = Du \]   \hspace{1cm} (10)

\[ \int_{\Lambda} \delta (Du)^T E (Du) \, d\Lambda - \int_{\Lambda} \delta u^T p \, d\Lambda - \int_{B_s} \delta u^T (b_s - M^T c) \, dB + \int_{B_m} \delta u^T Q^T [\mu E (Du) + c] \, dB = 0 \]   \hspace{1cm} (11)

3 INFINITE HIGH TUBE

An infinite vertical tube is chosen as a representative application. These conditions are present for example in tall silos, in vertical blood vessels and in funnels of erupting volcanos.

For resting or steadily moving hybrid material in an infinite high tube, exact analytical solutions are available. This allows an evaluation of the general performance of the numerical analysis based on the hybrid solid-liquid formulation.

Figure 2 shows a horizontal slice taken from a vertical infinite high plane tube. The constant area load \( p \) which is identical to the specific weight \( \gamma \) acts on the material. With respect to infinity the complete weight of the slice is transferred to the vertical walls and results in shear forces that hold the equilibrium. Between the two walls the shear stresses vary linearly in the horizontal direction and stay constant in the vertical direction. The contribution of the cut off
upper and lower parts of the tube represents the related boundary load $\sigma_{12}$ that acts on the top and bottom faces of the slice.

If no sliding is possible at the vertical walls the distribution of displacement is quadratic in the horizontal direction and constant in the vertical direction (Figure 2). The principal stresses are independent from the properties of the material. The major principal stress $\sigma_1$ (compression) is opposite equal to the minor principal stress $\sigma_{11}$ (tension). The angle is 45 degrees. Since tension is not permissible for granular material a relative movement at the walls evolves.

3.1 Analysis

The link between the exact formulation and the approximate formulation is the analysis for nonlinear symmetric distributions of vertical stresses over the cross section (Figure 6). No changes regarding the vertical and horizontal stresses are possible in the vertical direction.

\[
\frac{\partial \sigma_{11}}{\partial x_1} = 0 \quad \frac{\partial \sigma_{22}}{\partial x_2} = 0 \quad \frac{\partial \sigma_{12}}{\partial x_2} = 0
\]  

(12)

No change of the vertical strain in the horizontal direction is possible since then the solid shear stresses would increase according to the infinity of the height.

\[
\frac{\partial e_{11}}{\partial x_2} = 0
\]  

(13)

Shear stresses follow from the equilibrium:

\[
\sigma_{12} = -\gamma x_2
\]  

(14)

Normal stresses:

\[
\sigma_{11,s} = \sigma_{11} - c
\]  

(15)

\[
\sigma_{22,s} = \sigma_{22} - c
\]  

(16)

\[
\sigma_{22,s} = \frac{\nu}{1-\nu} \cdot \sigma_{11,s}
\]  

(17)

Boundary condition at the walls:
Equilibrium at the walls:
\[ \sigma_{12} = c + \mu \sigma_{22} \]  
\[ (18) \]

\( \sigma_{12} = -\frac{\gamma L}{2} \)  
\[ (19) \]

### 3.2 Constant vertical stress distribution

Horizontal strain:
\[ \varepsilon_{22} = 0 \]  
\[ (20) \]

![Figure 3: Boundary stresses and principal stresses in a slice of an infinite high vertical plane tube. a, elastic solid solution (left) and b, liquid solution (right)](image)

**Solid solution:**

A mere solid solution evolves in the following case. The applied vertical boundary load \( b_1 \) causes horizontal stresses \( \sigma_{22} \) that activate shear stresses \( \sigma_{12} \) by wall friction that hold the equilibrium to the weight of the silo slice (Figure 3a).

\[ \varepsilon_{11} = -\gamma L \frac{(1 + \nu)(1 - 2\nu)}{2\mu E\nu} \]  
\[ (21) \]

\[ \sigma_{11} = -\gamma L \frac{(1 - \nu)}{2\mu \nu} \]  
\[ (22) \]

For a given height \( H \) of the solution area it is possible to determine the displacements. Index \( t \) refers to the top face; index \( b \) refers to the bottom face. Index \( c \) refers to the centre; index \( w \) refers to the walls.
3.3 Nonlinear vertical stress distribution

A nonlinear vertical stress distribution over the cross section is possible in an infinite high vertical tube. It probably will not evolve with respect to the minimum of elastic deformation energy.

Derivation of the stress strain relations:

$$u_{\text{nc}} = u_{\text{nw}} + u_{\text{bc}}$$  \hspace{1cm} (23)

$$u_{\text{nw}} = \gamma HL \cdot \frac{(1 + v)(1 - 2v)}{2\mu E v}$$  \hspace{1cm} (24)

$$u_{\text{bc}} = \frac{\gamma L^2}{4E} (1 + v)$$  \hspace{1cm} (25)

The integral of horizontal strain is zero according to the vertical tube.

$$\varepsilon_{22} = -\frac{1 + v}{E} \cdot \sigma_{11} + c$$  \hspace{1cm} (27)

$$\int_{-\frac{L}{2}}^{\frac{L}{2}} \varepsilon_{22} \, dx_2 = 0 = -\frac{1 + v}{E} \int_{-\frac{L}{2}}^{\frac{L}{2}} \sigma_{11} \, dx_2 + cL$$  \hspace{1cm} (28)

3.4 Functional and Principle

Functional:

$$\Pi = \frac{1}{2} \int_A (Du)^T E(Du) \, dA - \int_A u_2 \frac{\partial C}{\partial x_2} \, dA - \int_A u_1 \gamma \, dA - \int_{b_h} u_1 (b_1 - c) \, dB + \int_{b_n} u_1 \mu (\sigma_{22,s} + c) \, dB$$  \hspace{1cm} (29)

Principle:

$$\int_A \delta (Du)^T E(Du) \, dA = \int_A \delta u_2 \frac{\partial C}{\partial x_2} \, dA - \int_A \delta u_1 \gamma \, dA - \int_{b_h} \delta u_1 (b_1 - c) \, dB + \int_{b_n} \delta u_1 \mu (\sigma_{22,s} + c) \, dB = 0$$  \hspace{1cm} (30)

4 APPROXIMATION

A fourth order approximation of the vertical displacement \(u_1\) in the horizontal direction and a linear approximation in the vertical direction require six degrees of freedom with respect to the symmetry of the tube.

A single degree of freedom is required for a cubic approximation of the horizontal displacement \(u_2\) since it is assumed to be constant in the vertical direction and to be zero in the center and at the walls of the tube. This degree of freedom is the horizontal strain \(\varepsilon_{22}\) in the
center which is the first derivation of the horizontal displacement. The digits t and b of the nodal values refer to the top face and the bottom face (Figure 4).

\[ u = F^T \bar{u} = \begin{pmatrix} t^T \\ 0^T \\ f \end{pmatrix} \begin{pmatrix} \bar{u}_1 \\ \bar{u}_2 \end{pmatrix} \]  

(31)

Displacement at the walls:

\[ u_w = h^T \bar{u}_w = \frac{H-x_t}{H} u_{tw} + \frac{x_t}{H} u_{bw} \]  

(32)

Restriction of the vertical tube:

\[ u_{bw} = 0 \]  

(33)

\[ u_{bc} = u_{bc} + u_{tw} \]

\[ u_{bc}' = u_{bc}' \]

\[ u_{bw} = u_{bw}' \]

---

**Figure 4**: Nodal values for the interpolation functions

The liquid pressure \( c \) is assumed to be constant in the vertical direction and quadratic in the horizontal direction. Due to symmetry two degrees of freedom are required. These degrees of freedom are the liquid pressure \( c_c \) in the center and \( c_w \) at the walls (Figure 4).

Strain interpolation matrix:

\[ B = D F^T \]  

(34)

The boundary load \( b \) acts at the top face and the bottom face of the slice. The quadratic distribution of the vertical component \( b_1 \) depends on values \( b_c \) at the center and \( b_w \) at the walls. The linear distribution of the horizontal component \( b_2 \) depends on the value \( b_{2w} \) at the walls. It is zero in the center.
Integration of area load:

\[ \int_{A} F_p dA = \gamma \int_{A} f dA \]

The horizontal area load is an interaction between solid and liquid parts:

\[ p_{2,L} = -p_{2,S} \]

Integration of partial area load:

\[ \int_{A} F_p dA = \begin{cases} \gamma_s \int_{A} f dA \\ -p_{2,w,S} \int_{A} g dA \end{cases} \]

\[ p_{2,w,S} \quad \text{Solid part (S) of the horizontal force } p_2 \text{ at the walls (w)} \]

It follows with the principle (30):

\[ \delta \bar{u}^T B \bar{E} B^T dA \bar{u} - \delta \bar{u}^T \int_{A} \frac{\partial g^T}{\partial \bar{X}_2} dA \bar{e} - \delta \bar{u}^T \int_{A} f dA - \delta \bar{u}^T \int_{A} g^T dB (\bar{h}_b - \bar{c}) + \ldots \]

\[ \ldots + \delta \bar{u}_w^T \mu \int_{\bar{h}_w} \frac{\partial f}{\partial \bar{X}_2} e^T B^T dB \bar{u} + \delta \bar{u}_w^T \mu \int_{\bar{h}_w} h g^T dB \bar{c} = 0 \]

5 EXAMPLES

Specific weight, Poisson’s ratio and coefficient of wall friction in the applications represent grain [2]. The modulus of elasticity is chosen according to [6] (e.g. peat).

\( \gamma = 0,009 \text{ MN/m}^2 \) specific weight
\( E = 1,000 \text{ MN/m}^3 \) Young’s modulus
\( \nu = 0,375 \) Poisson’s ratio
\( \eta = 0,001 \text{ MNs/m} \) viscosity
\( \mu = 0,4 \) coefficient of wall friction
\( L = 1,00 \text{ m} \) width
\( H = 20,00 \text{ m} \) height

5.1 Constant vertical stress distribution

The finite element analysis reproduces the exact solutions for constant vertical stresses (Section 3.2). The stresses are negative for granular material since tension is not permitted. In the following discussion omits the sign for compression while (partial) tension is indicated by a minus sign.

Solid solution:
\[ \sigma_{11} = 0.01875 \text{ MN/m}^2 \] (39)

The solid solution represents the state of rest in a high silo. The red color indicates the mere solid state of the hybrid material. Liquid pressure is zero. Solid stresses and displacements are identical with Section 3.2.

![Diagram showing solid solution](image)

**Figure 5**: Transformation from a, the solid state (red) by the hybrid states (b, dark red and c, violet) to d, the liquid state (blue)

Liquid solution:

\[ \sigma_{11} = 0.0045 \text{ MN/m}^2 \]
\[ c = 0.0045 \text{ MN/m}^2 \] (40)

The blue color indicates the mere liquid state of the hybrid material. Solid stresses and displacements are zero.

The liquid solution evolves only for absent or nearly absent bottom since the flow velocity in the steady state is very high. For even higher velocities a granular gas evolves that is not covered by the performance of coupled solid and liquid analysis.

Hybrid solution:

The hybrid solid liquid solution represents the common situation in tall silos if the material is moving with a constant velocity. This happens sometime after the beginning of discharging. The behavior is primarily solid, and the velocity is small. No horizontal displacements evolve for constant vertical stress distributions.
Transformation:

The two states analysis enables the transformation from the static solid state at the beginning of time to the steady liquid state at the end of time. Figure 5 shows the solid and liquid states and two intermediate hybrid states.

The red picture in Figure 5 represents the solid state. The first violet picture represents an intermediate hybrid state. It contains more red color which indicates that the solid part dominates the liquid part. The second violet picture represents another hybrid state. It contains more blue color since the behavior is primarily liquid.

5.2 Quadratic vertical stress distribution

Nonlinear vertical stress functions \( \sigma_{11} \) result in nonlinear distributions of solid and liquid parts over the cross section. The relation between both parts is determined by the relation of the first stress invariants \( I_{1,S} \) and \( I_{1,L} \) (Table 1). Limiting condition for the solution area is that one part cannot exceed 100 %. According to Section 3.3 evolve horizontal area load \( p_2 \) and horizontal strain \( \varepsilon_{22} \).

Table 1: Stresses, principal stresses, stress invariants, strains and horizontal load

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<thead>
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<th>6a</th>
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<td>( I_{1,L}/I_{1,S} )</td>
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</table>

Lower pressure in the centre:

Starting from the mere solid case only a decline of the vertical stresses in the center is possible to avoid tension. For lower vertical stresses in the center (Figure 6a) the partial solid stresses dominate in the center (red color). At the walls the liquid stresses finally exceed the solid stresses (violet color). If the vertical stresses in the center continue to decrease the solid stresses at the walls enter the not permitted tension range. This follows from the horizontal strain at the walls in the second column of Table 2.
Lower pressure at the walls:

Starting from the mere liquid case only an increase of the vertical stresses in the center is possible. For higher vertical stresses in the center (Figure 5b) the partial liquid stresses dominate in the center (blue color). At the walls the solid stresses finally exceed the liquid stresses (red color).

Transformation:

The mere solid solution (Figure 5a) turns to the hybrid solution (Figure 6a) if the constant stress function turns to a concave stress function. While the stress level decreases it approaches the mere liquid solution (Figure 5d). While the constant stress function turns into a convex stress function (which is barely possible) it turns to the hybrid solution (Figure 6b). While the stress level increases it finally approaches the mere solid solution again (Figure 5d).

Table 2: Transformation from the solid state (Fig. 5a) by the hybrid state (Fig. 6b) to the liquid state (Fig. 5d) and back to the solid state by the hybrid state (Fig. 6a), (x_2=0.5)

<table>
<thead>
<tr>
<th>Fig.:</th>
<th>5a</th>
<th>6a</th>
<th>5d</th>
<th>6b</th>
<th>5a</th>
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</thead>
<tbody>
<tr>
<td>(\sigma_{11,c})</td>
<td>0,01875</td>
<td>0,013050</td>
<td>0,004500</td>
<td>0,005925</td>
<td>0,01875</td>
</tr>
<tr>
<td>(\sigma_{11,w})</td>
<td>0,01875</td>
<td>0,008775</td>
<td>0,004500</td>
<td>0,007350</td>
<td>0,01875</td>
</tr>
<tr>
<td>(\sigma_{22})</td>
<td>0,01125</td>
<td>0,010125</td>
<td>0,004500</td>
<td>0,004650</td>
<td>0,01125</td>
</tr>
<tr>
<td>(c)</td>
<td>0</td>
<td>0,000750</td>
<td>0,004500</td>
<td>0,004400</td>
<td>0</td>
</tr>
<tr>
<td>(p_2)</td>
<td>0</td>
<td>0,042750</td>
<td>0</td>
<td>-0,014250</td>
<td>0</td>
</tr>
<tr>
<td>(\varepsilon_{11})</td>
<td>0,01031</td>
<td>0,00206</td>
<td>0</td>
<td>0,00241</td>
<td>0,01031</td>
</tr>
<tr>
<td>(\varepsilon_{22})</td>
<td>0</td>
<td>0,00392</td>
<td>0</td>
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<td>0</td>
</tr>
<tr>
<td>(\sigma_{12})</td>
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<td>0,00450</td>
<td>0,00450</td>
<td>0,00450</td>
<td>0,00450</td>
</tr>
<tr>
<td>(\sigma_1)</td>
<td>0,020858</td>
<td>0,01400</td>
<td>0,004500</td>
<td>0,010698</td>
<td>0,020858</td>
</tr>
<tr>
<td>(\sigma_2)</td>
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<td>0,00490</td>
<td>0,004500</td>
<td>0,001302</td>
<td>0,009142</td>
</tr>
<tr>
<td>(\alpha)</td>
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<td>40,7</td>
<td>45,0</td>
<td>36,6</td>
<td>25,1</td>
</tr>
<tr>
<td>(I_{1,L}/I_{1,S})</td>
<td>0</td>
<td>0,793</td>
<td>1,00</td>
<td>0,733</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 2 shows the development at the walls (x_2 = 0,50 m) during this process. The intermediate states result from the development of the vertical stress in the center (x_2 = 0) in the first line.

6 CONCLUSIONS

The computational method presented in this paper covers a wide range of possible applications. It is based on the simultaneous interaction of two materials in the same place at the same time. The linearity of the analysis is preserved. The unavoidable nonlinear effects are covered by obvious a priori considerations as usual in engineering. Further research is directed
towards more general applications and the investigation of the usefulness of the numerical analysis that has been developed for an infinite high tube.

Figure 6: a, Primarily solid behavior at the walls and nearly liquid behavior in the center (left). b, Primarily liquid behavior at the walls and nearly solid behavior in the center (right).

REFERENCES
TIME REVERSAL METHODS IN ACOUSTO-ELASTODYNAMICS

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Key words: Time Reversal, Elastodynamics, Elastic waves, Wave propagation, Finite Element, Inverse problems

Abstract. The aim of the article is to solve an inverse problem in order to determine the presence and some properties of an elastic “inclusion” (an unknown object, characterized by elastic properties discriminant from the surrounding medium) from partial observations of acoustic waves, scattered by the inclusion. The method will require developing techniques based on Time Reversal methods. A finite element method based on variational acousto-elastodynamics formulation will be derived and used to solve the forward, and then, the time reversed problem. A criterion, derived from the reverse time migration framework, is introduced, to help use to construct images of the inclusions to be determined. Our approach will be applied to configurations modeling breast cancer detection, using simulated ultrasound waves.

1 INTRODUCTION

Time reversal (TR) is a subject of very active research for over two decades. Many international teams are currently working on the subject from theoretical, physical and numerical points of view. It was originally experimentally developed by M. Fink in 1992 in acoustics and showed very interesting features [1].

Time reversal is a procedure based on the reversibility property of wave propagation phenomena in non-dissipative media. As a consequence, one can “time-reverse” developed signals, by letting them propagate back in time to the location of the source (or scatterers) that emitted them originally. The initial experiment, proposed by M. Fink, was to refocus, very precisely, a recorded signal after passing through a barrier consisting of randomly distributed metal rods. Theoretically, as well as an inverse problem solved in
ideal circumstances, TR method should yield the exact solution. However, there is always the possibility that under some (realistic!) conditions, the time reversed process will fail. This may happen due to several reasons: measurement noise, availability of only partial information in space or in time, and lack of knowledge about the medium properties. Since then, numerous applications of this physical principle have been designed, in seismology, for locating the epicenter of an earthquake from measurements taken on the ground [2] and medical imaging [3]. The first mathematical analysis can be found in [4] for a homogeneous medium and in [5], [6] for a random medium.

In a previous Note [16], we have shown the feasibility of a TR method in an acousto-elastic medium. We propose here to extend it by considering more complex acousto-elastic medium that can mimic, for instance, breast tissue configurations. We will apply our approach to identify an “inclusion”, or to differentiate between two close inclusions, eventually with different elastic properties, corresponding to different breast tumors, for example, benign and malignant. Indeed, elastic properties of tumor often help to differentiate them: typically, a benign tumor corresponds to normal breast tissues, with a Young modulus between 1 and 70 KPa, whereas malignant tumors have a Young modulus varying from 15 to 500 KPa (see for instance [7]).

2 Forward Problem

We first formulate the mathematical forward problem. We consider a two-dimensional fluid-solid domain $\Omega$ made of two parts, an acoustic one $\Omega_f$ and an elastic one $\Omega_s$.

![Figure 1: Acousto-elastic medium that mimics breast tissue](image)

We will assume that $\Omega$ is half an ellipse (see figure 1). The acoustic part of the domain $\Omega_f$ corresponds to a homogeneous fluid, characterized by its density $\rho_f$ and its Lamé
parameter $\lambda_f$. We denote by $\partial \Omega_f$ the boundary of $\Omega_f$ and $n$ is the outward unit normal to the boundary. Introduce the pressure $p(x, t)$ on a time $t$, $x = (x_1, x_2) \in \Omega_f$, and $f(x, t)$ is a given source, for instance a Ricker function, the acoustic wave equation in $\Omega_f$ is written
\[
\frac{1}{\lambda_f} \frac{\partial^2 p}{\partial t^2} - \text{div} \left( \frac{1}{\rho_f} \nabla p \right) = f ,
\] (1)
together with initial homogeneous conditions. We assume that the boundary $\partial \Omega_f$ can be split into $\partial \Omega_f = \Gamma_f \cup \Gamma_I$, where $\Gamma_I$ denotes the interface between the fluid and solid part, assumed, for simplicity, to be horizontal. We supplement the system with absorbing boundary conditions [15] on $\partial \Omega_f$. Denoting by $V_p = \sqrt{\frac{\lambda_s}{\rho_s}}$ the wave velocity in the fluid, the absorbing boundary conditions on $\Gamma_f$ are written
\[
\frac{\partial p}{\partial t} + V_p \frac{\partial p}{\partial r} + V_p \frac{p}{2r} = 0
\] (2)
On the part $\Gamma_I$, we add an interface condition for the pressure $p(x, t)$, that will be presented below, see (5). We then introduce the governing equations of linear elastodynamics for $\Omega_s$, the solid part of the domain, characterized by the density $\rho_s$, and the Lamé parameters $\lambda_s$ and $\mu_s$. We assume that the boundary $\partial \Omega_s$ can be split into $\partial \Omega_s = \Gamma_s \cup \Gamma_f$. Denoting by $u(x, t) = (u_1(x_1, x_2, t), u_2(x_1, x_2, t))$ the velocity on a time $t$, at a point $x = (x_1, x_2) \in \Omega_s$, we have
\[
\rho_s \frac{\partial^2 u}{\partial t^2} - \nabla \cdot (\mu_s \nabla u) - \nabla \left( (\lambda_s + \mu_s) \nabla \cdot u \right) = 0 ,
\] (3)
Remark that writing the equation above in terms of velocity (e.g. the time derivative of the displacement) instead of displacement, allows us to derive a pressure-velocity fluid-solid formulation, which will make easier the handling of the transmission conditions during the derivation of the variational formulation, as we will see below.

This equation is supplemented with homogeneous initial conditions and absorbing boundary conditions on $\Gamma_s$, as proposed in [14],
\[
A \frac{\partial u}{\partial t} = \tau(u) \cdot n ,
\] (4)
where the matrix $A$ is a diagonal $N \times N$ matrix, with $A_{11} = -\sqrt{\rho_s(\lambda_s + 2\mu_s)}$, $A_{22} = -\sqrt{\rho_s\mu_s}$ for horizontal boundaries, and the contrary for vertical boundaries. A general expression of $A$ can be found in [14] for more complex geometries of the boundary. Finally, we introduce the transmission conditions at the fluid-solid interface $\Gamma_I$:
\[
\frac{1}{\rho_f} \frac{\partial p}{\partial n} = \frac{\partial u}{\partial t} \cdot n ,
\] (5)

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\[
\frac{\partial p}{\partial t} \mathbf{n} = \tau(u) \mathbf{n} .
\] (6)

These conditions express the continuity of the normal component (5) and of the stress tensor (6) and appear naturally in the pressure-velocity variational formulation, that will be basis of the finite element method. Putting all these equations together, one can derive the following variational formulation in the fluid-solid domain:

\[
\int_{\Omega} \frac{1}{\lambda_f} \frac{\partial^2 p}{\partial t^2} q \, d\omega + \int_{\Omega} \frac{1}{\rho_f} \nabla p \cdot \nabla q \, d\omega \\
+ \int_{\Gamma_f} \frac{\partial \mathbf{u}}{\partial t} \cdot \mathbf{n} q \, d\sigma + \int_{\Gamma_f} (\frac{1}{\lambda_f \rho_f} \frac{\partial p}{\partial t} + \frac{p}{2\tau \rho_f}) q \, d\sigma = \int_{\Omega} f q \, d\omega ,
\] (7)

\[
\int_{\Omega_s} \rho_s \frac{\partial^2 \mathbf{u}}{\partial t^2} \cdot \mathbf{v} \, d\omega + \int_{\Omega_s} \lambda_s \text{div} \mathbf{u} \text{div} \mathbf{v} + 2\mu_s \tau_{ij}(\mathbf{u}) \tau_{ij}(\mathbf{v}) \, d\omega \\
- \int_{\Gamma_v} \frac{\partial p}{\partial t} \mathbf{v} \cdot \mathbf{n} d\sigma - \int_{\Gamma_s} \mathbf{n} \frac{\partial \mathbf{u}}{\partial t} \cdot \mathbf{v} d\sigma = 0 .
\] (8)

3 Time Reversed Problem

In a second step, we formulate the time reversed acousto-elastic problem. Examples of time reversal techniques, numerical or experimental, can be found (among others) in [1, 9, 10, 11, 12]. We first introduce the time-reversed wave equation for the acoustic part of the domain \( \Omega_f \). We denoted by \( p^R(\mathbf{x}, t') \) the time-reversed pressure, defined by \( p^R(\mathbf{x}, t') = p(\mathbf{x}, T_f - t) \), \( \mathbf{x} \in \Omega_f \), where \( T_f \) denotes the final time. Since the wave equation involves only second order time derivatives, this definition ensures that the reversed field \( p^R(\mathbf{x}, t') \) is a solution to the wave equation

\[
\frac{1}{\lambda_f} \frac{\partial^2 p^R}{\partial t'^2} - \text{div} \left( \frac{1}{\rho_f} \nabla p^R \right) = 0 ,
\] (9)

together with (TR) initial conditions and (TR) absorbing boundary conditions on \( \Gamma_f \), analogous to (2). In addition, on the boundary \( \Gamma_{SRA} \), modeling a source-receivers array (SRA) where the forward signal is recorded (see Fig. 1), we set \( p^R(t') = p(T_f - t) \) which is the (recorded) source of the TR.

Similarly, we also introduce the elastic time-reversed problem associated to equation (3). We denote by \( \mathbf{u}^R(\mathbf{x}, t') = (u_1^R(x_1, x_2, t'), u_2^R(x_1, x_2, t')) \) the time-reversed velocity solution to linear elastodynamics, that solves
\[ \rho_s \frac{\partial^2 u^R}{\partial t'^2} - \nabla \cdot (\mu_s \nabla u^R) - \nabla ((\lambda_s + \mu_s) \nabla \cdot u^R) = 0, \quad (10) \]

together with (TR) initial conditions and absorbing boundary conditions analogous to (4). Finally, we derive the time-reversed continuity transmission conditions at the interface \( \Gamma_I \)
\[ \frac{1}{\rho_f} \frac{\partial p^R}{\partial t'} \cdot \mathbf{n} = - \frac{\partial u^R}{\partial t'} \cdot \mathbf{n}, \quad (11) \]

\[ \frac{\partial p^R}{\partial t'} \mathbf{n} = \tau(u^R) \mathbf{n}. \quad (12) \]

Similar to the forward problem, we introduce the time-reversed variational formulation
\[ \int_{\Omega_f} \frac{1}{\rho_f} \frac{\partial^2 p^R}{\partial t'^2} q d\omega + \int_{\Omega_f} \frac{1}{\rho_f} \nabla p^R \cdot \nabla q d\omega + \int_{\Gamma_I} \frac{1}{\rho_f} \frac{\partial u^R}{\partial t'} \cdot \mathbf{n} q d\sigma + \int_{\Gamma_I} \left( \frac{1}{\rho_f} \frac{\partial p^R}{\partial t'} + \frac{p^R}{2\tau \rho_f} \right) q d\sigma - \int_{\Gamma_{SRA}} f q d\sigma = 0 \quad (13) \]

\[ \int_{\Omega_e} \rho_e \frac{\partial^2 \mathbf{u}^R}{\partial t'^2} \cdot \mathbf{v} d\omega + \int_{\Omega_e} \lambda_e \text{div} \mathbf{u}^R \text{div} \mathbf{v} + 2\mu_e \tau_{ij}(\mathbf{u}^R) \tau_{ij}(\mathbf{v}) d\omega - \int_{\Gamma_I} \frac{\partial p^R}{\partial t'} \mathbf{v} \cdot \mathbf{n} d\sigma - \int_{\Gamma_{SRA}} k \frac{\partial \mathbf{u}^R}{\partial t'} \cdot \mathbf{v} d\sigma = 0. \quad (14) \]

In order to create synthetic data, the forward and reversed formulations are approximated by the FreeFem++ package [13] which implements a finite element method in space. In this study we use a \( P_2 \) finite element method. The advancement in time is performed by using a second order in time central finite difference scheme, so that it is time reversible also on the numerical level.

### 4 Numerical results

In this section, we describe numerical results obtained for a scatter identification problem, in the case of two scatters located in the elastic part. The principle of the numerical process is as follows: an incident wave is generated by a point source such that after a time \( T_f \) the total field is negligible. On the boundary \( \Gamma_{SRA} \) located in the fluid part, the forward signal is recorded. Then, we perform numerically a time-reversed computation, by back propagating the recorded scattered data from the SRA. However, we do not assume we know the physical properties or the number of the inclusions, nor their locations. Hence,
the recorded data are back propagated in the medium without the inclusions. Finally, we intend to image the unknown scatterers in the medium - responsible of the diffraction of the incident wave - by using correlation method between the forward $u^I$ and the reversed wave $u^R$ in the same spirit as those involved for instance in time reverse migration [8]. Here, we have considered the following RTM (Reverse Time Migration) criterion:

\[
RTM(x) = \int_{0}^{T_f} u^R_{R}(T_f - t, x) \times u^I(t, x) dt.
\]  

To illustrate our purpose, we consider the medium sketched in Figure 1, made of fluid part (top) and of a elastic one (bottom), the elastic part sketching a breast tissue geometry and is a heterogeneous medium, as it contains a skin layer, i.e. a very thin layer. The SRA is an horizontal line as sketched on Figure 1.

For the fluid part, we choose $\rho = 1000 kg/m^3$ and $\lambda = 2.25 GPa$, for the solid part, the same value of $\rho$ with $\lambda = 1.83 GPa$ and $\mu = 18.33 kPa$, and for the skin (inside the solid part), $\rho = 1150 kg/m^3$, $\lambda = 6.66 GPa$ and $\mu = 66.66 kPa$. There are two elliptical inclusions with different size, shape, and elastic properties. The first one represents a benign tumor with $\rho = 1000 kg/m^3$, $\lambda = 2.16 GPa$ and $\mu = 21.66 kPa$, and the second one a malignant tumor, with the same $\rho$, $\lambda = 2.99 GPa$ and $\mu = 30 kPa$. Note that both inclusions are penetrable, which means that the reflection of the incident wave highlighting the inclusion is quite weak. Finally, the source used to generate the acoustic wave in the fluid part is a Ricker function of the form

\[
f(x, t) = (1 - 2\pi^2(\nu_0 t - 1)^2)e^{-\pi^2(\nu_0 t - 1)^2},
\]

with a central frequency $\nu_0 = 100 kHz$ and a corresponding wavelength equal to $\lambda_W = 12 mm$.

To verify the (in)sensitivity of the method with respect to the noise in the data, we added Gaussian noise to the recorded field $p^S$ with

\[
p^S_{Noise} = (1 + Coeff \ast randn) \ast p^S
\]

where $randn$ satisfies a centered reduced normal law and $Coeff$ is the noise level, taken equal to 10% in our simulations.

Hence, the scatterers are illuminated by an incident acoustic field, that is first transmitted to the elastic medium through the interface $\Gamma_I$, and then scattered by the inclusions, before to be recorded by the SRA. The SRA being located in the fluid part, they are able to record only a scalar quantity (the pressure $p(x, t)$), and not a vector velocity $u(x, t)$.

However, as shown on images below, where the correlation image between the forward and the reversed wave is depicted (only in the elastic layer), one is able to determine the existence and location of the malignant tumor. The definition of more quantitative criteria to determine the presence and the properties of these inclusions is the subject of our future work.
5 Conclusion

We proposed a time-reversal approach for acousto-elastic non homogeneous wave equations. Numerical results have been presented and show satisfactory and promising results in a heterogeneous fluid-solid medium (breast tissue with skin), using only partial information, that is pressure recorded data in the fluid part. By cross-correlating the incident field with the time-reversed scattered field, we were able to determine properties of these inclusions and to differentiate two inclusions, even with different elastic properties. We have now to evaluate quantitatively the obtained elasticity parameters, probably by introducing different cost functions, in the same spirit as what is derived for inverse problems. As usual in this context, optimization based algorithm could be necessary to achieve this part.

REFERENCES


[9] F. Assous, M. Kray, F. Nataf, Time-reversed absorbing conditions in the partial 


breast cancer detection. IEEE Transactions on Microwave Theory and Techniques 

and scatterer identification. Computer methods in applied mechanics and engineering 


[14] L. Halpern, Etudes des conditions aux limites absorbantes pour des schémas 
umériques relatifs a des équations hyperboliques linéaires, Ph.D Thesis, Paris VI 
University, 1980.


[16] F. Assous, M. Lin, Time reversal for obstacle location in elastodynamics from acoustic 
AN ANALYSIS OF THREE-DIMENSIONAL NON-PLANAR CRACK PROPAGATION PHENOMENON WITH SMOOTHED PARTICLE HYDRODYNAMICS METHOD

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Key words: SPH, Fatigue, Crack propagation, Non-planar crack, Fracture mechanics

Abstract. In the present study, the non-planar crack propagation problems in the 3D body are solved, extending our previous study on the smoothed particle hydrodynamics (SPH) method applied to the fatigue crack propagation of the planar cracks in the 3D body. To solve the propagation of the non-planar crack, the crack front particles are given the information of the slope and the position of the crack surface in addition to the crack length. To confirm the validity of the proposed method, a fatigue test of the CT specimen with an additional horizontal hole is carried out and the result is compared with the computed one successfully.

1 INTRODUCTION

The fatigue damage is the critical problem for almost all the mechanical structures. Fatigue crack propagation is one of the dominant phenomena of the damage. Accordingly, some meshing numerical analyses for the crack propagation problem, represented by X-FEM [1], have been investigated. However, in general, it is difficult to solve some complex situations, such as the process of penetrating the thickness of a plate, or connecting multiple cracks or defects [2,3]. On the other hand, mesh-less numerical analyzes, like a particle method, is expected to solve such problems easily.

In the preceding study, we applied the smoothed particle hydrodynamics (SPH) method [4] to the linear fracture mechanics and the fatigue crack propagation and proposed the method to solve the propagation of the planar crack in the 3D body with such complex situations [5].

In the present study, the method to solve the propagation of the non-planar cracks in the 3D body is proposed. In addition, to confirm the validity of the method, a fatigue test of the non-planar crack is carried out and the result is compared with the computed result.
2 ANALYSIS METHOD

2.1 Basic algorithm for fatigue crack propagation

In the present method, the basic algorithm for the crack propagation is the same as the method for the planar cracks [5]. The method consists of two sections, such as the SPH stress analysis section and the fatigue crack propagation analysis section. At first, the stress distribution of the 3D body is computed in the SPH section, and the result is sent to the crack propagation analysis. The support domain size in the SPH is twice the particle size.

In the crack propagation analysis, the values of the stress intensity factor of the crack front particle $i$, $K_i$, is calculated simply as follows:

$$K_i = \sigma_{1,i} (\pi \Phi)^{1/2}$$

(1)

where $\sigma_{1,i}$ is the maximum principal stress and $\Phi$ is the size of the particle. In the $n$th analysis step, the fatigue cycle increment $\Delta N_n$ is given and the increment of the crack length in the particle $L_{i,n}$ is calculated as follows:

$$\Delta L_{i,n} = \frac{da}{dN_i} \Delta N_n$$

(2)

where $\frac{da}{dN_i}$ is the fatigue crack growth rate of the particle. It is obtained by equation (1), given stress ratio $R$ and Paris Erdgan Law [6]. The crack length of the particle in this step $L_{i,n}$ is calculated as follows:

$$L_{i,n} = L_{i,n-1} + \Delta N_n$$

(3)

where $L_{i,n-1}$ is the crack length of the particle in $(n-1)^{th}$ analysis step. When $L_{i,n}$ becomes the same value as $\Phi$, the particle becomes the fractured particle. The decreasing of the stiffness due to the crack propagation is released by removing the fractured particle.

2.2 Non-planar crack modeled by particles

Fig. 1 shows the example of the non-planar crack in the 3D body. The non-planar crack in Fig. 1 (a) is modeled by the particles as shown in Fig. 1(b). In the figure, the particles $i$ and $j$ are already removed due to the crack propagation and the particles $k$ and $l$ are placed on the upper side and the lower side of the cracked surface, respectively. Before the particles $i$ and $j$ are fractured, the particles $k$ and $l$ were the neighboring particle each other. However, when both of the particles $i$ and $j$ are fractured, the crack appears between the particles $k$ and $l$, then, the particles should not be the neighboring particle in the figure.

To realize the above state, the particles on the same position as the particle $l$ in the figure are searched in the nine cross sections, A to I in Fig. 2, of all the groups of the neighboring particles. As shown in Fig. 3, the neighboring particles of the particle $k$ are numbered by the relative positions between the particle $k$. In case of the cross section A in Fig. 2, the particles shown in Fig. 4 are searched. In case of the figure, the particles No. 14 and 16 are the removed particles and the particle No. 17 is the same state as the particle $l$ in Fig. 1(b). Then, in the figure, the particle No. 17 is excluded from the group of neighboring particles of the particle $k$. 

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Figure 1: Non-planar crack in 3D body

Figure 2: Searching planes in group of neighboring particles

Figure 3: Numbers for neighboring particles

Figure 4: Plane A in Fig. 2
2.3 Crack propagation algorithm for non-planar crack

To calculate the propagation of the non-planar crack, the slope and the position of the crack surfaces in the crack front particles should be concerned. Then, in the present method, the crack front particles have information of the slope and the position of the crack surface as shown in Fig. 5 in addition to the crack length. The axis of $\zeta$ in the figure is decided as the same direction of $x$, $y$ or $z$ which is most close to the direction of $\sigma_1$ in the initial crack front. Thus, $\zeta$-$\eta$-$\zeta$ is $x$-$y$-$z$, $y$-$z$-$x$ or $z$-$x$-$y$. As shown in the left side of the figure, the information of the slope is given as $\theta_\zeta$ and $\theta_\eta$. They are the angles between the orthogonal plane of $\sigma_1$ and the axis of $\zeta$ and $\eta$, respectively. As shown in the right side of the figure, the position is given as the distance from bottom $\zeta$-$\eta$ plane. The new crack front particle receives $h_1$, $h_2$, $h_3$ or $h_4$ of the fractured particle as its $h_3$, $h_4$, $h_1$ or $h_2$ and the other values are calculated by $\theta_\zeta$ and $\theta_\eta$.

When the crack front particle is fractured, the new crack front particles are searched in the sub groups of the neighboring particles I to IV in Fig. 6. For example, in case of Fig. 7, the sub group II consists of the neighboring particles No. 6, 14 and 23 (see Fig. 3). If the group does not consist of any other crack front particle nor removed particle when the particle $i$ is fractured, one of these will be defined as a new crack front particle. If $h_2$ of the particle $i$ is larger than 0 and smaller than $\Phi$, the particle No. 14 will be defined as the new crack front particle and it receives $h_2$ of the particle $i$ as its $h_4$. If $h_2$ of the particle $i$ is smaller than 0,
the particle No. 6 will be defined as the new crack front particle and it receives the sum of $h_2$ of the particle $i$ and $\Phi$ as its $h_4$. If $h_2$ of the particle $i$ is larger than $\Phi$, the particle No. 23 will be defined as the new crack front particle and it receives the difference of $h_2$ of the particle $i$ and $\Phi$ as its $h_4$. Using the above method, the non-planar crack propagation is analyzed.

3 FATIGE TEST

To confirm the validity of the method, a fatigue crack propagation test was carried out. Fig. 8 shows the geometry of the fatigue specimen. The specimen is the half inch CT specimen [7] with an additional horizontal hole. The hole is 10mm in diameter and places 8mm below from the center line and 25 mm from the back surface of the specimen. The specimen is made of ductile cast iron. The tensile cyclic load was applied to the specimen by an electro-hydraulic servo fatigue testing machine.

![Figure 8: CT Specimen with an additional horizontal hole](image)

4 COMPUTATIONAL AND TESTED RESULTS

Fig. 9 shows the tested and the computed results of the crack propagation of the CT specimen with an additional horizontal hole. The computed specimen consists of 70,000 particles and they are placed at regular intervals, meaning that the diameter of a particle is 0.5 mm.

As shown in Fig. 9 (a), the tested result showed that the initial crack propagated to horizontal direction and the crack changed its direction to the additional hole step by step. Finally, the crack passed though the edge of the hole. As shown in Fig. 9 (b), the computed result shows the smoothed crack propagation and the result shows almost the same crack shape as the tested result.
5 CONCLUSIONS

- The method for the 3D planar crack propagation by SPH is extended to solve the 3D non-planar crack propagation.
- The non-planar crack propagation of CT specimen with an additional horizontal hole is computed in a smooth manner.
- The computed result shows almost the same crack shape as the tested result.

REFERENCES

A COMPUTATIONAL FRAMEWORK FOR THERMAL COUPLING IN HYBRID FIRE SIMULATION

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Key words: Hybrid Fire Simulation, Thermal Coupling, Sequentially-Coupled, Fully-Coupled, Transient Analysis.

Abstract. In structural fire engineering, it is crucial to estimate the global structural behavior in a realistic scheme. This necessity arises from the reason that the single element testing doesn’t represent the global behavior of the structure correctly due to the possible load redistribution into alternative load paths and change of static systems in case of global fire. Therefore, hybrid simulation method can be accounted as a key method, which fulfills the possibility of study of the global structural behavior in structure with coupling the numerical simulation and experimental testing. In this method, the numerical simulation procedure of the whole structure is coupled and controlled with the outcomes of the experiment performed on a single part of the structure, which is critical or difficult to study numerically.

So far, several attempts have been made to study hybrid fire simulation. There, however, exist severe shortcomings in so-far research: - the correct consideration of the stiffness and material properties for the heated element and their degradation during fire exposure, - retaining the compatibility and the equilibrium between the substructures, - the automatic real-time interaction between the substructures and also - realistic consideration of the thermal coupling between substructures with regard to the transfer of the heat from fire exposed component to adjacent elements.

In hybrid fire simulation, the thermo-mechanical coupling can be studied realistically, when the heat exposed to the single compartment, its transfer to the adjacent substructures and the effect of two latter on the mechanical response of the structure is considered. In the current paper, this purpose is studied on a steel structure benchmark with two different approaches: sequentially-coupled thermal-stress analysis and fully-coupled thermal-stress analysis. Here, the mathematical and mechanical aspects of each approach and their difference regarding the response of the structure will be investigated. Also, their application in the hybrid fire simulation and the importance of the real-time issue in these approaches are outlined. In this paper, the numerical model of the intended benchmark which interacts automatically with another numerical model, representing the experimental substructure.
exposed to fire is studied. Therefore, the implementation of hybrid fire simulation and different aspects of the thermal coupling including the existence of heat transfer and mechanical and thermal properties will be discussed.

1 INTRODUCTION

Fire is one of the most important hazards in structural engineering, since it is vital to study the resistance of the whole structure in a certain time period of fire exposure. Single element testing cannot represent completely the correct global structural behavior and it is because of possible load redistribution and changes in static system of the structure. Therefore, the performance of structures in fire has to be investigated in the full scale. In one hand, the full-scale fire tests are costly and on the other hand, pure numerical simulations on the large scale structures would be afflicted with uncertainty due to existing complexities in some sub-parts of the structure. Hybrid fire simulation counts as a new method, which overcomes the existing limitations and provides the capability to study the performance of structures globally.

Hybrid fire simulation provides the tool to study the global behavior of structures under fire loadings. It couples the numerical simulation representing the whole structure and an experimental test, performed on the parts which will be exposed to fire in a fire test experiment. In this method, the mechanical equilibrium of the global structure will be solved and controlled incrementally by receiving the measured data from the substructure exposed to fire and simultaneously the numerical simulation updates the commands for proceeding the test procedure in a real time. Therefore, the strength degradation and change of material properties in the physical substructure is considered in the mechanical response of the whole structure.

The first idea of combining numerical simulation and physical testing was proposed by Takanashi et al. [1] in 1970s who did the coupling for estimation of seismic behavior of structures referring as “online testing”. This technique then was followed by many researchers in earthquake engineering, represented as “Hybrid testing” [2-5]. However, due to the existence of thermal effects, procedures in fire engineering are different from seismic engineering and there should be some other adjustments that meet the requirements of structural fire design.

Korzen et al. [6] firstly explained the idea of separating the whole structure to sub-parts in structural fire engineering with suggesting a substructuring method. They applied some fire tests with updating thermo-mechanical boundary conditions of the element exposed to fire in interaction with adjacent substructure. This method still didn’t consider the automatic real-time communication between the numerical part and the experimental part of the hybrid simulation. Also, the equilibrium of displacement and forces was only based on the numerical part without taking into account the stiffness of the experimental part.

Mostafaei [7, 8] then aimed at developing a hybrid modeling approach to be used for the analysis of the global structural behavior of a six-storey reinforced concrete building with a compartment fire scenario located on the ground floor. The experimental part of his hybrid model consists of a reinforced concrete column that was tested at full scale inside a furnace and the mechanical and thermal load application was performed in two consecutive steps. Mostafaei’s approach lacked also an automated controlling interface between the two substructures, which is error-prone and excludes reproducibility in any other fire test facility.
Also, the solution evolution neglected an iterative loop to achieve displacement compatibility with the thermal expansion and accumulated an error.

Sauca et al. [9, 10] discussed the drawbacks of previous approach with implementing a new method, which assures displacement compatibility and fulfilling of stability with independency from the stiffness ratio between the substructures. [9]. Major shortcomings of their study is lack of consideration of continuous degradation of the stiffness with continuous increase of temperature due to fire in calculation of stiffness ratio of the substructures. They assumed the stiffness of the physical substructure as an initial elastic tangent stiffness and to remain constant, which is far from the reality of the structural behavior in fire. The stiffness calculation in numerical simulation was also considered as a predetermined elastic matrix.

The alternative phrase “Consolidated Testing” was proposed by Fontana et al. [11] for thermo-mechanical modeling of global structural behavior. In this method, the idea was to test a single element as a part of a whole structure and to apply the results of the global numerical simulation to control the test in real-time. Schulthess et al. [12, 13, 14] developed for the first time the basic requirements for the hybrid fire simulation method in the real time for a benchmark in laboratory scale, which considered an automatic communication for study of mechanical coupling between the fire-exposed substructure and the adjacent sub-parts, but it still lacks a precise study of the thermal coupling in interaction of the two substructures. A precise view to thermal coupling in hybrid fire simulation is required. Therefore, the focus of this paper is on the study of thermal coupling and the effect of heat transfer from the fire-exposed substructure to the adjacent substructures as well as their influence on the mechanical and thermal equilibrium of the global structure at elevated temperatures.

2 THERMAL COUPLING MECHANISM IN HYBRID FIRE SIMULATION

In hybrid fire simulation the global structure is divided into two substructures, which one part is easier to be studied numerically and one other part is complicated or not straightforward for numerical simulation and therefore it is implemented in experimental testing facilities. In the interface between two substructures, the numerical simulation part gives the displacement and temperature to the physical substructure in order to control experimental procedure and on the other hand with obtaining the measured data from the compartment exposed to fire, the procedure and equilibrium equation of the numerical simulation can be controlled in every increment of FE simulation. It is of importance to consider both mechanical coupling and thermal coupling rigorously according to the global structural behavior in fire. For considering the thermal coupling in a realistic way, not only the single element tested in experiment is going to be exposed to direct temperature due to fire test facility, but also the temperature distribution and heat transfer from the physical component to the adjacent substructures have to be considered. Therefore, in the physical substructure the temperature can be increased with a constant rate and then the induced heat and the temperature distribution in the adjacent components may be studied also in each simulation-time increment. So, the heat flux vector at the point of the interface has to be determined and controlled in each increment of simulation to control also temperature compatibility at the interface besides displacement compatibility to be able to control the equilibrium of forces in the global structure. With considering the produced heat flux and temperature distribution in the adjacent substructures, not only the fire-exposed component
changes in material property and stiffness, but also the stiffness would reduce in the adjacent components and due to temperature- and time-dependent material properties, expansion, thermal creep and strength degradation occur also in the non-exposed-to-fire components. This phenomenon would affect the stress analysis of the global structure and therefore it has to be controlled in every time increment with the displacement compatibility at the interface to fulfill the stiffness relationship for the whole structure.

In hybrid fire simulation in every increment of the simulation time the transfer of the heat from the physical substructure to the numerical substructure is influencing the stress analysis of the whole structure with affecting the time- and temperature-dependent material properties and stiffness degradation due to temperature. The temperature increase in the component exposed to fire test, can be defined according to a specific protocol, which deduce the temperature distribution in the physical substructure as well as in the interface of sub-parts independently from the mechanical response. Therefore, heat transfer analysis can be considered with two different approaches at the interface of two substructures. These approaches are presented in the following sub-sections.

2.1 Sequentially coupled thermal-stress analysis

In this simplified approach, the distribution of the temperature and heat at the interface of two substructures can be studied primarily for a pure transient heat transfer analysis on the global structure. The heat equation as finite element discretization is as follows:

\[
[C][T] + [K_c] \{T\} = \{R_T\}
\]  

(1)

Where \([C]\) is the heat capacity matrix, \([K_c]\) is the conductivity matrix, \(T\) represents the temperature field and \(\{R_T\}\) is the residual thermal vector.

Physical substructure is exposed to a temperature increase with a constant temperature rate for each time increment of the simulation. The constant temperature increase rate for the physical substructure may provide though a nonlinear temperature distribution in the adjacent substructure which can be specified in each time increment of the global numerical simulation. The temperature-time increment history for the numerical substructure can be as an input for the stress analysis of the global structure in hybrid fire simulation to study the mechanical coupling of two substructures consecutively after their thermal coupling. Considering temperature distribution in both substructures will necessarily affect the stiffness relationship and displacement equilibrium of the structure. The important point in a sequentially analysis, is the finite element compatibility in FE simulation of both pure heat transfer analysis and following static analysis.

This simplified approach would avoid the simultaneous study of heat equation and stress analysis, with performing the thermal coupling and mechanical coupling sequentially at the interface of the two substructures. Therefore, this method can be accounted as an intermediate or preliminary step for the next approach, which will be explained.

The advantage of this simplified method is saving calculation time in the transient heat analysis of the numerical simulation of hybrid fire simulation, since the temperature history would be primarily defined in the adjacent substructures and then hybrid fire simulation studies consecutively the global structural behavior according to the predefined thermal
coupling from previous analysis. Though in pure heat transfer analysis of the sequentially approach, the target temperature is applied on the physical element itself and not to the gas around it in fire test facility. Therefore, in hybrid fire simulation in sequential stage, the deviations in the temperature increase rate in the furnace of fire test facility for physical element in each increment and the difference of target temperature in the gas in the furnace with the existing temperature of the specimen, may cause an incompatibility for the temperature distribution history in the adjacent substructure regarded to the existing temperature in specimen.

This approach can be applied primarily in a pure numerical hybrid simulation which avoids the existent errors in experiment environment in order to study the effect of thermal coupling in equilibrium of the structure. A schematic overview of the algorithm of the hybrid fire simulation using sequentially coupled analysis is shown in Figure 1.

**Figure 1**: Sequentially coupled algorithm of thermal coupling in hybrid fire simulation
2.2 Fully-coupled thermal stress analysis

In this approach the thermal analysis and stress analysis are studied simultaneously at each time increment, so the temperature distribution at the physical substructure, the numerical substructure and their interface will be studied with the stress analysis simultaneously, which is affected by the change of temperature and time dependent material properties, degradation of stiffness both in physical component and numerical component and also the thermal expansion. The equation of the fully coupled analysis will be as below:

\[
\begin{bmatrix}
K_{uu} & K_{u\theta} \\
K_{\theta u} & K_{\theta\theta}
\end{bmatrix}
\begin{bmatrix}
\Delta u \\
\Delta \theta
\end{bmatrix}
= 
\begin{bmatrix}
R_u \\
R_{\theta}
\end{bmatrix}
\]

in which \(K_{uu}\) and \(K_{\theta\theta}\) are the submatrices regarding displacement and temperature in the coupled Jacobian matrix. \(K_{u\theta}\) represents the coupling effect of temperature on the equation of displacements as thermal expansion and \(K_{\theta u}\) is submatrix regarding the influence of displacement on thermal response which may be assumed zero. \(R_u\) and \(R_{\theta}\) are mechanical and thermal residual vectors and \(\Delta u\) and \(\Delta \theta\) are displacement and temperature change in each increment time. The algorithm of the fully-coupled thermal stress analysis applied in hybrid fire simulation is shown in Figure 2.

![Figure 2: Fully-coupled algorithm of thermal coupling in hybrid fire simulation](image-url)
In the second approach, in comparison to the simplified approach, the temperature distribution in the whole structure will be applied in the adjacent substructures in the same time of performing the hybrid simulation which is a more rigorous view to thermo-mechanical coupling, so displacement compatibility and the temperature distribution compatibility would be studied in the same time in a fully coupled manner. This would although bring of course more calculation time in the numerical simulation to control the transient fully coupled thermal stress analysis by checking the temperature distribution, the convergence of iterations and fulfilling the equilibrium of forces in each increment. This parameter can affect the real-time issue of the hybrid fire simulation which is a necessity in fire analysis. Calculation time of the numerical simulation in this procedure has to be checked and synchronized with the time which will be needed in experimental set up for reaching to temperature and displacement target in the machine. Therefore, as an intermediate step to hybrid fire simulation the first approach can be utilized to save the calculation time and to simplify the numerical simulation procedure which has to be performed in hybrid analysis.

3. NUMERICAL FRAMEWORK OF HYBRID FIRE SIMULATION

Since the heat transfer study in hybrid fire simulation is a novel topic, different parameters in the numerical simulation and their importance have to be investigated primarily. Therefore, in this paper, both substructures are modeled purely numerical, which they are explained further.

3.1 Thermo-mechanical benchmark problem

To study the method of hybrid fire simulation, it is of great importance to choose an appropriate benchmark problem which can be implemented in laboratory scale and will be provable with pure physical testing.

The benchmark used in this study is referred to the benchmark problem in [12], since a precise study of pure mechanical coupling in the implementation of hybrid fire simulation between numerical simulation and experimental testing were successfully concluded for this benchmark. It consists of a static system for a simply supported beam connected at its mid span through a hinge to a rod (Figure 3a). The rod is the structural element which is supposed to be in a fire test furnace and the temperature increases through it with a predefined specific temperature-time protocol. The beam acts as the adjacent component, which is exposed to the heat transferred from the rod and a nonlinear temperature increase occurs in beam. The whole benchmark is applied to a constant external load \( P(t) \) in the mid-span of the beam. Therefore, the internal forces in the rod and supports of the beam are stiffness proportionate. As a first step from time \( t_0 \) to \( t_1 \), the load reaches to \( P(t) \) and it remains constant for the rest of the procedure (Figure 3b). On the other hand, in the first step temperature is constant at ambient and then a constantly increasing predefined temperature protocol will be applied to the gas in the furnace around the rod. By increasing the temperature at the rod, the internal force in the rod decreases and due to its elongation, there will be a deflection in the mid-span of the beam, which it causes an increase in the reaction forces of the supports of the beam and therefore the equilibrium of the forces with external load will be fulfilled. But later on, with increasing the temperature in the beam, both the stiffness of the beam and rod degrades and the equilibrium of forces have to still be fulfilled and checked. The figure below represents the benchmark
problem and loading and temperature protocols.

![Diagram of benchmark system, mechanical load application, and temperature increase history](image)

**Figure 3:** a) Benchmark system; b) Mechanical load application on system; c) Temperature increase history of the rod

### 3.2 Physical and numerical substructures of the benchmark problem

Both substructures of hybrid fire simulation are modeled numerically in ABAQUS. The first numerical model which is representable for numerical substructure is the global structure of the benchmark. The beam element is modeled with a 3D solid element to be able to assign temperature degrees of freedom in ABAQUS (DC3D8). The dimensions of the global structure are considered according the realistic dimensions for the physical substructure, which will be an experimental specimen e.g. implemented in a furnace in the laboratory scale. The fire-exposed substructure in the global model is a user-defined element (UEL) which its properties are specified. It acquires its properties through an automated interaction with the physical element in the fire compartment. In this study, the physical component is demonstrated also as a numerical model which simulates a dog bone shaped solid model representing the shape of the specimen in the laboratory scale that can be used in the testing equipment for the next step of coupling a numerical simulation with an experimental testing. In this context, the physical substructure model corresponds to a dog bone shaped specimen in laboratory dimensions of 5·10 mm from steel grade S235. These two FEM models have to interact in an automated way with each other with the help of a middle-ware server, which creates communications with two FEM model as a threading network. The physical substructure model is analyzed by a transient fully-coupled thermal-stress analysis and it...
gives the temperature, thermal expansion and actual force of the specimen in each increment as an output. These measured data have to be transferred to the global model. So in global model the displacement compatibility is checked, and the heat flux vector at the interface point of two substructures is determined according to the temperature of physical substructure and the reference temperature at the adjacent substructure and then the equation of displacement and the equation of heat are solved either with fully coupled analysis or either with static analysis having a predefined temperature history in adjacent substructure as the second step of sequentially coupled analysis, so the iteration convergence in both approaches have to be checked for the equilibrium in each increment.

Requirement of an automated communication interface between two substructures demands the physical component model to be equipped also with four user-defined subroutines to be capable of achieving the temperature, displacement and sending the measured elongation and restoring force respectively. Figure 4 demonstrates the computational implementation of the numerical model representing testing element with the automated server.

![Figure 4: Implementation of user subroutine in physical substructure for automated communication in hybrid fire simulation](image-url)
3.3 Computational procedure of the solution

To perform a purely numerical hybrid fire simulation with an automated middle-ware server, it is crucial to make the receiving and sending of the measured values at the interface between both substructures compatible and synchronized. Therefore, it is important to apply sending and receiving socket functions in user subroutines of FEM models and server with the property of blocking mode to be able to synchronize the two-way automated communication. When the global model achieves the thermal expansion due to increase of temperature from another numerical model, the solver has to suggest a new target displacement since displacement compatibility will get out of balance at the interface point. The displacement is applied on physical element model as the displacement command in testing machine may be performed and then displacement in the gauge length of specimen model and respecting force have to be sent back to update the stiffness matrix of the fire-exposed user-defined element and check the convergence for the equilibrium of forces. This procedure is iterated until the convergence is fulfilled and a new increment of global model is started. Therefore, the controlling parameter for the automated communication of hybrid fire simulation for two purely numerical models, has to be each iteration of the global model. In other words, each iteration of simulation time of global model can include one or more increment of the simulation time of the physical substructure model.

4 CONCLUSIONS

In this paper a framework for thermo-mechanical coupling of the hybrid fire simulation has been presented which studies the heat transfer and its effect on the behavior of global structure in fire. In particular, the effect of heat flux and temperature distribution in the hybrid fire simulation from fire-exposed experimental component to adjacent substructures for a specified benchmark problem are considered. This consideration provides a more rigorous study of the thermal coupling in hybrid fire simulation.

Two different approaches for thermal coupling are presented as sequentially coupled and fully-coupled analysis and the outcomes applying each method in hybrid fire simulation are discussed.

It is important to investigate the application of this advanced aspect regarding thermal coupling of hybrid fire simulation, in later stages in a coupled numerical simulation-experimental fire test. This accompanies further challenges in adjusting the numerical simulation time increments with physical time scale, especially in the evolution of temperature during the transient analysis and in convergence of the mechanical equilibrium with plastic material properties.

REFERENCES


A MOLECULAR DYNAMICS STUDY OF THE INTERFACE TEMPERATURE IN ULTRASONIC METAL WELDING

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Key words: Molecular Dynamics Simulations, Ultrasonic Metal Welding, Temperature Evolution, Coupled Problems

Abstract. In this study, mechanical and thermal behavior of the mating interface during ultrasonic metal welding is investigated using molecular dynamics (MD) simulations. In ultrasonic welding process, the reciprocating motion of the sonotrode together with the application of the external pressure on the mating parts are the sources of friction heat generation, high temperature gradient at the interface and plastic deformations.

The rapid process of ultrasonic welding, which takes a few seconds at the longest, involves coupled mechanical and thermal processes. Therefore, MD simulations have been employed to elucidate the nano-mechanics of this complex coupled process within the picosecond timescale. To this end, the atomic scale simulations of the microstructure at and in the vicinity of the mating interface have been carried out.

This contribution addresses the interactive effects of the process parameters on the interface temperature evolution and the diffusion behavior of the interface atoms at the atomic scale. The results of this work are compared to the results from macro scale investigations.

1 INTRODUCTION

Ultrasonic metal welding (USMW) is a solid state consolidation process, during which the growing interface temperature is far below the melting point of the participating metals. During this process, the formation of a bond occurs through a combined effect of the applying pressure normal to the mating parts and the high frequency frictional vibrations of a sonotrode on top of the mating parts. Formation of the bond during the USMW involves moderate to strong plastic deformations as well as friction heat generation and softening of the material at the vicinity of the bond interface. Different aspects of the USMW process have been studied over decades. Microscopic inspections of the bond as
well as real time monitoring of the bond formation and the interface temperature gradient have been carried out to better understand the role of the process parameters in this complex process. Krzanowski [1] observed dynamic recovery or recrystallization in aluminum wires during ultrasonic bonding. Hazlett and Ambekar [2] stated that four bonding mechanisms may occur during ultrasonic welding depending on the mating parts, such as melting of the interface, mechanical interlocking, interfacial atomic forces and interfacial diffusion. Elangovan et al. [3] stated that an increasing clamping force decreases the generated interface temperature and leads to formation of the work piece rather than welding. Ding and Kim [4] showed that a higher bond force results in an insignificant higher temperature rise and does not necessarily result in a better wire bondability. Mostafavi et al. [5] investigated the microstructure of different weld samples under the influence of different pressures and vibration amplitudes of the welding sonotrode. They realized that for a high welding pressure, the boundaries at the contact regions of the aluminum strands are recognizable even after the process ends. They also stated that increasing the vibration amplitude in USMW of multi-strand single core aluminum cables is more efficient in interface temperature rise than increasing the applied pressure. Bai and Yang [6] gave an approximately linear relation between the deformation of surface asperities and ultrasonic vibration amplitude.

However, in-situ investigations of the interface temperature and observation of the bond formation require a big amount of time and precise measuring techniques. Therefore, in recent years MD simulations have been employed to simulate the nano-mechanics of many mechanical processes. Patil et al. [7] proposed a non-linear wear law in disc-pad braking system. Chen et al. [8] studied the microstructure evolution, heat dissipation and generation of mixing layers in the region near the contact interface during nanoscale friction. Chen et al. [9] studied the atomic structure and computed the interfacial energy in Ni-Cr alloys by means of MD simulations. Jiao et al. [10] established an atomic model for the study of linear friction welding between Ni and Al, where they studied the flattening of the surface roughness and the pore closure during the process. Song et al. [11] studied plastic deformation and atomic diffusion behavior in the process of linear friction welding between dissimilar Ti-based alloys.

Various theoretical and numerical models have been proposed in order to study the mechanism of the bond formation and the change in interface temperature, most of which are based on fundamentals of continuum mechanics.

This study employs MD simulations to investigate the nano-mechanics of the interface. The coupled effect of two parameters, namely constant sliding velocity and compression rate on the interface temperature and diffusion behavior of the interface atoms are discussed.

2 SIMULATION METHOD

MD simulations are carried out to discuss the effect of compression rate and sliding velocity on the nanostructure of the interface. In the MD simulations method, atomic
trajectories are obtained through integrating the classical Newtonian equations of motion for a system of N atoms as particles. A force field or potential is used to compute the forces between the atoms in those equations. The velocity and the positions of the atoms are updated based on their interaction potentials.

2.1 Computational model and boundary conditions

MD simulations are performed inside LAMMPS (Sandia National Laboratories)[12]. The velocity-verlet algorithm is used for the numerical integration of the Newtonian equations of motion. For the purpose of visualization of the atomistic simulation data, the open visualization tool Ovito [13] is used. The simulation box consists of two blocks of a monoatomic aluminum FCC structure. The box is filled with a total number of 322,873 atoms. Fig. 1 (left) shows the geometry of the structure. Each block has the dimensions of $60.75 \times 40.5 \times 16.2\text{ Å}^3$. Three types of atom description are set for the computational model, namely rigid atoms, thermostat atoms and Newtonian atoms. The region of rigid moving atoms moves as a single entity. The thermostat atoms were used to ensure heat dissipation during sliding.

![Figure 1: Geometry of the model (left), temperature evolution of the interface (right)](image)

Pressure of the sonotrode and the amplitude of the vibrations are translated into compression rate and sliding velocity in this study. In a reference model the rigid atoms of the upper block are moved at a constant compression rate $v_y = 0.7 \text{ Å/ps}$ and a constant sliding velocity $v_x = 0.9 \text{ Å/ps}$. The computation is set for 88000 steps with a time step of 0.001 ps. Finally, cool down of the model is set for another 50000 steps.
2.2 Applied methodology

In the present work, the embedded atom method (EAM) interatomic potential developed by Mishin et al. [14] is used (see Eqn. 1). This interatomic potential gives a better description of metallic atoms interactions than a two-body potential and accounts for the effect of electron density surrounding each atom and accurately modeling the surface energy [8].

\[
U_{EAM} = \sum_i^N \left[ F_i(\rho_i) + \frac{1}{2} \sum_{j \neq i}^N \phi_{ij}(r_{ij}) \right], \quad \rho_i = \sum_{j \neq i}^N \rho_j(r_{ij}), \tag{1}
\]

where i, j describe the types of the atoms, \( r_{ij} \) is the scalar distance between atoms i and j and \( \phi_{ij} \) is the pairwise interaction potential. \( \rho_i \) is the electron density of atom i due to all its neighbors and \( F_i(\rho_i) \) illustrates the energy arising from embedding atom i in an electron gas of density \( \rho_i \).

In a MD computational model, kinetic energy and potential energy of each atom can be calculated at any particular time step. In order to compute the temperature as a global quantity, temperature must be averaged over a certain number of atoms. To this end, kinetic energy of a system with \( N \) atoms as in Eqn. 2 is set equal to the kinetic energy from Eqn. 3, which results in the thermodynamic temperature of the system as in Eqn. 4.

\[
U_{KE} = \frac{1}{2} \sum_i^N m_i v_i^2, \tag{2}
\]

\[
U_{KE} = \frac{3}{2} N k_B T, \tag{3}
\]

\[
T = \frac{1}{3} \frac{m}{N k_B} \sum_i^N v_i^2, \tag{4}
\]

where \( k_B \) is the Boltzmann constant.

3 RESULTS AND DISCUSSION

The effect of a percentage-wise increase in compression rate and sliding velocity is studied. In each simulation only one of these two parameters is varied.

3.1 Temperature evolution of the interface atoms

Figure 2 shows the snapshots of the interface temperature once the upper block reaches the lower block. An initial sudden increase of the interface temperature occurs due to the high atomic repulsion energy. This can be seen on the graph in Fig. 1 as well. A global maximum of the interface temperature is achieved at the end of the process. After
removing $v_x$ and $v_y$, cool down of the interface takes place and the interface temperature monotonically decreases (see Fig. 1).

As shown in Fig. 3, increasing $v_x$ increases the interface temperature, whereas a clear pattern for the interface temperature change with increasing $v_y$ cannot be recognized.

### 3.2 Diffusion behavior analysis

Fig. 4 shows the mean square displacement (MSD) of the middle atoms at the interface. To this end, the total squared displacement from the original position of each atom, $(dx^2 + dy^2 + dz^2)$, summed and averaged over all the interface atoms is given in Eqn. 5. The slope of the MSD vs. time is proportional to the diffusion coefficient of the atoms at the interface. As Hazlett and Ambekar [2] claimed, there may be grain boundary diffusion across the bond interface rather than bulk diffusion during the bond formation process. Increasing the sliding velocity helps the atom transfer and diffusion. On the
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contrary, increasing the compression rate prevents the atom transfer and does not change the diffusion process significantly.

\[ r^2(t) = \frac{1}{N} \left[ \sum_i^N |r_i(t) - r_i(0)|^2 \right]. \]  

Figure 4: Change in MSD of the interface atoms with \( v_x \) (top) and \( v_y \) (bottom)
3.3 Correlation between MD, experiments and FE simulations results

In our previous work, results from experiments and FE simulations regarding the interface temperature have been reported in detail [5]. Fig. 5 shows the mean values of the interface temperature for different couples of process parameters in USMW of multi-strand single core aluminum cables from experiments and FE simulations. As shown, increasing the vibration amplitude increases the interface temperature continuously, due to the effective friction heat generation. Increasing the applied pressure increases the interface temperature due to plastic deformations, until a threshold value is reached. A high temperature at the bonding interface is not the only crucial factor in formation of a good bond in USMW, but also the frictional sliding motion of the parts against each other is important as it disperses impurities, oil and metallic oxides at the interface effectively and leaves clean parts for bonding. The results from the simplified atomic scale simulations in the current study are in good agreement with these results from experiments and FE simulations.

![Figure 5: Interface temperature for different couples of process parameters [5]](image)

4 CONCLUSIONS

A study of the mating interface in USMW is done through MD simulations. The main conclusions and achievements of this study are summarized as follows:

- Interface temperature increases as sliding velocity increases. With an increase in the compression rate, interface temperature stays nearly constant.

- Atomic diffusion at the interface increases as sliding velocity increases.

- MD simulations confirm the effect of process parameters on the interface temperature, which has been established by experiments and FE simulations.

- MD simulations are capable of describing the mechanical and thermal characteristics of the interface at nanoscale.
Material and process related parameters obtained from atomistic simulations can be integrated in multi-scale approaches as in [15], where a link between molecular and continuum models of brittle fracture was proposed.

REFERENCES


A PSEUDOTHERMAL APPROACH FOR SIMULATING THE RESIDUAL STRESS FIELD CAUSED BY SHOT BLASTING

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Key words: Shot blasting, residual stresses, weld simulation, pseudothermal loading

Abstract. Industrial practice often prescribes cleaning of steel surfaces prior to welding with shot blasting. Shot blasted components have been considered free of residual stresses. Hence, recent studies show that these residual stresses from mechanical surface treatments are not negligible. A simulation of the surface treatments and their mechanical effect in full scale though, is not possible under modern computational capabilities. Instead, a straightforward, pseudothermal approach is proposed and tested in the present study, in order to introduce an initial residual stress field from shot blasting by application of thermal strains. This engineering concept is applied for validation reasons on a small-scale specimen, where a measured profile of residual stresses from shot blasting is simulated with preciseness. Subsequently a component with dimensions of real weldments is modelled, so that simplifications reducing the computational time to acceptable levels can be derived.

LIST OF NOTATIONS

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>E</td>
<td>Young’s modulus (MPa)</td>
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<tr>
<td>f</td>
<td>yielding function</td>
</tr>
<tr>
<td>f_s(u)</td>
<td>resisting force as a function of displacement u (N)</td>
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<tr>
<td>H</td>
<td>tangent modulus of bilinear σ-ε material behaviour [MPa]</td>
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<tr>
<td>p(t)</td>
<td>external transient loading (N)</td>
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<tr>
<td>T</td>
<td>temperature (°C)</td>
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<tr>
<td>t</td>
<td>time (s)</td>
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<tr>
<td>u</td>
<td>displacement (mm)</td>
</tr>
<tr>
<td>ε</td>
<td>strain (-)</td>
</tr>
<tr>
<td>α_se</td>
<td>secant coefficient of thermal expansion</td>
</tr>
<tr>
<td>δ_ij</td>
<td>Kronecker’s delta</td>
</tr>
<tr>
<td>ν</td>
<td>Poisson’s ratio (-)</td>
</tr>
<tr>
<td>σ</td>
<td>stress (MPa)</td>
</tr>
<tr>
<td>σ_eq</td>
<td>von Mises effective stress (N/mm²)</td>
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</tbody>
</table>
1 INTRODUCTION

Steel plates are usually considered free of residual stresses (RS) prior to welding, although it is well understood that there are RS from the rolling process, especially in the case of cold rolled plates. Nevertheless, significant deviation of simulated welding residual stresses (WRS) with the respective measured profiles was met in an ongoing research project [1]. The investigated component was a fillet weld made of S355 with real yield strength of 400 MPa. It was simulated with a previously validated engineering approach for calculating the WRS of weldments [2], [3], [4] etc. The simulation provided very good agreement with the measurements in the fusion zone (FZ), the heat affected zone (HAZ) and the parent material (PM) near them. However, compressive stresses in an order of magnitude of -200 MPa were met in the PM away from the HAZ, an effect that could not be reflected by the numerical model. The above-mentioned very good agreement of numerical and experimental results near the critical weld section led to the conclusion that the simulation was valid and a different effect than welding should account for these compressive RS.

Previous investigations by Shaw et al. [6] and Hensel et al. [7] have proven that most of the widely applied surface treatments, such as shot blasting or glass peening, lead to the introduction of non-negligible compressive RS on the surface, of a different magnitude in each case though. The through-depth RS profiles, which were measured in [6] for different surface treatments of a mechanical component of a 20MnCr5 steel [8], are presented in Figure 1. This material is reported to exhibit a yield strength of 398 MPa at room temperature, ultimate tensile strength of 562 MPa and Young’s modulus of 219 GPa [9]. It becomes evident from these measurements, that even for surface treatments like shot blasting, where no obvious, significant deformation of the surface takes place, non-negligible residual stresses can be introduced. Based on these findings, it was concluded that in the above-mentioned case of fillet welds of S355, shot-blasting, which was applied on the surface of the plates prior to welding to remove the mill scale and foreign matter, had to be accounted for the compressive RS.

In the case presented in [6], the peak RS near the surface were measured to be -329 MPa, i.e. 83 % of the yield limit. In the case of the S355 fillet welds, residual stress profiles with significant deviation in the range of -200 MPa to -300 MPa were measured, fluctuating between 50 % and 75 % of the yield strength. Detailed results will be published in [1], [10]. Such discrepancies are expected, as the profiles were measured on the surface of the specimen and the effect of these surface treatments is localized around the impact locus. Moreover, different batches of 20MnCr5 exhibit significant deviation regarding yield strength, which is predominant for introduced RS, and there is no reference to the strength of the specific applied batch provided in [6].

RS introduced by shot blasting in the weld region are rationally considered to be relieved by the thermal input during subsequent welding. It’s becoming evident though that in order to properly simulate WRS away from the weld as well, RS from shot blasting have to be considered in subsequent simulations. Nonetheless, a direct, full-scale simulation of shot blasting treatment is not possible. It would require the simulation of a great number of impacts, raising an unfeasible numerical problem with modern computational capabilities. The present study investigates the possibility of applying a fictitious thermal load in a pseudothermal analysis instead, in order to generate a compressive RS field similar to that of shot blasting. The present method is not foreseen to act predictively but to reproduce measured profiles of residual
stresses from shot blasting as input for the simulation of WRS in existing weldments. Prerequisite is to minimize the computational effort so that it can be applicable in practice.

2 THEORETICAL BACKGROUND

A quasi-static solution is applied for the present study, governed by eq. 1,

\[ f_s(u) - p(t) = 0. \]  (1)

Total mechanical strain is decomposed to elastic and plastic parts (eq. 2),

\[ \varepsilon_{\text{mech}} = \varepsilon_{\text{el}} + \varepsilon_{\text{pl}}. \]  (2)

The stress \( \sigma \) is proportional to the elastic strain \( \varepsilon_{\text{el}} \) according to Hooke’s law for linear isotropic material behaviour, which is presented in the following equation (eq. 3) in terms of Young’s modulus and Poisson’s ratio and in tensor notation,

\[ \varepsilon_{ij} \sigma_{ij} = \frac{1}{E} (\sigma_{ij} - \nu (\sigma_{kk} \delta_{ij} - \sigma_{ij})), \]  (3)

where \( \delta_{ij} \) is the Kronecker delta. Von Mises yield criterion (eq. 4),

\[ f(\sigma, \sigma_y) = \sigma - \sigma_y = 0, \]  (4)

is widely applied for metallic materials, where \( \sigma_y \) is the von Misses equivalent stress (eq. 5),

\[ \sigma_y = \sqrt{\frac{1}{2} \left( \frac{1}{3} \text{tr} \left( \sigma \right)^2 \right)}, \]  (5)
The pseudothermal loading is applied as thermal strains based on the temperature dependent coefficient of thermal expansion $\alpha_{se}$

$$\varepsilon^{th}_{se} = \alpha_{se}(T) \cdot (T - T_{ref}).$$

3 INVESTIGATED CASES

3.1 Proposed approach and previous considerations

Goal of the present study was the generation of RS from shot blasting based on an existing measured profile, which would act as input for subsequent weld simulation. According to textbook knowledge, when an area of a metallic component is heated rapidly like in the case of welding, restraining of the zone from neighbouring cold material leads to the introduction of plastic strains and in extension RS. When no other phenomena such as microstructural transformations that influence their magnitude take place, RS in this area are tensile. This effect can be reproduced by numerical approaches and has been thoroughly investigated by the authors of the present study in the past [2], [3], [4], [5] etc. As the generated profile of RS in the present case should be compressive, it was assumed that the respective area of the component should be cooled contrary to welding. Initial expectations dictated the application of temperature lower than the ambient, which whenever possible would follow the measured RS qualitatively in the depth direction. It was believed that in this way it would be more straightforward to generate the measured RS profile and its peaks and valleys. Once again, according to common knowledge, the magnitude of the introduced RS is higher for a restrained (during the application of heating/cooling) component and therefore, restraints were applied on the faces of the investigated components as described-below. Selection of the restraints was arbitrary and such that would not lead to numerical difficulties, based on previous knowledge of the authors. Finally, it was decided that the RS field after removal of the boundary conditions would be compared with the measured one, as the component with the generated RS profile should be restraint-free for application in subsequent analyses.

3.2 Investigated components

Two components were investigated in the present study; a small-scale one made of 20MnCr5 steel (component A) and a larger one made of S355 (component B). It was evident even before present study that a very fine mesh of the order of magnitude of 10 μm would be needed in order to reproduce RS profiles, which variate significantly at the top 100 μm near the surface. Nevertheless, the same mesh has to be subsequently applied to a weld simulation, whereby modelling of a real size component with this element sizes is not possible under modern computational restrictions. Hence, a component with dimensions of 5 mm x 5 mm x 5 mm and finer mesh was modelled at first. Goal was to validate the feasibility of the method by introducing the through-depth profile of RS from shot blasting measured in [6]. The upper 1 mm of the component was meshed with elements of varying thickness from 0.0025 mm at the top layer to 0.0255 mm at the bottom. Trough-thickness element size was 1 mm for the rest of the component. A universal transverse and longitudinal element dimension of 0.1 mm was applied (x and y direction). Component A along with the respective applied mesh is presented in Figure 2.
Component B had dimensions of 1000 mm x 365 mm x 10 mm, identical with the components investigated in [1]. In this case, as modelling with the above-mentioned mesh is prohibitive for subsequent welding simulations, a simplified approach is proposed alternatively. A universal element size of 0.3 mm is applied, which is of the same order of magnitude with the mesh in the HAZ during weld simulations. It is assumed for the present study that only 100 mm adjacent to the weld line in both directions are shot blasted. Component A along and the respective applied mesh are presented in Figure 3 and 4 respectively.

![Figure 2: Component A](image-url)
3.3 Investigated materials

Effective material properties of 20MnCr5 and S355 were adopted from [8] and [1] respectively ν and α_{se} were assumed equal to 0.28 and 12 x 10^{-6} for both materials based on a range of values found in [11]. Bilinear elastic-plastic material models were applied for simulating the σ-ε behaviour taking into consideration the Bauschinger effect (kinematic hardening). The applied properties are presented in Table 1.
Table 1: Material properties of 20MnCr5 and S355

<table>
<thead>
<tr>
<th>Material Property</th>
<th>20MnCr5</th>
<th>S355</th>
</tr>
</thead>
<tbody>
<tr>
<td>E [MPa]</td>
<td>218,000</td>
<td>210,000</td>
</tr>
<tr>
<td>$\sigma_y$ [MPa]</td>
<td>398</td>
<td>400</td>
</tr>
<tr>
<td>H [MPa]</td>
<td>2,261</td>
<td>2,330</td>
</tr>
<tr>
<td>v [-]</td>
<td>0.28</td>
<td>0.28</td>
</tr>
<tr>
<td>$\alpha_{se}$ [-]</td>
<td>$12 \times 10^{-6}$</td>
<td>$12 \times 10^{-6}$</td>
</tr>
</tbody>
</table>

3.4 Pseudothermal analysis

Commercial FE software ANSYS was applied for all simulations [12]. Temperature was applied as nodal loads for simulating the effect of shot blasting. For both components, solution was carried out in 3 steps. In the first one boundary conditions and loads were applied and in the second and third, the loads and the restraints were respectively removed.

In the case of component A, applied temperature on each node was a function of its depth. This was enabled through an appropriate function $A(d)$ identical to the shape of the measured RS profile. The applied temperature on each node was equal to $A(d)$, where $d$ was the depth of the node, multiplied with the loading factor $T_{\text{load}}$. The values of 0.5, 1 and 2 are tested for this factor. Function $A(d)$ is compared in Figure 5 with the RS profile measured in [6] for shot blasting. All the faces of the component apart from the top one were restrained to the direction normal to their plane, thus modelling a plate of infinite width.

In the case of component B and due to the unavoidably coarser mesh, such a distribution of temperature was not possible. Instead a universal differential temperature of -500 °C was applied at the nodes of the top and bottom face (both sides were shot blasted) for 50 mm in each direction adjacent to the centerline. Once again, all the faces of the component apart from the top one were restrained to the direction normal to their plane.

![Figure 5: A(d) and RS measured in [3], both in depth direction](image-url)
4 RESULTS AND DISCUSSION

4.1 Component A

The stress contours of component A for $T_{\text{load}} = 1$, prior and after removal of boundary conditions, are presented in Figure 6. The qualitative distribution of RS meets initial expectations with compressive stresses of large magnitude arising at the top face. Compressive stresses of lower magnitude are met in the rest component. As expected, removal of external restraints leads to stress relaxation on the boundaries of the component. However, the distribution of RS remains same qualitatively at its center. The through-depth profile of RS for the different values of $T_{\text{load}}$ is presented in Figure 7 for better understanding.

In all three cases, the shift up of the RS profile due to stress relaxation after removal of restraints is evident. Nonetheless, it is expected that this effect is going to be negligible away from the boundaries for a larger component. Moreover, when a larger component is investigated, restraints of subsequent analyses could be applied for shot blasting as well and a removal of boundary conditions would not be necessary. A different effect of the restraints is expected in this case. For $T_{\text{load}} = 0.5$ the RS profile is qualitatively similar to the measured one but lies significantly higher. When the load is increased ($T_{\text{load}} = 1$ and $2$) a plateau of RS near the surface is met, although temperature distribution followed the peaks and valleys of the measured RS according to function A(d). The introduced plasticity and the accompanied redistribution of stiffness is to be accounted for this inability of the numerical model to reproduce exactly the RS profile. The effect is becoming even more evident from the extension of the plateau when $T_{\text{load}}$ is increased from $1$ to $2$, causing the widening of the plastic zone.

In any case, the method seems promising, as the calculated RS profile for $T_{\text{load}} = 2$ after removal of external restraints lies within the boundaries of the measured RS although the peaks and valleys are not reproduced. As it is mentioned above such a detailed analysis would be anyway impossible for a larger component due to mesh size restrictions.

Figure 6: Component A – Contours of residual stresses introduced for $T_{\text{load}} = 1$, prior (A) and after (B) removal of restraints – results in N/mm²
4.2 Component B

The contours of RS and Von Mises plastic strains for component B prior and after to the removal of external restraints are presented in Figure 8 and Figure 9 respectively. As expected compressive stresses are met on the surface of the area where differential temperature of \(-500\) °C is applied. Comparing the two contours, the above-stated expectation that stress relaxation would not cause such a significant change at the center of a larger component is validated.

The through-thickness RS profile at the center of the specimen is illustrated in Figure 10, in order to enable a better overview. A linear, symmetric distribution of stresses is evident. It is as expected compressive near the outer surfaces and moves to the tensile region at a depth larger than 4 mm. Symmetry is attributed to the simultaneous application of the thermal loads on both upper and bottom faces. The residual stresses inner to the external upper and bottom faces, where the thermal load was applied, are introduced due to equilibrium reasons. As expected, the fluctuating profile of the measured RS cannot be reproduced due to the coarser mesh and homogenous surface loading. Nevertheless, compressive stresses of the same order of magnitude as those measured in [1] are introduced near the surface, without significant computational effort. Questions arise however, how an erroneous modelling of the RS at depths deeper than 1 mm, where measurements for validation are more difficult, could affect a subsequent simulation of WRS. Component’s significant ratio of length to width is to be accounted for the higher magnitude of longitudinal stresses.
Figure 8: Component B, results prior to removal of restraints – A) Contours of residual stresses (results in N/m²) – B) Contours of Von Mises plastic strain

Figure 9: Component B, results after removal of restraints – A) Contours of residual stresses (results in N/m²) – B) Contours of Von Mises plastic strain

Figure 10: Component B – RS profile in depth direction at the center of the component
5 CONCLUSIONS AND FUTURE WORK

A pseudothermal modelling approach for introducing RS from shot blasting prior to welding simulations has been proposed and tested in the present study. Thermal strains are imposed on the upper layer of a component, so that the desired RS profile can be introduced. Significant simplifications have to be adopted, due to mesh restrictions, but the results seem promising. The influence of the RS from shot blasting is expected to be negligible in any case near the HAZ and FZ of weldments, as the welding heat input erases previously introduced plastic strains and RS. The current method could improve the agreement of simulated and measured RS profiles on shot blasted surfaces away from the weld section. Nevertheless, the following additional investigations are proposed for further validation and better calibration of the approach:

- Arbitrary restraints were applied in the present study, whose removal for subsequent simulations would influence significantly the RS profiles. This influence of stress relaxation was less significant for the larger component validating initial expectations. Additional analyses, with boundary conditions of subsequent welding simulations can be applied, in order to further test the influence of external restraints.
- Profile of measured RS could not be reproduced, even in the case where a very fine mesh was applied and therewith, pseudothermal loading with fluctuation in depth direction similar to the measurements could be applied. The nonlinear material behaviour lead to either underestimation of RS with qualitatively better agreement, or to introduction of RS quantitatively closer to the real ones but with different distribution. Nevertheless, this would not deter the application of the method on larger components as the above mentioned necessary mesh restrictions would anyway allow only the creation of a homogenous stress field at the top layer. Applying more complex or even fictitious material model could enable better agreement with measured profiles.
- Finally, a coupled simulation of shot blasting with a subsequent weld simulation is proposed, so that the improvement in the calculation of WRS can be documented is proposed.

6 ACKNOWLEDGEMENT

The present study was carried out in the framework of the first author’s doctoral thesis [10].

REFERENCES


A REGULARIZED DAMAGE MODEL FOR STRUCTURAL ANALYSES OF CONCRETE DAMS IN THE PRESENCE OF ALKALI-SILICA REACTION

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Key words: Alkali-silica reaction, regularization, nonlocal formulation, strain localization, concrete dam

Abstract. Alkali-silica reaction is a chemical phenomenon that affects concrete structures built some decades ago and subject to a very wet environment, e.g. dams. The starting point of this work is a bi-phase damage model present in the literature. In general, finite element solutions with damage models for material having a softening behaviour exhibit a sensitivity to the element size and do not converge to physically meaningful solutions as the mesh is refined. In literature, some regularization techniques have been proposed and the fracture energy one has been implemented in the bi-phase chemo-damage model. The limit of this approach is that the solution remains mesh-dependent, so if the mesh is refined the damage localizes in a band of width fixed by the element size. In this work the nonlocal formulation of this damage model has been developed, validated with simple examples and applied to an existing concrete gravity dam, subject to service loading and affected by the ASR. A comparison between fracture energy regularization approach and nonlocal formulation is performed.

1 INTRODUCTION

Concrete is one of the most used materials in civil engineering, but its durability can be reduced by several chemical phenomena, among them the alkali-silica reaction (ASR) plays a fundamental role. During ASR amorphous silica of aggregates reacts with the high alkaline solution in concrete micro pores to form a hydrous alkali-calcium-silica gel, which expands and causes increase of displacements in concrete structures. Another key dissipative phenomenon related to ASR is micro-cracking, which results in non-symmetric,
progressive degradation of mechanical properties (strength and stiffness). In [1] a phenomenological two-phase isotropic damage model for the evaluation of the effects of ASR has been proposed. This model, which extends the one originally proposed in [11] takes into account the simultaneous influence of both humidity and temperature through two uncoupled diffusion analyses: the heat diffusion analysis and the moisture diffusion analysis. The solution of these two analyses are considered as input for a consequent mechanical analysis, used to define the response due to ASR.

The model in [1] has been implemented with fracture energy pseudo-regularization, hence, as damage develops, the boundary value problem may still become ill-posed and the damage pattern obtained in numerical analyses is mesh-dependent. Such difficulties can be solved implementing a real regularization technique, as proposed in the literature ([2]-[4]). In all regularized models the introduction of a material characteristic length fixes the width of the zone in which damage localizes, thus preventing strain localisation into a line with consequent zero energy dissipation. In this work a nonlocal formulation of the bi-phase damage model is proposed for the description of ASR-induced degradation. Non-locality has been introduced replacing strain invariants with their nonlocal counterpart, obtained by weighted average. This approach has been validated on a simple example, then it has been applied to a real case of existing concrete gravity dam.

2 BI-PHASE CHEMO-MECHANICAL DAMAGE MODEL

At the mesoscale concrete affected by ASR is composed of two phases (the solid skeleton and the gel), so the macroscopic stress is written as the sum of the effective stress \( \sigma' \) (acting on the skeleton) and of the stress \(-bp1\) (acting on the gel)

\[
\sigma = (1 - D) [2G e + K (tr\varepsilon - \alpha \theta)1 - bp 1]
\]

with

\[
p = (1 - D) M (b tr\varepsilon - \zeta_g - \alpha_g \theta)
\]

where: \( G \) and \( K \) are respectively the shear and bulk moduli of the homogenized concrete skeleton; \( M \) and \( b \) are the Biot’s modulus and the Biot’s coefficient; \( \alpha_e \) and \( \alpha_g \) are respectively the volumetric coefficients of thermal expansion for the concrete skeleton and the gel; \( \zeta_g \) is the gel volume content; \( D \) is the damage variable, governed by the activation function, written in terms of strain invariants \((tr\varepsilon \text{ and } J_2)\) in the following form

\[
f = (1 - D)^2 4G^2 J_2 - 9a_t (1 - D)^2 [(K + Mb^2) tr\varepsilon - Mb \zeta_g] + 3b_t (1 - D) [(K + Mb^2) tr\varepsilon - Mb \zeta_g] h(D) - k_t h(D)^2
\]

where: \( tr\varepsilon = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} \) is the first strain invariant and \( J_2 = \frac{1}{2} e : e \) is the second one; \( a_t, b_t, k_t \) are material parameters governing the shape and dimensions of the elastic domain; \( h \) is the herdening-softening function.
In the previous Equation $\sigma_e/\sigma_0$ is the ratio between the stresses at the elastic limit and at peak, $D_0$ defines the damage level corresponding to the peak stress and $c$ governs the negative slope of the softening part of the function $h(D)$. In finite element approach, the coefficient $c$ is used to scale the fracture energy density of the material in such a way that each finite element can dissipate the correct amount of energy, independently of its size. This method, called as "fracture energy regularization", prevents the occurrence of spurious mesh dependency in the structural global response. The evolution of $\zeta_g$, which depends on temperature and humidity, is not reported here for brevity and reference is made to [1] for further details.

3 REGULARIZED MODELS

In the context of standard continuum theories, damage-induced softening constitutive models typically cause ill-posedness of the initial boundary value problem. In order to introduce a remedy, various regularization techniques have been proposed in the literature, especially for damage models (as one used in this work). Among them, the following approaches are cited:

(i) Fracture energy pseudo-regularization: the parameters governing the material softening are modified with the mesh size in order to have a fixed value of the fracture energy associated with the finite element. It can not be considered a real regularization method as the length introduced is a mesh-dependent numerical parameter and not a material one.

(ii) Nonlocal integral models ([2]-[3]): the inelastic behaviour at a point is governed by a weighted average over a representative volume of the strains or strain invariants.

The nonlocal regularization methods introduce a characteristic material length in the formulation, which fixes the width of the zone in which damage localises, thus preventing strain localisation into a line with consequent zero energy dissipation. Usually, for material likes concrete this length depends on the aggregates size. In 3.1 and 3.2 the two above cited methods are presented and in 3.3 a simple numerical test is performed.

3.1 Fracture energy approach

The simplest but crude remedy to pathological mesh-dependence, popular in engineering applications, is to adjust the softening part of the stress-strain diagram as a function of the element size. When this is done properly, the energy dissipated in a band of cracking
elements does not depend on the width of the band. The fracture energy regularization introduces a modification of the softening parameters according to the mesh size, such that to impose the same energy dissipation per unit area even with mesh refinement. This can be considered as a numerical “trick” to obtain a physically sense overall response, for this reason it is known as a pseudo-regularization method.

The method is based on the assumption that dissipation always takes place in a band one element thick, irrespective of the element size. The constitutive law is modified in such a way that the energy dissipated over a completely fractured finite element is equal to an assigned value depending on the fracture energy $G_f$ (which is a material property, independent of the specimen size) and on the element size. The area below the softening part of the $\sigma - \varepsilon$ curve represents the energy dissipated per unit volume (or specific fracture energy $g_f$) in uniaxial test. This is related to the corresponding fracture energy $G_f$ through the material characteristic length $w$ (i.e., $G_t = g_t w$) representing the width of the crack band front. For each element, the “material characteristic length” $w$ is substituted by the “element characteristic length” $l_e$, which depends on the mesh and measures the numerical width of the fracture process zone. The specific fracture energy $g_f$ is then scaled for each element so that $g_f l_e = G_f$.

The fracture energy density $g_f$ is defined as the area below the stress-strain curve and it depends on parameter $c$ through Equation 4. For $c < 1$, the $\sigma - \varepsilon$ curve has a snap-back branch, while for $c = 1$ the slope is discontinuous at the peak. Values of $c > 1$ are adopted in all cases. Examples of fracture energy density scaling for varying $c$ are shown in Figure 1.

![Figure 1](image.png)

**Figure 1**: Specific fracture energy definition with different parameter $c$ values.
3.2 Nonlocal model

A computationally efficient and theoretically sound localization limiter is provided by the nonlocal averaging, which is in principle applicable to any type of constitutive model. The idea of a nonlocal continuum originally appeared in elasticity [9].

The nonlocal approach replaces a certain variable by its nonlocal counterpart obtained by weighted averaging over a spatial neighborhood of each point under consideration. Thus the response at a point \( x \) depends not only on the state and internal variables at that point, but also on those of point \( s \), belonging to a proper neighborhood of the point. The characteristic length defines the size of this neighborhood.

If \( \alpha(x) \) is some “local“ field in a domain \( V \), the corresponding nonlocal field is defined by

\[
\langle \alpha(x) \rangle = \int_V \alpha'(x, s) \alpha(s) ds \tag{5}
\]

where \( \alpha'(x, \xi) \) is a given nonlocal weight function.

In this work the nonlocal model presented in [2], which defines the weighted average of a strain measure, has been developed, implemented and used. The basic non-local variables at a point \( x \) are assumed to be the average strain invariants, i.e. the weighted averages over the volume \( V \) of the local strain invariants

\[
\langle J_\varepsilon(x) \rangle = \int_V W(x - s) J_\varepsilon(s) ds \tag{6}
\]

\[
\langle tr\varepsilon(x) \rangle = \int_V W(x - s) tr\varepsilon(s) ds \tag{7}
\]

where \( W(x - s) \) is the weighting function, adequately defined to normalise the averaging. In Equations 6 and 7 and in what follows the symbol \( \langle \cdot \rangle \) denotes the weighted average value of the quantity \( \cdot \). \( W(x - s) \) is assumed as the normalised Gauss function and the average is extended to the whole body so that \( V \) coincides with the body volume:

\[
W(x - s) = \frac{1}{W_0(x)} \exp\left( -\frac{\|x - s\|^2}{2l^2} \right) \tag{8}
\]

with

\[
W_0(x) = \int_V \exp\left( -\frac{\|x - s\|^2}{2l^2} \right) ds \tag{9}
\]

The length \( l \) is a material parameter which can be related to the width of the zone in which damage phenomena localise. No particular provisions need to be introduced for points near the boundary of the body since \( W_0(x) \) in Equation 9 already normalises the averaging.

The non-local model is then obtained by replacing in the loading functions the averages of the strain invariants. The resulting non-local loading functions \( F \) is
\[ F = (1 - D)^2 4G^2 \langle J_2 \rangle - 9a_t (1 - D)^2 [(K + Mb^2) \langle tr\varepsilon \rangle - Mb\zeta_g]^2 + \\
+ 3b_t (1 - D) [(K + Mb^2) \langle tr\varepsilon \rangle - Mb\zeta_g] h(D) - k_t h(D)^2 \] (10)

Note that non-locality only intervenes in the damage activation function, while the stress-strain Equation 1 remains local.

3.3 Plane strain tension test

In order to clarify the limits of the fracture energy regularization and the effectiveness of the nonlocal regularization, these methods have been tested on a simple example subject to a linearly increasing displacement applied on one base. A bi-dimensional specimen in plane strain tension conditions has been considered, meshed with different finite element sizes (see Figure 2). To trigger localization, the strength is slightly reduced in the central part of the specimen. The analyses have been performed by a finite element Matlab code where the local and nonlocal models have been implemented.

Figure 3 (a) and (b) depict the global response in terms of reaction force as a function of axial displacements obtained with fracture energy regularization and nonlocal formulation. In both cases, as expected, the global response is quite similar for all considered meshes. On the contrary, the damage pattern, shown in Figure 4, is completely different: when using fracture energy regularization damage localizes in one element thick band and hence considerably changes by modifying the mesh (see Figure 4 (a)); when using nonlocal regularization instead the width of the localization band is fixed by the material length and thus does not change with the mesh size (see Figure 4 (b)).

4 STRUCTURAL ANALYSIS OF A GRAVITY DAM SUBJECT TO ASR

The comparison between fracture energy regularization approach and nonlocal formulation has been developed considering an existing concrete dam: Fontana dam is a gravity dam (maximum height, length, and thickness at the basis equal to 146, 720 and 114 m, respectively) located in Graham County, North Carolina (United States). Its construction was completed in 1946, but only 3 years later a pattern of cracking was first observed, together with an upstream movement of the structure. In late 1972, inspectors found a large longitudinal crack near the left abutment, in both the upstream and downstream walls of the foundation drainage gallery inside the dam (for more details see [10]).

The bi-phase model, both in local and nonlocal formulation, accounts for the simultaneous effect of the temperature and humidity. A weakly coupled approach has been followed: a preliminary heat diffusion analysis and moisture diffusion analysis allowed to compute the varying fields of temperature and humidity, which have been the input of the subsequent chemo-damage analysis. The preliminary thermal and humidity analyses have been performed using Abaqus software. Furthermore, with the same program the parameter
Figure 2: Specimen geometry for the simple tension test at imposed displacements; typical elements dimensions: (a) 10 mm, (b) 5 mm and (c) 2 mm.

Figure 3: Comparison of the global response in terms reaction force vs of axial displacements between (a) local and (b) nonlocal approach.
representing the reaction evolution has been calculated and used in Matlab in order to compare the local and nonlocal model results.

The 2D dam section has been discretized by plane strain 3-nodes element. To check the regularization properties of the two models we have considered two meshes with different refinements (with typical finite element dimension of 50 and 20 cm).

For this dam no detailed monitoring data are available, only the crack geometry due to ASR is known from [10]. For this reason, the damage material parameters have been calibrated considering this crack formation and direction.

For the annual variation of temperature, saturation degree for the water and reservoir level, in this work reference has been made to what reported in [11] (see Figure 5).

To determine the initial temperature and of saturation degree fields within the dam, a preliminary heat diffusion analysis and a preliminary moisture diffusion analysis have been performed respectively.

In these first steady state analyses the stabilized temperature and saturation degree in the internal nodes, starting from the initial uniform field of the two variables, have been evaluated by assuming as boundary conditions the mean values of temperature, saturation degree and reservoir level. The second step consisted of transient analyses, in which the assumed sinusoidal annual variation of air temperature and saturation degree, shown in Figure 5 (b) and (c) respectively, have been applied. Furthermore, a sinusoidal reservoir level variation (Figure 5 (a)) has been considered. In Figure 6 (a) the histories of tem-

**Figure 4**: Contour plot of the damage, from the largest FE size (on the left) to the smallest one (on the right) for: (a) fracture energy regularization and (b) nonlocal formulation.
Figure 5: History of Fontana (a) reservoir level, (b) air temperature and (c) saturation degree for the water.

Figure 6: Histories of (a) temperature and (b) saturation degree of some nodes (A, B and C) of Fontana dam (10 years of the full analysis).

The diffusion analyses have been performed in Abaqus and the reaction extent evolution could then be computed. Then, the chemo-mechanical analysis has been implemented in the Matlab code considering both the local and nonlocal models. In Figure 7 the damage contour plot after 15 years with different meshes is shown: as discussed in the section 3.1, with fracture energy regularization (green outline) the band of the damaged area depends strongly on the finite element dimension (it becomes smaller when the mesh size is reduced). On the contrary, instead, with nonlocal formulation (orange outline), the damage pattern remains almost unchanged passing from a mesh to another. The same Figure emphasizes that using the pseudo-regularization technique the results in terms of the global response remain quite good: the same vertical crest displacements have been
obtained for the two meshes, similarly to what happened with nonlocal formulation.

Figure 7: Damage contour plot after 15 years and crest vertical displacement evolution with coarse and refined meshes; fracture energy regularization at the top and nonlocal formulation at the bottom.

5 Conclusions

Concrete dams are strategic structures that may be subject to many degradation phenomena, such as alkali-silica reaction, which causes displacements increase, cracks and material expansion. These effects can be studied through a bi-phase damage model, present in the literature, which has been implemented using a fracture energy regularization technique in order to avoid sensitivity to the element size and non-convergence to physically meaningful solutions as the mesh is refined. This method is a pseudo-regularization approach since the characteristic length introduced for scaling the material fracture energy depends on the element size. For this reason, in this work the nonlocal formulation of the bi-phase chemo-damage model has been developed. It consists in replacing the strain
invariants with their nonlocal counterpart obtained by weighted averaging. The new version of the model has been validated with simple tensile tests in plane strain conditions. It has been demonstrated that with nonlocal model the damage localization band remains almost unchanged when the mesh is refined, as opposed to what happens with fracture energy regularization (the damage concentrates in a band one element thick). With both the methods, the global response in terms of reaction forces vs axial displacements is similar for all the considered meshes. Then, the comparison between the two approaches has been developed for an existing gravity dam, thus showing the effectiveness of the model also in structural analyses of real structures.

REFERENCES


ENERGY-MOMENTUM TIME INTEGRATIONS OF A NON-ISOTHERMAL TWO-PHASE DISSIPATION MODEL FOR FIBER-REINFORCED MATERIALS BASED ON A VIRTUAL POWER PRINCIPLE

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Abstract. Fiber-reinforced plastics (FRP) are composite materials made of an isotropic polymer matrix reinforced with organic or inorganic fibers. The major contribution to the internal dissipation in FRP is due to the isotropic matrix material. However, internal dissipation in the fibers has to be taken into account if Carbon or Kevlar fibers, respectively, are applied [1], or by using organic fibers, applied in the automotive industry [2]. Therefore, we introduce in this presentation a new two-phase dissipation model at finite strains with independent viscoelastic behaviour in the matrix and the fibers.

This model is based on the multiplicative split of the deformation gradient \( \mathbf{F} := \mathbf{F}_e \mathbf{F}_v \) of the composite in an elastic and viscous deformation gradient \( \mathbf{F}_e \) and \( \mathbf{F}_v \), respectively, as well as on the multiplicative split of the fiber deformation gradient \( \mathbf{F}_F := \mathbf{F}_F^e \mathbf{F}_F^v \) in an elastic and viscous fiber deformation gradient \( \mathbf{F}_F^e \) and \( \mathbf{F}_F^v \), respectively. However, the time-dependent matrix behaviour depends directly on the principal invariants of the symmetric elastic right Cauchy-Green tensor \( \mathbf{C}_e := [\mathbf{F}_e]^T \mathbf{F}_e \). Analogously, the trace of the elastic fiber right Cauchy-Green tensor \( \mathbf{C}_F := [\mathbf{F}_F^e]^T \mathbf{F}_F^e \) determines the time evolution of the viscous fiber deformation.

In the internal power of a mixed principle of virtual power, we consider free energy functions \( \Psi_M^{vis} \) and \( \Psi_F^{vis} \), depending on matrix and fiber invariants. In the external power, the non-negative internal dissipation with respect to a positive-definite viscosity tensor or a positive fiber viscosity parameter, respectively, is introduced. In this way, we derive the viscous evolution equations by variation. The internal power also includes mixed fields for the thermo-elastic matrix and fiber behaviour. Algorithmic terms in the virtual external power provide energy-momentum time integrations of this two-phase model.
1 INTRODUCTION

In Reference [3], a mixed finite element formulation for fiber-reinforced continua is presented, which is derived from a principle of virtual power. The reason for choosing this principle is the comfortable derivation of energy-momentum schemes of higher-order for coupled problems and mixed finite elements. This can be explained by the Simo-Taylor-Pister functional

\[
\Pi_{\text{STP}}(\varphi, \tilde{J}, p) := \int_{\mathcal{B}_0} \Psi_{\text{iso}}(\varphi) \, dV + \int_{\mathcal{B}_0} \Psi_{\text{vol}}(\tilde{J}) \, dV - \int_{\mathcal{B}_0} p G(\varphi, \tilde{J}) \, dV
\]

with \( G(\varphi, \tilde{J}) := \tilde{J} - \det(\nabla \varphi) \) in Reference [4]. This Hu-Washizu functional introduces an independent volume dilatation field \( \tilde{J} \) and volume pressure field \( p \), during a deformation \( \varphi \) of a reference configuration \( \mathcal{B}_0 \) with the isochoric strain energy function \( \Psi_{\text{iso}} \) and the volumetric strain energy function \( \Psi_{\text{vol}} \). The symbol \( \nabla \) denotes the partial derivative with respect to any material point \( X \in \mathcal{B}_0 \). The energy-momentum time integration of this functional requires the preservation of the balance law corresponding to the strain energy density \( \Psi(\varphi, \tilde{J}) := \Psi_{\text{iso}}(\varphi) + \Psi_{\text{vol}}(\tilde{J}) \) on a time step \([t_n, t_{n+1}]\), given by

\[
\int_{\mathcal{B}_0} \Psi_{\varphi}^{t_{n+1}}(\varphi, \tilde{J}^{t_{n+1}}) \, dV - \int_{\mathcal{B}_0} \Psi_{\varphi}^{t_n}(\varphi, \tilde{J}^{t_n}) \, dV = \int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} \left[ \frac{\partial \Psi}{\partial \varphi} \cdot \dot{\varphi} + \frac{\partial \Psi}{\partial \tilde{J}} \cdot \dot{\tilde{J}} \right] \, dV \, dt
\]

We denote by the symbol ‘·’ a single tensor contraction. This balance law can be easily satisfied with the weak form

\[
\int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} \delta p \, G(\varphi, \tilde{J}) \, dt = 0 \quad \text{with} \quad G(\varphi, \tilde{J}) := \tilde{J} - \det(\nabla \varphi)
\]

by substituting the pressure \( p \) for the test function \( \delta p \). Hence, it is more appropriate to enforce the constraint \( G \) on the velocity level as on the variable level, if an energy-momentum time integration of higher-order is the goal of the simulation. The weak form in Eq. (3) can be directly derived by the principle of virtual power in Reference [3].

2 THE PRINCIPLE OF VIRTUAL POWER

In Reference [3], damping in the fibers is neglected. Therefore, in this paper, we take into account a two-face model of damping, which assume an independent viscoelastic behaviour of the fibers and the matrix. According to Reference [3], we start with the kinetic power functional

\[
\mathcal{T}(\varphi, \dot{\varphi}, \dot{p}) := \int_{\mathcal{B}_0} [\rho_0 \, \mathbf{v} - \mathbf{p}] \cdot \dot{\mathbf{v}} \, dV - \int_{\mathcal{B}_0} \dot{\mathbf{p}} \cdot [\mathbf{v} - \dot{\varphi}] \, dV + \int_{\mathcal{B}_0} \mathbf{p} \cdot \ddot{\varphi} \, dV
\]

where \( \mathbf{v} \) and \( \mathbf{p} \) denotes the Lagrangian velocity and momentum field, respectively, and \( \rho_0 \) the mass density in the initial configuration \( \mathcal{B}_0 \). A superimposed dot indicates a time
derivative. Recall that according to Reference [3], the variation has to be performed with respect to the independent fields in the argument of the power functionals. This means, the variation is performed with respect to temporally continuous time rate fields and temporally discontinuous Lagrange multiplier fields. This variation is indicated by the symbol ‘\(\delta\)' [3]. The exception is the temporally discontinuous field \(\tilde{\Theta}\) in the internal power functional

\[
\dot{H}^{\text{int}} := \dot{H}^{\text{int}}(\varphi, \dot{\bar{F}}, \tilde{\mathbf{C}}, \dot{\bar{C}}_v, \dot{\bar{C}}_F, \dot{\bar{C}}_P, \dot{\bar{C}}_M, \dot{\bar{C}}_V, \tilde{\dot{\Theta}}, \dot{\bar{\eta}}, \dot{\bar{\Theta}}, \mathbf{F}, \mathbf{S}, \mathbf{S}_V, \mathbf{S}_F) \\
= \frac{1}{2} \int_{\mathcal{B}_0} \left[ 2 \left( \frac{\partial \Psi_M}{\partial \mathbf{C}} - S_v \right) A_v^0 + S_F A_0 - S_v \right] : \dot{\tilde{\mathbf{C}}} \, dV + \frac{1}{2} \int_{\mathcal{B}_0} \left[ 2 \left( \frac{\partial \Psi_M}{\partial \mathbf{C}_V} - S_{V} \right) \right] : \dot{\tilde{\mathbf{C}}}_V \, dV \\
+ \frac{1}{2} \int_{\mathcal{B}_0} \left[ 2 \left( \frac{\partial \Psi_F}{\partial \mathbf{C}_F} - S_{F} \right) \right] \dot{\tilde{\mathbf{C}}}_F \, dV + \int_{\mathcal{B}_0} \left[ \mathbf{F} S - \mathbf{P} \right] : \dot{\bar{F}} \, dV + \int_{\mathcal{B}_0} \left[ \frac{\partial \Psi_M}{\partial \mathbf{S}} \right] : \dot{\bar{S}} \, dV \\
+ \int_{\mathcal{B}_0} \mathbf{P} : \nabla \varphi \, dV - \int_{\mathcal{B}_0} \tilde{\dot{\bar{\eta}}} \left[ \dot{\tilde{\Theta}} - \Theta \right] \, dV + \int_{\mathcal{B}_0} \left[ \eta + \frac{\partial \Psi}{\partial \Theta} \right] \dot{\Theta} \, dV + \int_{\mathcal{B}_0} \frac{\partial \Psi_F}{\partial \mathbf{C}_F} \dot{\tilde{\mathbf{C}}}_F \, dV
\]

which is no Lagrange multiplier, but replaces the time rate of a thermal displacement field. This is possible due to the fact, that the free energy does not depend on a thermal displacement field, but on the temperature field \(\Theta\). We denote the independent entropy density field by \(\eta\), which is associated with the free energy \(\Psi := \Psi_M + \Psi_F\) of the \(n_{\text{dim}}\)-dimensional body \(\mathcal{B}_0\), additively split in the matrix function \(\Psi_M\) and the fiber function \(\Psi_F\). The prescribed structural tensor of the fibers is denoted by \(\mathbf{A}_0 = \mathbf{A}_0(X)\), and

\[
A_v^0 := \frac{1}{n_{\text{dim}}} \det(\mathbf{C}) \mathbf{C}_v^{-1}
\]

denotes the volumetric structural tensor with respect to the independent right Cauchy-Green tensor \(\mathbf{C}\). We indicate by the superscript ‘\(-1\)’ the inverse of a tensor, and by the symbol ‘\(\cdot\)’ a double tensor contraction. The independent scalar-valued fields \(S_F\) and \(S_V\) designate the volumetric and fiber stress, which are energy-conjugated to the fiber strain \(\tilde{\mathbf{C}}_F\) and the volumetric strain \(\tilde{\mathbf{C}}_V\). The total second Piola-Kirchhoff stress tensor is denoted by the independent second-order tensor field \(\mathbf{S}\). In contrast to Reference [3], we introduce the independent deformation gradient field \(\bar{\mathbf{F}}\) and the independent first Piola-Kirchhoff stress field \(\mathbf{P}\). In the last term of Eq. (5), we introduce an independent viscous internal variable \(\mathbf{C}_v^\alpha\) of the fibers, which is scalar-valued, in contrast to the symmetric internal variable tensor field \(\mathbf{C}_v\) of the matrix material.

Conservative and non-conservative external force terms and Dirichlet as well as Neumann boundary terms are included in the external power functional. We take into account the conservative, mass-specific gravitational force \(\mathbf{B}\) and the traction load \(\mathbf{T}\) on the Neumann boundary \(\partial_{I_{\mathcal{B}_0}}\). A transient inward boundary heat flux is introduced as thermal Neumann load \(\bar{Q}\) on the boundary \(\partial_{Q_{\mathcal{B}_0}}\). The heat conduction law in the considered
fiber-reinforced body \( \mathcal{B}_0 \) is given by

\[
Q := - \left[ \frac{k_{F0} - k_0}{C_F} A_0 + k_0 \tilde{C}^{-1} \right] \nabla \Theta
\]

where \( k_{F0} := \det(\tilde{F}) k_F \) and \( k_0 := \det(\tilde{F}) k \) denote the material conductivity coefficients of the fibers and the matrix, respectively (cp. Reference [5]). The corresponding dissipation by conduction of heat is given by

\[
D^{\text{cdu}} := - \frac{1}{\Theta} \nabla \Theta \cdot Q
\]

The viscous driving force in the matrix material, defined by the tensor

\[
\Sigma_v := \mathbf{V}(C_v) : \dot{\mathbf{C}}_v
\]

with respect to the positive-definite viscosity tensor

\[
\mathbf{V}(C_v) := \frac{1}{4} \left( V_{\text{vol}} - \frac{V_{\text{dev}}}{n_{\text{dim}}} \right) C_v^{-1} \otimes C_v^{-1} + \frac{V_{\text{dev}}}{4} \Gamma_{\text{sym}} : C_v^{-1} \otimes C_v^{-1}
\]

is also introduced in the external power functional. The associated deviatoric and volumetric viscosity parameters are designated by \( V_{\text{dev}} > 0 \) and \( V_{\text{vol}} > 0 \), respectively. As Dirichlet boundaries, we take into account a heat sink of the body by means of a constant ambient temperature \( \Theta_\infty \) and the corresponding boundary heat flux \( \lambda \) on the boundary \( \partial \Theta \mathcal{B}_0 \). A temperature open-loop control on the boundary \( \partial \dot{\Theta} \mathcal{B}_0 \) is realized by a prescribed temperature time evolution \( \dot{\Theta}(t) \) with the corresponding boundary entropy \( h \). And finally, a mechanical Dirichlet boundary \( \partial \varphi \mathcal{B}_0 \) for introducing a bearing with the reaction force \( \mathbf{R} \) is also taken into account. These external forces and boundaries leads to the external power functional

\[
\Pi^{\text{ext}} := \Pi^{\text{ext}}(\varphi, \dot{\mathbf{C}}, \dot{C}_v, \dot{\mathbf{C}}_V, \dot{\mathbf{C}}_F, \dot{\Theta}, \dot{\Theta})
\]

\[
= \int_{\mathcal{B}_0} \frac{1}{2} \tilde{S} : \dot{\mathbf{C}} \, dV + \int_{\mathcal{B}_0} \frac{1}{2} \tilde{S}_V \dot{C}_V \, dV + \int_{\mathcal{B}_0} \frac{1}{2} \tilde{S}_F \dot{C}_F \, dV
\]

\[
- \int_{\mathcal{B}_0} \rho_0 \mathbf{B} \cdot \dot{\varphi} \, dV - \int_{\partial \mathcal{B}_0} \mathbf{T} \cdot \dot{\varphi} \, dA + \int_{\partial \mathcal{B}_0} \frac{\dot{\Theta}}{\Theta} \dot{Q} \, dA
\]

\[
+ \int_{\mathcal{B}_0} \frac{1}{\Theta} \nabla \dot{\Theta} \cdot \dot{\mathbf{Q}} \, dV + \int_{\partial \mathcal{B}_0} \frac{\dot{\Theta}}{\Theta} (D^{\text{cdu}} + D^{\text{int}}) \, dV + \int_{\mathcal{B}_0} \dot{\mathbf{C}}_v : \Sigma_v \, dV
\]

\[
+ \int_{\partial \Theta \mathcal{B}_0} \lambda \left[ \dot{\Theta} - \Theta_\infty \right] \, dA - \int_{\partial \mathcal{B}_0} h \left[ \dot{\Theta} - \dot{\Theta}_\infty \right] \, dA - \int_{\partial \varphi \mathcal{B}_0} \mathbf{R} \cdot [\dot{\varphi} - \dot{\varphi}] \, dA
\]

\[
+ \int_{\mathcal{B}_0} \dot{C}_F^v \Sigma_F^v \, dV + \int_{\mathcal{B}_0} \tilde{M}_F \left[ L_F(\dot{C}_F) - L_F^v(\dot{C}_F^v) \right] \, dV
\]
where the first four rows with integral terms in Eq. (11) are also applied in Reference [3]. The first row with space integrals introduces algorithmic stresses for achieving an energy-momentum scheme. In this paper, however,

\[ D^{\text{int}} := D^{\text{int}}_M + D^{\text{int}}_F \]  

includes beside the internal dissipation

\[ D^{\text{int}}_M := \dot{C}_v : \nabla(C_v) : \dot{C}_v \geq 0 \]  

of the matrix material also the new internal dissipation \( D^{\text{int}}_F \) of the fibers. The last row of Eq. (11) is new and includes the viscous time evolution of the fiber material in the first term, and in the last term, an algorithmic stress in order to achieve the energy-momentum time integration of the viscoelastic fiber material. According to Reference [3], the space-time weak formulation follows from the incremental principle of virtual power

\[
\int_{t_0}^{t_{n+1}} \left[ \delta_s \tilde{T}(\dot{\phi}, \dot{v}, \dot{p}) + \delta_s \tilde{H}^{\text{int}}(\dot{\phi}, \dot{\tilde{F}}, \dot{\tilde{C}}_v, \dot{\tilde{C}}_V, \dot{\tilde{C}}_F, \dot{\Theta}, \dot{\eta}, \dot{\Theta}, \dot{\Theta}, \dot{P}, \dot{S}, S_V, S_F) \\
+ \delta_s \tilde{H}^{\text{ext}}(\dot{\phi}, \dot{\tilde{C}}_v, \dot{\tilde{C}}_V, \dot{\tilde{C}}_F, \dot{\tilde{C}}_F, \dot{\tilde{C}}_V, \dot{\tilde{C}}_F, \dot{\tilde{C}}_F, \dot{\tilde{C}}_F) \right] \, dt = 0
\]  

As mentioned above, the viscoelastic constitutive formulation of the fibers is new, and therefore not described in Reference [3]. Therefore, we summarize this model in Section 3.

3 THE VISCOELASTIC CONSTITUTIVE MODEL OF THE FIBERS

In Reference [6] is already shown, that the derivation of a viscoelastic material model for fibers from a three-dimensional constitutive model for isotropic materials is successful. Therefore, we derive a fiber viscoelasticity formulation from the constitutive model of the matrix material in Reference [3].

3.1 The free energy

The idea is based on the well-known multiplicative split of the deformation gradient in a viscous and an elastic product tensor. In the case of the fiber deformation, we assume

\[ F_F = F_F^e F_F^v \]  

with the fiber deformation gradients

\[ F_F := a_t \otimes a_0 \quad F_F^e := a_t \otimes \bar{a} \quad F_F^v := \bar{a} \otimes a_0 \]  

defined by the stretched fiber direction vector \( a_t \) in the tangent space \( T_x B_t \) at the current configuration \( B_t \), the fiber direction vector \( \bar{a} \) in the linear space \( \mathcal{Y}_F \) (‘intermediate fiber configuration’) and the unit direction vector \( a_0 \) with \( \| a_0 \| = 1 \) in the tangent space \( T_x B_0 \) at the initial configuration \( B_0 \) (see Figure 1). The symbol \( \otimes \) denotes the standard dyadic
tensor product. In principle, we assume a generalized Maxwell element with an elastic branch and a viscoelastic branch. In the case of large deformations, we therefore define the fiber free energy

\[ \Psi_F = \Psi_{F,\text{ela}} + \Psi_{F,\text{vis}} \] (17)

The elastic free energy depends on the squared fiber stretch \( \tilde{C}_F \), given by

\[ \tilde{C}_F := a_t \cdot a_t = a_0 F^T F a_0 = C a_0 \otimes a_0 = C A_0 = C_F : I \] (18)

with the structural tensor \( A_0 := a_0 \otimes a_0 \) of the fiber family, the right Cauchy-Green tensor \( C := F^T F \) of the body \( B_0 \), the unity metric tensor \( I \) with respect to \( B_0 \), and the right Cauchy-Green tensor

\[ C_F := F^T F = [C] A_0 \] (19)

of the fiber family. The superscript ‘\( T \)’ denotes the transposition of a second-order tensor. Hence, we define a free energy function \( \Psi_{F,\text{ela}} := \tilde{\Psi}_{F,\text{ela}} (\tilde{C}_F) \). The viscoelastic free energy depends on the elastic fiber stretch

\[ C_{F,\text{vis}} := C_F : \tilde{I} = [F_F]^T F_F : \tilde{I} = [F_F^u]^{-T} F_F F [F_F^u]^{-1} : \tilde{I} = [F_F^u]^{-T} C [F_F^u]^{-1} : \tilde{I} \] (20)

where \( \tilde{I} \) designates the unity metric tensor of the linear space \( \mathcal{V}_F \). By using the index notation of tensor products, we arrive at

\[ C_{F,\text{vis}} = C^T : [F_F^u]^{-1} [F_F^u]^{-T} = C^T : [C_F^u]^{-1} = C [C_F^u]^{-1} : I \] (21)
where the second-order tensor $C_F^{v}$ denotes the viscous right Cauchy-Green tensor

$$C_F^{v} = [C_F^{v}]^T F_F^{v} = [a_0 \otimes \bar{a}] \cdot [\bar{a} \otimes a_0] = [\bar{a} \cdot \bar{a}] A_0 =: C_F^{v} A_0$$  \hspace{1cm} (22)

The scalar-valued field $C_F^{v}$ denotes the new viscous internal variable of the fiber family. The inverse of the viscous right Cauchy-Green tensor of the fiber family is defined by

$$[C_F^{v}]^{-1} := [F_F^{v}]^{-1} [F_F^{v}]^{-T}$$  \hspace{1cm} (23)

where the inverse of the deformation gradient $F_F^{v}$ satisfies the relation

$$a_0 = [F_F^{v}]^{-1} \bar{a} =: \tilde{\lambda}_F [a_0 \otimes \bar{a}] \cdot \bar{a} = \tilde{\lambda}_F [\bar{a} \cdot \bar{a}] a_0 = \tilde{\lambda}_F C_F^{v} a_0$$  \hspace{1cm} (24)

Thus, the multiplier $\tilde{\lambda}_F$ denotes the inverse of the viscous internal variable, and Eq. (23) reads

$$[C_F^{v}]^{-1} = \frac{1}{(C_F^{v})^2} [a_0 \otimes \bar{a}] \cdot [\bar{a} \otimes a_0] = \frac{1}{(C_F^{v})^2} [a_0 \otimes a_0] C_F^{v} = \frac{1}{C_F^{v}} A_0$$  \hspace{1cm} (25)

Employing Eq. (25) in Eq. (21), we obtain the elastic fiber stretch

$$C_F^{v} = C \frac{1}{C_F^{v}} A_0 : I = [C : A_0] \frac{1}{C_F^{v}} = \tilde{C}_F$$  \hspace{1cm} (26)

Accordingly, we define the viscous free energy function $\Psi_F^{vis} := \Psi_F^{vis}(C_F^{v}) = \Psi_F^{ela}(\tilde{C}_F[C_F^{v}]^{-1})$, which means we apply the same free energy function as in the elastic branch, but with a different argument and generally different material constants (cf. Reference [7]).

### 3.2 The viscous dissipation and evolution equation

According to the Clausius-Plank inequality and the definition of the entropy, the viscous internal dissipation in the fibers is given by

$$D_F^{int} := \frac{1}{2} S_F \dot{C}_F - \dot{\Psi}_F^{ela} - \dot{\Psi}_F^{vis} = \frac{\dot{C}_F}{2 C_F} - \dot{\Psi}_F^{ela} - \dot{\Psi}_F^{vis} = M_F L_F - \dot{\Psi}_F^{ela} - \dot{\Psi}_F^{vis} \geq 0$$  \hspace{1cm} (27)

Here, we introduced the Mandel stress $M_F := \dot{\Psi}_F^{ela} S_F$, energy-conjugated to the fiber strain rate $L_F$. The time rate of the free energy pertaining to the elastic branch takes the form

$$\dot{\Psi}_F^{ela} = 2 \frac{\partial \Psi_F^{ela}}{\partial \dot{C}_F} \frac{\dot{C}_F}{2} = 2 \tilde{C}_F \frac{\partial \Psi_F^{ela}}{\partial \dot{C}_F} L_F =: M_F^{ela} L_F$$  \hspace{1cm} (28)

and the time rate of the free energy associated with the viscoelastic branch reads

$$\dot{\Psi}_F^{vis} = \frac{\partial \Psi_F^{vis}}{\partial C_F} \frac{\dot{C}_F}{C_F} = 2 C_F^{v} \frac{\partial \Psi_F^{vis}}{\partial C_F} \left[ \frac{\dot{C}_F}{2 C_F} - \frac{C_F^{v}}{2 C_F} \right] =: M_F^{vis} [L_F - L_F^{v}]$$  \hspace{1cm} (29)
Consequently, the viscous dissipation in the fibers are given by

\[ D_{\text{int}}^\text{vis} := [M_F - M_F^{\text{ela}} - M_F^{\text{vis}}] L_F + M_F^{\text{vis}} v_F \geq 0 \]  

(30)

The Clausius-Plank inequality can be fulfilled by setting

\[ M_F := M_F^{\text{ela}} + M_F^{\text{vis}} \]  

(31)

and by defining the viscous evolution equation

\[ M_F^{\text{vis}} \cdot \dot{C}_F^{\text{vis}} = \sum v_F \]  

(32)

as viscous driving force associated with the viscosity constant \( V_F > 0 \). The viscous fiber dissipation then takes the form \( D_{\text{vis}}^\text{vis} = V_F (\dot{L}_F^u)^2 \geq 0 \). Eq. (32) represents an ordinary differential equation for the viscous internal variable \( C_F^{\text{vis}} \), which reveals the equivalent form of the viscous fiber dissipation

\[ M_F^{\text{vis}} L_F^v = \frac{C_F}{C_F^{\text{vis}}} \frac{\partial \Psi_F^{\text{vis}}}{\partial C_F} \dot{C}_F^{\text{vis}} = - \frac{\partial \Psi_F^{\text{vis}}}{\partial C_F} \dot{C}_F^{\text{vis}} \quad \text{and} \quad V_F (\dot{L}_F^u)^2 = \frac{V_F}{(2 C_F^{\text{vis}})^2} \dot{C}_F^{\text{vis}} \dot{C}_F^{\text{vis}} \]  

(33)

By taking into account Eq. (33), the viscous evolution equation can be written as

\[ Y_F = \frac{V_F}{(2 C_F^{\text{vis}})^2} \dot{C}_F^{\text{vis}} \quad \text{with} \quad Y_F := - \frac{\partial \Psi_F^{\text{vis}}}{\partial C_F^{\text{vis}}} \]  

(34)

as non-equilibrium stress of the fiber family.

4 THE VISCOUS ALGORITHMIC FIBER STRESS

The energy-momentum time integration of the viscoelastic fiber formulation requires the exact fulfillment of the gradient theorem

\[ \Psi_F^{\text{vis}}_{t_{n+1}} - \Psi_F^{\text{vis}}_{t_n} = \int_{t_n}^{t_{n+1}} \dot{\Psi}_F^{\text{vis}} \, dt \equiv \int_0^{1} \frac{\Psi_F^{\text{vis}}}{\Psi_F^{\text{vis}}} \, d\alpha \]  

(35)

on each time step \([t_n, t_{n+1}]\), or on the normalized time interval \([0, 1]\), respectively (compare Reference [3]). We indicate by a superimposed \( \circ \) the derivative with respect to \( \alpha \in [0, 1] \). We satisfy this constraint by means of the algorithmic Mandel stress \( \bar{M}_F^{\text{vis}} \) in the external power of the variational formulation.

Remark 4.1 In Reference [3], the energy-momentum time integration of the viscous free energy of the matrix material is only based on the algorithmic elastic Mandel stress, which modifies the equations of motion only. This leads in the isothermal case to an unmodified viscous evolution equation of the matrix material. Motivated by References [8], in which the viscous evolution equation is modified by a discrete derivative, we here modify also the viscous Mandel stress of the fibers. In this way, the equations of motion as well as the viscous evolution equation are modified. Note that, in contrast to References [8], the modification in this paper is higher-order accurate, and not restricted to second-order accurate energy-momentum time integrations.
As described in detail in Reference [9], we determine the variational parameter field \( \bar{M}_F^v \) by using a separate constrained variational problem. Here, we define the Lagrange functional

\[
\mathcal{F}_F^v(\bar{M}_F^v, \mu_F^v) := \mu_F^v \mathcal{G}_F^v(\bar{M}_F^v) + \int_0^1 F_F^v(\bar{M}_F^v) \, d\alpha
\]

(36)

with the Lagrange multiplier \( \mu_F^v \) and the definitions

\[
F_F^v(\bar{M}_F^v) := \frac{(\bar{M}_F^v)^2}{2} \quad \text{and} \quad \mathcal{G}_F^v(\bar{M}_F^v) := \psi_{vis}^{F_{n+1}} - \psi_{vis}^{F_n} - \int_0^1 G_F^v(\bar{M}_F^v) \, d\alpha
\]

(37)

with the constraint function

\[
G_F^v(\bar{M}_F^v) := [M_{vis}^v + \bar{M}_F^v] [L_F^v - L_v^v]
\]

(38)

A functional minimization subject to the constraint \( \mathcal{G}_F^v = 0 \) leads to the Euler-Lagrange equations

\[
\frac{\delta \mathcal{F}_F^v}{\delta \bar{M}_F^v} = \mathcal{G}_F^v = 0
\]

(39)

These Euler-Lagrange equations lead to the algorithmic Mandel stress function

\[
\bar{M}_F^v := \mu_F^v [L_F^v - L_v^v]
\]

(40)

with the Lagrange multiplier

\[
\mu_F^v := \frac{\psi_{vis}^{F_{n+1}} - \psi_{vis}^{F_n} - \int_0^1 M_{vis}^v [L_F^v - L_v^v] \, d\alpha}{\int_0^1 [L_F^v - L_v^v]^2 \, d\alpha}
\]

(42)

Note that the Lagrange multiplier \( \mu_F^v \) depends on the material point \( \mathbf{X} \in \mathcal{B}_0 \), but not on the normalized time \( \alpha \in [0, 1] \).

5 THE WEAK FORMULATION

With the following exceptions, the weak formulation in Reference [3] applies also in this paper by taking into account the internal dissipation in Eq. (12) and the free energy in Eq. (17). First, in this paper, we obtain the weak equation of motion

\[
\int_{t_{n+1}}^{t_n} \int_{\mathcal{B}_0} \delta \varphi \cdot [\dot{\mathbf{p}} - \rho_0 \mathbf{B}] \, dV \, d\alpha + \int_{t_{n+1}}^{t_n} \int_{\mathcal{B}_0} \mathbf{P} : \nabla (\delta \varphi) \, dV \, dt
\]

(43)
where the weak stress power term is formulated with the independent first Piola-Kirchhoff stress tensor. Second, the fiber stress equation includes the algorithmic viscous Mandel stress, so that we arrive at the weak form

$$\int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} \delta_s \dot{C}_F \left[ 2 \frac{\partial \Psi_F}{\partial C_F} + \tilde{S}_F + \frac{\bar{M}_F^v}{C_F} - S_F \right] dV dt = 0$$  \hspace{1cm} (44)$$

where the algorithmic fiber stress $\tilde{S}_F$ fulfills the gradient theorem with respect to $\psi_{ela}^F$ (see Reference [3]). As we introduce the deformation gradient and the first Piola-Kirchhoff stress tensor as independent fields, we obtain the additional weak forms

$$\int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} \delta_s \dot{\mathbf{F}} : \left[ \dot{\mathbf{F}} - \nabla \dot{\varphi} \right] dV dt = 0 \quad 0 = \int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} \delta_s \dot{\mathbf{F}} : \left[ \bar{\mathbf{P}} \mathbf{S} - \mathbf{P} \right] dV dt$$  \hspace{1cm} (45)$$

Finally, we obtain the weak form of the new viscous evolution equation of the fiber family, given by

$$\int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} \delta_s \dot{C}^v_F \left[ -Y_F - \frac{\bar{M}_F^v}{2 C_F^v} + \frac{V_F}{2 C_F^v} L^v_F \right] dV dt = 0$$  \hspace{1cm} (46)$$

Note that a further advantage of the existence of the additional algorithmic stress $\bar{M}_F^v$ besides the algorithmic stress $\tilde{S}_F$ is, that each free energy part of the fiber family possesses its own algorithmic modification. Hence, neglecting one part of the fiber free energy allows for the neglect of the corresponding algorithmic stress term.

### 6 THE DISCRETE VISCOUS EVOLUTION EQUATION OF THE FIBERS

Usually, viscous evolution equations are solved at each Gaussian quadrature point in space, because the missing boundary conditions suggests to solve a viscous evolution equation pointwise as initial boundary value problem. But, due to the derivation of the viscous evolution equation as additional weak form in Eq. (46), it is also possible to solve the viscous evolution equation of the fibers as elementwise field equation, analogous to the fiber stress equation in Eq. (44). In this way, we obtain one matrix differential equation in time for each finite element, instead one scalar differential equation for each Gaussian quadrature point of a finite element. For higher order finite elements with many Gaussian quadrature points, this can be more efficient. Hence, the discretization of the viscous fiber evolution equation, in this paper, is distinct from the matrix evolution equation in Reference [3] in two ways:

1. the existence of an algorithmic stress in the viscous evolution equation,
2. the solution procedure by using spatially discretized discrete equations.

We discretize the viscous evolution equation in Eq. (46) on the parent domain $\mathcal{B}_0$ associated with each finite element in space as well as with respect to the normalized time.
\( \alpha \in [0, 1] \) on each time step \([t_n, t_{n+1}]\) with the time step size \( h_n = t_{n+1} - t_n \) in time. Hence, we discretize the weak form

\[
\int_0^1 \int_{\mathcal{B}} \delta_x \frac{\partial}{\partial x} C_F^v \left[ -Y_F - \frac{\dot{M}_F^v}{2 C_F^v} + \frac{V_F}{2 C_F^v} L_F^v \right] \mathrm{d}V \mathrm{d}\alpha = 0
\]

(47)

with the viscous strain rate

\[
L_F^v = \frac{C_F^v}{2 h_n C_F^v}
\]

(48)

As we aim at a higher-order accurate space-time approximation, we employ for the test function the Galerkin approximation

\[
\delta_x \left( \frac{\partial}{\partial x} C_F^v \right)(\chi, \alpha) = \sum_{J=1}^{k} \sum_{B=1}^{\tilde{n}_{node}} \tilde{M}_J(\alpha) \tilde{N}_B(\chi) \left[ \frac{\partial}{\partial x} C_F^v \right]_{J}^B = \left( \tilde{c}(\alpha) \otimes \tilde{N}(\chi) \right)^T \tilde{C}_F^v
\]

(49)

where \( \tilde{M}_J(\alpha) \) denotes a one-dimensional Lagrange polynomial of degree \( k - 1 \) with respect to \( \alpha \) (see Reference [3]), and \( \tilde{N}_B(\chi) \) the standard spatial shape functions with respect to the considered spatial parent domain (tetrahedral or hexahedral finite elements, for instance). In a matrix notation, we combine these temporal shape functions in the column vector \( \tilde{c}(\alpha) \), and the spatial shape functions in the column vector \( \tilde{N}(\chi) \). The nodal values of the variations of the internal variable field are combined in the column vector \( \tilde{C}_F^v \). Thereby, the symbol \( \otimes \) denotes the standard Kronecker matrix product, and the superscript \( 'T' \) the transposition of a matrix. The temporally continuous viscous internal variable field is then approximated by

\[
C_F^v(\chi, \alpha) = \sum_{I=1}^{\tilde{n}_{node}} \sum_{A=1}^{k+1} M^I(\alpha) \tilde{N}_A(\chi) \left[ C_F^v \right]^A_I = \left( \tilde{c}(\alpha) \otimes \tilde{N}(\chi) \right)^T \tilde{C}_F^v + \left[ M^I(\alpha) \otimes \tilde{N}(\chi) \right] \tilde{c}_F^v
\]

(50)

The polynomials \( M^I(\alpha) \) denote the one-dimensional Lagrange polynomials of degree \( k \) with respect to \( \alpha \) (see also Reference [3]). In the matrix notation, the unknown nodal values of the internal variable field are then included in the column vector \( \tilde{C}_F^v \), and the prescribed initial values in the column vector \( \tilde{c}_F^v \). The \( k \) polynomials \( M^I(\alpha), I = 2, \ldots, k+1 \), are combined in the column vector \( \tilde{c}(\alpha) \). Employing Eqs. (49) and (50) in the weak form in Eq. (47), we arrive at the matrix equation

\[
\mathbf{Y}^{\text{mat}} + \mathbf{Y}^{\text{alg}} = \mathbf{\Sigma}
\]

(51)

The material stress vector \( \mathbf{Y}^{\text{mat}} \) includes the viscous non-equilibrium stress, derived from the viscous free energy. The algorithmic stress vector \( \mathbf{Y}^{\text{alg}} \) includes the algorithmic Mandel stress \( \tilde{M}_F^v \), and the viscous driving force \( \mathbf{\Sigma} \) the viscosity constant \( V_F \) and the viscous strain rate \( L_F^v \). For variational consistency, we apply exactly \( k \) Gauss points in time (see [3, 9]).
7 THE NUMERICAL EXAMPLE

As numerical examples, we consider examples from References [3, 9] for a direct comparison. These include a fiber-reinforced turbine rotor, whose mesh is derived from Reference [10]. In the numerical examples, we demonstrate the above introduced Dirichlet and Neumann boundary conditions as well as the obtained energy-momentum consistency.

REFERENCES


NON-LINEAR FINITE ELEMENT MODELLING OF LIGHT-TO-HEAT ENERGY CONVERSION APPLIED TO NANOENCAPSULATED PHASE CHANGE MATERIALS

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Key words: Finite Element Method, Multiphysics Problems, Thermoelasticity, Phase Change, Joule heating

Abstract. In nature, physical phenomena tend to exhibit their effects simultaneously and, depending on the situation of study, their interactions cannot be neglected. For instance, nanofluids, which are composed of both fluid and nanosolids, are currently used for thermal energy storage in concentrated solar power plants and couple thermal and mechanical fields. Notice that owing to some limitations of solar collectors, fluids combined with nanoparticles are under research currently to absorb solar energy by light-to-heat conversion of energy. On this ground, the aim of the present work is to develop a numerical formulation within the finite element method (FEM) to study the light-to-heat energy conversion, phase-change and thermal stresses in nanosolids. For this purpose and in a first and good approximation, it is assumed that the light is converted into heat by the Joule heating—a non-linear term which quadratically depends on the electric field. Therefore, the set of three coupled governing equations is composed of: balance of linear momentum for the mechanical field, balance of energy for the thermal field and balance of electric current for the electric field. These equations are rewritten in a weak form, which is more amenable in the context of the FEM, and they are implemented in a numerical code. Finally, several benchmarks are presented to validate the numerical results against analytical solutions developed by the authors.

1 INTRODUCTION

The rapid development of societies nowadays increases more and more the consumption of energy around the world. In order to fight against the consequences of climate change, renewable energies are growing in importance. Among the different types of renewable
energies, solar energy and more specifically solar thermal energy are of special interest [1]. A main application of solar thermal energy is concentrated solar power (CSP) plants [2], where phase change materials (PCMs) are combined with heat transfer fluids (HTF) to enhance both sensible and latent energy storage. In order to improve the efficiency of these systems, the addition of nanoencapsulated phase change materials (nePCMs) is currently under research [3, 4]. The combination of nanoparticles with a fluid is known as nanofluid [5].

Due to the limitations that solar collectors present such as corrosion, considerable heat losses and limitations on the incident flux, fluids mixed with nanoparticles are under research instead to absorb directly the solar energy [6]. This combination of liquids with nanoparticles is also known as solar nanofluids [7].

Currently, to the best of the author’s knowledge, a solar nanofluid containing nePCMs has not been attempted by the experimental community due to the fact that the increase in temperature achieved by solar radiation is not sufficient to melt the core of nePCMs. However, the aim of this work is to provide a general numerical framework to analyse the behaviour of a generic nanoparticle by including thermomechanical phase change with light-to-heat conversion. In particular, this work presents a numerical formulation within the finite element (FE) method [8]. Previously, a consistent thermodynamic approach is performed to obtain the set of three-dimensional governing equations. Then, these equations are discretised by following FE standard procedures and implemented in the research code FEAP [9], which belongs to the University of California at Berkeley (USA). In order to validate the code, numerical solutions are compared with analytical ones developed by the authors.

Table 1 summarizes the mathematical notation used through the present work.

2 GOVERNING EQUATIONS

Three coupled partial differential equations are required to describe light-to-heat conversion in nePCMs. These equations are often called governing equations and are composed of balance equations and of boundary conditions.

2.1 Balance equations

Consider a general domain of study Ω, boundary ∂Ω and outward normal n containing solid and liquid phases. Four balance equations must be considered: linear and angular momentum balances, energy balance and electric charge balance for the whole domain.

2.1.1 Mechanical balance

The strong form of the linear momentum balance reads:

$$\rho \dot{u} = \nabla \cdot \sigma + f$$  \hspace{1cm} (1)

Table 1 summarizes the mathematical notation used through the present work.
Table 1: Notation.

<table>
<thead>
<tr>
<th>Mathematical operators</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\dot{}())</td>
<td>First time derivative</td>
</tr>
<tr>
<td>(\ddot{}())</td>
<td>Second time derivative</td>
</tr>
<tr>
<td>(())</td>
<td>First order tensor</td>
</tr>
<tr>
<td>(\underbrace{()}_2)</td>
<td>Second order tensor</td>
</tr>
<tr>
<td>(\underbrace{()}_4)</td>
<td>Fourth order tensor</td>
</tr>
<tr>
<td>(()^T)</td>
<td>Transpose</td>
</tr>
<tr>
<td>(\text{tr}())</td>
<td>Trace</td>
</tr>
<tr>
<td>((()\cdot()))</td>
<td>Dot product</td>
</tr>
<tr>
<td>((()\cdot()\cdot()))</td>
<td>Double contraction product</td>
</tr>
<tr>
<td>((()\otimes()))</td>
<td>Tensor product</td>
</tr>
</tbody>
</table>

where \(\rho, \ddot{u}, \sigma, f\) denote mass density, acceleration, Cauchy stress tensor and body force vector, respectively. The stress tensor is related to the traction vector \(t\) by the Cauchy relation: \(t = \sigma \cdot n\). The Cartesian components of the displacement vector are defined as \(u = (u, v, w)\).

Secondly, the angular momentum balance is automatically satisfied by the symmetry of the Cauchy stress tensor: \(\sigma = \sigma^T\).

### 2.1.2 Energy balance

The energy balance is written in the present work in terms of enthalpy, which is defined as:

\[
H = \int_{T_{ref}}^{T} \rho c \, d\theta + \rho L h (T - T_m) \tag{2}
\]

where \(c, L\) denote heat capacity and latent heat, respectively. The variable \(T\) represents temperature and \(T_{ref}\) and \(T_m\) denote reference temperature at which enthalpy is calculated and melting temperature, respectively. Finally, \(h (T - T_m)\) is the Heaviside step function, which is defined as follows:

\[
h (T - T_m) = \begin{cases} 
0 & \text{if } T < T_m \\
1 & \text{if } T > T_m
\end{cases} \tag{3}
\]
According to the previous definitions, the local form of eq. (2) becomes:

\[
\frac{dH}{dt} + \nabla H \cdot \dot{u} = -\nabla \cdot q + j \cdot E
\]  

(4)

where \( \dot{u}, q, j \) and \( E \) denote velocity, heat flux vector, electric flux vector and electric field, respectively. The last term in eq. (4) represents the contribution of Joule heating.

Notice that the phase change problem considered within the energy balance in the present work is that of pure substances. More specifically, the algorithm used in the present work to solve phase change numerically is the enthalpy method reported in [10].

2.1.3 Electric charge balance

The strong form of the electric charge balance may be expressed as:

\[
\frac{d\rho_f^q}{dt} = -\nabla \cdot j
\]

(5)

where \( \rho_f^q \) denotes the free electric charge.

Notice that a source/sink term does not exist in eq. (5) due to the fact that electric charge is neither created nor destroyed [11].

2.2 Constitutive equations

Constitutive equations describe the behaviour of the media contained in the domain of study.

2.2.1 Thermomechanical constitution

The constitutive equation of the solid phase that relates strain, temperature and stress is:

\[
\sigma_s = C : \varepsilon - \beta (T - T_{ref})
\]  

(6)

where \( C, \varepsilon \) and \( \beta \) denote the fourth-order elastic tensor, the infinitesimal strain tensor and the second order thermoelastic tensor, respectively.

Tensors \( C \) and \( \beta \) are defined as follows:

\[
C = \lambda I \otimes I + 2\mu I^{sy}
\]

\[
\beta = (3\lambda + 2\mu) \alpha I
\]

(7)

where \( I, I^{sy} \) denote second and symmetric part fourth order identity tensors, respectively [12]. In turn, \( \alpha, \lambda \) and \( \mu \) denote the coefficient of thermal expansion and Lamé parameters, respectively. Lamé parameters are defined as:
\[
\lambda = \frac{E\nu}{(1 + \nu)(1 - 2\nu)}, \quad \mu = \frac{E}{2(1 + \nu)}
\]  
(8)

where \( E \) and \( \nu \) represent Young’s modulus and Poisson’s ratio, respectively.

The constitutive equation for a static fluid phase is:

\[
\sigma_l = p I
\]  
(9)

where \( p \) is the thermodynamic pressure of the fluid. In the present work, as an approximation, the liquid phase is assimilated to a fluid at rest given that the liquid volume inside the nanoparticles (at the order of nanometers) is reduced and consequently, dynamic effects can be neglected. Therefore, the pressure in the fluid can be computed as the spherical part of the stress tensor in the solid phase:

\[
p = \frac{1}{3} \text{tr} \left( \sigma_s \right)
\]  
(10)

2.2.2 Heat conduction

The relation between heat flux and temperature is:

\[
q = -\kappa \cdot \nabla T
\]  
(11)

where \( \kappa \) denotes the thermal conductivity tensor.

2.2.3 Electricity conduction

The relation between electric flux and electric field is:

\[
j = \gamma \cdot E
\]  
(12)

where \( \gamma \) denotes the electric conductivity tensor.

2.3 Boundary conditions

The boundary conditions are composed of Dirichlet (also known as first-type) or Neumann (second-type) expressions:

\[
\begin{align*}
\text{Dirichlet} & \quad u = \bar{u} \quad T = \bar{T} \quad V = \bar{V} \\
\text{Neumann} & \quad \sigma \cdot n = \bar{t} \quad q \cdot n = \bar{q} \quad j \cdot n = \bar{j}
\end{align*}
\]  
(13)

where \( \bar{u}, \bar{T}, \bar{q}, \bar{V} \) and \( \bar{j} \) are the prescribed displacements, temperature, traction, thermal flux, voltage and electric flux, respectively. The variable \( V \) represents voltage.

Finally, these governing equations are written in weak forms and discretised to be implemented in the numerical code FEAP.
3 NUMERICAL BENCHMARKS

In this section, several validations of the formulation are performed by comparing numerical and analytical solutions developed by the authors. For the validations, it is assumed that the variation of free electric charge with time is negligible. Material properties of tin (Sn) are considered; see [10] for further detail.

Two different cases are studied to validate the numerical implementation. In case I, a thermomechanical problem with phase change is defined while in case II, a steady state problem of electro-thermoelasticity without phase change is the object of study.

3.1 Case I

An analytical solution is developed for a one-dimensional half-space domain, with a time-dependent temperature prescribed at its free end. The domain is traction free. More detail about the analytical solution is given in [10].

In this case, for the validations, prescribed and initial temperatures are respectively: \( T_0 = 583 \text{ K} \) (above melting temperature \( T_m = 504.95 \text{ K} \)), \( T_i = 323 \text{ K} \).

![Figure 1: Comparison of analytical and numerical temperature distributions (left) and axial displacement (right) for three different times along the one-dimensional geometry.](image)

For these numerical simulations, 200 elements are used. Eight-noded brick elements with standard shape functions of Lagrange-type are used to interpolate the results. The maximum relative error is lower than 1% between analytical and numerical solutions of temperature and lower than 4% between those of displacement. Notice that the validation of the axial displacement in Figure 1 is only done for the solid phase.
3.2 Case II

An analytical solution is developed for a one-dimensional body for a steady state study. In this case, voltage and temperature values (below the melting temperature $T_m = 504.95$ K) are prescribed at both ends of the one-dimensional geometry. The body is traction free and one of the ends is mechanically fixed ($v_1 = 0$).

In this case, for the validations, prescribed values of temperature and voltage are respectively: $T_1 = 303$ K, $T_2 = 353$ K, $V_1 = 0$ V, $V_2 = 0.1$ V. Subscripts 1 and 2 refer to left and right ends of the one-dimensional geometry, respectively.

![Graphs showing analytical and numerical distributions of voltage, temperature, and axial displacement along the one-dimensional geometry.](image)

Figure 2: Comparison of analytical and numerical voltage distribution (left, upper row), temperature distribution (right, upper row) and axial displacement (lower row) along the one-dimensional geometry.
For these numerical simulations, 200 elements are used. Eight-noded brick elements with standard shape functions of Lagrange-type are used to interpolate the results. The maximum relative error is lower than 0.1% between analytical and numerical solutions for the three magnitudes shown in Figure 2.

4 CONCLUSIONS

In this work, a FE formulation is proposed to deal with thermoelasticity with light-to-heat energy conversion. By comparing numerical and analytical solutions, it can be observed that a good agreement exists between both results. Therefore, the numerical model is validated and could be a useful tool to conduct multiphysics numerical analysis or predicting the stresses developed in nePCMs.

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REFERENCES


THERMO-MECHANICAL COUPLING IN FIBER-REINFORCED CONTINUA: MIXED FINITE ELEMENT FORMULATIONS AND ENERGY-MOMENTUM TIME INTEGRATION

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Key words: Mixed finite element method, higher-order energy-momentum scheme, fiber-reinforced material, polyconvex strain energy function, anisotropic thermoelasticity

Abstract. Our research activity is motivated by accurate dynamic simulations of fiber-reinforced materials in light-weight structures. In order to accomplish this, we have to take various steps. The material behavior is formulated with an anisotropic, polyconvex strain energy function. We combine different mixed element formulations (e.g. see Reference [2] or [3]) with a Galerkin time integrator as shown in Reference [5]. This reduces the volumetric locking effect of an incompressible matrix material as well as the locking effect due to stiff fibers. In addition, we increase the accuracy by using Galerkin-based higher-order time integrators. Since in long-term simulations a high energy error is a strong problem, we apply the mixed finite element formulations to an energy-momentum time integration scheme (see Reference [6]). In the next step, we extend the material formulation by adding a thermo-mechanical coupling as shown in Reference [7]. Here we also describe the directional heat conduction of the fiber. As numerical examples with multiple material domains and families of fibers serve cooks cantilever beam as in Reference [5]. The Dirichlet boundary conditions are modelled by the Lagrange-multiplier method (see Reference [7]) and as Neumann boundary condition a pressure distribution is used.

1 INTRODUCTION

The accurate dynamic simulation of fiber-reinforced materials in light-weight structures plays an increasing role. Meanwhile these materials are used in many areas such as
aircrafts, automobiles and wind power plants. In addition to the low density and the high modulus of elasticity, the thermal properties also play a crucial role. For example the low thermal expansion of the matrix part, as well as the possibility to conduct the heat directionally with the fibers. Therefore, in this paper, we present the dynamic behavior of a thermoelastic anisotropic continuum, where the different fibers and the matrix part have different thermal parameters.

By using the mentioned materials, we have on the one hand volumetric locking effects of an incompressible matrix material and on the other hand, locking effects due to stiff fibers. A first formulation that prevents volumetric locking successfully is described in Reference [1]. Here, the volumetric dilatation is approximated independently from the deformation gradient. Furthermore, this formulation was improved again in Reference [2] by approximating the cofactor also as an independent field. A possibility to overcome the locking of the fiber is shown in Reference [3]. Here an independent approximation of the right Cauchy-Green tensor for the anisotropic part of the strain energy function is done. In Reference [5] this method is reformulated in the fourth invariant and another field for the fifth invariant is introduced. In addition, the invariant method can also be represented in tensors, but the results for both methods are the same (see Reference [5]). The tensor variant has the advantage to use several fibers without further implementation effort for the element formulation.

In order to perform exact dynamic simulations and therefore to enable long-term simulations, it is necessary to provide higher-order time integrators. Thereby Galerkin-based higher-order time integrators are a good option. In addition, a high energy error is a strong problem and so we have to apply energy-momentum time integration schemes (see Reference [6]).

It is only logical to combine these methods and thus to combine the advantages of these methods. On the basis of Reference [7], we combine the Hu-Washizu functionals shown in Reference [5] with the mixed principle of virtual power and thus obtain a thermo-mechanical formulation for the various mixed elements and a Galerkin-based higher-order time integrators. Here, the Dirichlet boundary conditions are modelled by the Lagrange-multiplier method and a Neumann boundary condition in the form of a pressure distribution will also be provided. In addition, we extend the continuum in such a way, that we can model different families of fibers and directional heat conduction of the fibers.

In the current paper, we first define the continuum model and the finite element formulation. Then, with the help of the mixed principle of virtual power, we obtain the weak forms. Finally, we make various numerical studies on cook’s cantilever beam. Here we can show the excellent convergence behaviour of the mixed elements and the positive effect on the computational time. In addition, the advantages of using different fibres in the same continuum can be demonstrated, as their different properties can be used more purposefully.
2 CONTINUUM MODEL

As continuum model, we consider an anisotropic material with \( n_F \) fiber directions \( a_0^i \), moving in the Euclidean space \( \mathbb{R}^{n_{\text{dim}}} \) with the constant ambient temperature \( \Theta_\infty \). With the structural tensor \( M_i = a_0^i \otimes a_0^i \), the right Cauchy-Green tensor \( C = F^T F \) and the absolute temperature \( \Theta \), we define the strain energy function, which is split into a single matrix part \( \Psi_M \) and multiple fiber parts \( \Psi_{F_i} \), given by

\[
\Psi(C, \Theta, M) = \Psi_M(C, \Theta) + \sum_{i=1}^{n_F} \Psi_{F_i}(C, \Theta, M_i) \tag{1}
\]

By taking into account \( J = \det[F] = \sqrt{\det[C]} \), we assume the specific dependencies

\[
\Psi_M(C, \text{cof}[C], J, \Theta) = \Psi_{\text{iso}}^M(C, \text{cof}[C], J) + \Psi_{\text{vol}}^M(J) + \Psi_{\text{cap}}^M(\Theta) + \Psi_{\text{coup}}^M(\Theta, J) \tag{2}
\]

\[
\Psi_{F_i}(C, \text{cof}[C], J, \Theta, M_i) = \Psi_{\text{ela}}^{F_i}(C, \text{cof}[C], J, M_i) + \Psi_{\text{cap}}^{F_i}(\Theta) + \Psi_{\text{coup}}^{F_i}(\Theta, C, M_i) \tag{3}
\]

The elastic part of the matrix part \( \Psi_M \) is split into an isochoric part \( \Psi_{\text{iso}}^M \) and a volumetric part \( \Psi_{\text{vol}}^M \). The thermo-elastic free energy of the matrix is subdivided into a heat capacity part \( \Psi_{\text{cap}}^M \), and the part of the thermo-mechanical coupling effect, which takes the form

\[
\Psi_{\text{coup}}^M(\Theta, J) = -2n_{\text{dim}}\beta_M(\Theta - \Theta_\infty)J \frac{\partial \Psi_{\text{vol}}^M(J)}{\partial J}, \tag{4}
\]

where \( \beta_M \) ist the coefficient of linear thermal expansion for the matrix part. For the fibres, the thermal part is separated in the same way. We assume heat capacity parts \( \Psi_{\text{cap}}^{F_i} \) as well as parts of the thermo-mechanical coupling

\[
\Psi_{\text{coup}}^{F_i}(\Theta, C, M_i) = -2\beta_{F_i}(\Theta - \Theta_\infty)\sqrt{I_4} \frac{\partial \Psi_{\text{ela}}^{F_i}(I_4, \ldots)}{\partial I_4}, \tag{5}
\]

with the fourth invariant \( I_4(C, M_i) = \text{tr}[CM_i] \) and the coefficients of linear thermal expansion for the fiber parts \( \beta_{F_i} \).

3 FINITE ELEMENT FORMULATION

For the formulation of finite element discretizations in space, we use Hu-Washizu functionals \( \Pi_{HW} \). With the assumed temperature field \( \tilde{\Theta} \) and the entropy density field \( \eta \) as the corresponding Lagrange multiplier, the complete functional of the internal energy is

\[
\Pi^\text{int} = \Pi_{HW} + \int_{B_0} \eta(\Theta - \tilde{\Theta})dV \tag{6}
\]

The functional of the standard displacement element reads

\[
\Pi_{HW}^D(q, \Theta) = \int_{B_0} \Psi(C(q), \Theta, M)dV \tag{7}
\]
The introduction of an independent variable for the volumetric dilatation \( \tilde{\Psi} \), we arrive at the hydrostatic pressure. The corresponding functional takes the form

\[
\Pi_{HW}^D(q, \Theta, \tilde{J}, \tilde{p}) = \Pi_{HW}^D + \int B_0 \tilde{p} (J(q) - \tilde{J})dV \quad \text{with} \quad \tilde{p} = 1.5e6
\]  

(8)

With the introduction of an independent variable for \( \tilde{\Psi} \), we obtain the displacement-pressure element introduced by Simo et al. in [1]. Here, the corresponding Lagrange multiplier \( \tilde{p} \) plays the role of the hydrostatic pressure. The corresponding functional takes the form

\[
\Psi_M(\ldots) = \Psi_{iso}^M(C, \text{cof}[C], \tilde{J}) + \Psi_{vol}^M(\tilde{J}) + \Psi_{cap}^M(\Theta, \tilde{J}) + \Psi_{cap}^{cup}(\Theta, \tilde{J})
\]

(9)

\[
\Psi_F(\ldots) = \Psi_{ela}^F(C, \text{cof}[C], \tilde{J}, M_i) + \Psi_{cap}^F(\Theta) + \Psi_{cap}^{cup}(\Theta, C, M_i)
\]

(10)

A third functional is shown in Reference [2]. Here an additional field for the cofactor of \( C \) is introduced, such that we arrive at the functional

\[
\Pi_{HW}^{CoFEM}(q, \Theta, \ldots, H, B) = \Pi_{HW}^D + \int B_0 (\text{cof}[C(q)] - H)dV \quad \text{with} \quad \text{cof}[C(q)] - H
\]

(11)

\[
\Psi_M(\ldots) = \Psi_{iso}^M(C, H, \tilde{J}) + \Psi_{vol}^M(\tilde{J}) + \Psi_{cap}^M(\Theta) + \Psi_{cap}^{cup}(\Theta, \tilde{J})
\]

(12)

\[
\Psi_F(\ldots) = \Psi_{ela}^F(C, H, \tilde{J}, M_i) + \Psi_{cap}^F(\Theta) + \Psi_{cap}^{cup}(\Theta, C, M_i)
\]

(13)

Especially for anisotropic material formulations another element (called SKA element) is presented in Reference [3]. This introduces an additional field \( C_A \) for the anisotropic part \( \Psi_{ani}^M \) of the material formulation. The anisotropic part of the stress tensor is represented by the corresponding Lagrange multiplier \( S_A \). Here, we arrive at

\[
\Pi_{HW}^{CoSKA}(q, \Theta, \ldots, C_A, S_A) = \Pi_{HW}^{CoFEM} + \int B_0 \frac{1}{2} S_A : (C - C_A)dV \quad \text{with} \quad \text{cof}[C(q)] - H
\]

(14)

\[
\Psi_M(\ldots) = \Psi_{iso}^M(C, \text{cof}[C], \tilde{J}) + \Psi_{vol}^M(\tilde{J}) + \Psi_{cap}^M(\Theta) + \Psi_{cap}^{cup}(\Theta, \tilde{J})
\]

(15)

\[
\Psi_F(\ldots) = \Psi_{ela}^F(C_A, \text{cof}[C_A], \sqrt{\text{det}[C_A]}, M_i) + \Psi_{cap}^F(\Theta) + \Psi_{cap}^{cup}(\Theta, C_A, M_i)
\]

(16)
At last we add the additional fields $H_A$ and $\tilde{J}_A$ and the corresponding Lagrange multipliers $B_A$ and $\tilde{p}_A$ we get the CoCoA element as shown in Reference [5]

$$\Pi^{\text{CoCoA}}_{HW}(q, \ldots) = \Pi^{\text{CoSKA}}_{HW} + \int_{B_0} B_A : (\text{cof}[C] - H_A) dV + \int_{B_0} \tilde{p}_A (J - \tilde{J}_A) dV \quad \text{with (17)}$$

$$\Psi_M(\ldots) = \Psi_M^{\text{iso}}(C, H, \tilde{J}) + \Psi_M^{\text{cap}}(\Theta) + \Psi_M^{\text{coup}}(\Theta, \tilde{J}) \quad (18)$$

$$\Psi_{F_i}(\ldots) = \Psi_{F_i}^{\text{la}}(C_A, H_A, \tilde{J}_A, M_i) + \Psi_{F_i}^{\text{cap}}(\Theta) + \Psi_{F_i}^{\text{coup}}(\Theta, C_A, M_i) \quad (19)$$

Now, we apply the mixed principle of virtual power in Reference [7]. In this way, we can extend this formulation to dynamic problems. The basis is the total energy balance

$$\dot{T}(\dot{q}, \dot{v}, \dot{p}) + \dot{\Pi}^{\text{ext}}(\dot{q}, \dot{\lambda}, \tilde{\Theta}) + \dot{\Pi}^{\text{int}}(\dot{q}, \dot{\theta}, \dot{\Theta}, S_A, C_A, \tilde{p}, \dot{J}, B, \dot{H}, \tilde{p}_A, \dot{J}_A, B_A, \dot{H}_A) = 0 \quad (20)$$

where the time derivative of the kinetic energy

$$\dot{T}(\dot{q}, \dot{v}, \dot{p}) = \int_{B_0} (\rho_0 v - p) \cdot \dot{v} dV + \int_{B_0} \dot{\tilde{p}} \cdot (\dot{q} - v) dV + \int_{B_0} p \cdot \dot{q} dV \quad (21)$$

is defined by the velocity $v$, the linear momentum $p$ and the mass density $\rho_0$. As external power functional, we assume

$$\dot{\Pi}^{\text{ext}}(\dot{q}, \lambda, \tilde{\Theta}) = -\int_{\partial B_0} t \cdot \dot{q} dA - \int_{\partial B_0} \lambda \cdot (\dot{q} - \dot{q}^{\text{ref}}) dA + \int_{B_0} \frac{1}{\Theta} \nabla \tilde{\Theta} \cdot Q dV. \quad (22)$$

Here, Dirichlet boundary conditions are modelled by Lagrange multipliers $\lambda$. $\dot{q}^{\text{ref}}$ denotes the time evolution of Dirichlet boundary displacement vector, $t$ denotes the traction load.
for the Neumann boundary conditions and
\[
Q = - \left[ \sum_{i=1}^{np} J^i \frac{k_F - k_m}{C : M_i} M_i + kJC^{-1} \right] \nabla \Theta
\] (23)
denotes the Piola heat flux vector derived from Duhamel’s law (see Reference [7]). Here \(k_m\) and \(k_F\) denotes the material conductivity coefficients for matrix and fibers. By variation with respect to the variables in the argument from Eqn. 20 (as shown in Reference [7]), we get the following weak forms of the CoCoA element:

\[
\int_T \int_{\partial B_0} [\text{Div}[\mathbf{FS}] - \mathbf{p}] \cdot \delta \mathbf{q} \, dV \, dt = 0 \quad \int_T \int_{\partial B_0} \left[ \mathbf{p} - \mathbf{q} \right] \cdot \delta \mathbf{v} \, dV \, dt = 0
\]

\[
\int_T \int_{\partial B_0} [-\mathbf{t} - \mathbf{X}] \cdot \delta \mathbf{q} \, dA \, dt = 0 \quad \int_T \int_{\partial B_0} \left[ \mathbf{q} - \mathbf{q}^\text{ref}(t) \right] \cdot \delta \mathbf{x} \, dA \, dt = 0
\]

\[
\int_T \int_{B_0} \Theta \, \delta \mathbf{q} \, dV \, dt = 0 \quad \int_T \int_{B_0} \left[ \rho_0 - \mathbf{q} \right] \cdot \delta \mathbf{v} \, dV \, dt = 0
\]

\[
\int_T \int_{B_0} \left[ \frac{\text{Div}[Q]}{\Theta} + \dot{\mathbf{q}} \right] \delta \mathbf{v} \, dV \, dt = 0
\]

\[
\int_T \int_{B_0} \frac{1}{2} \left[ C_A - \dot{\mathbf{C}} \right] : \delta S_A \, dV \, dt = 0 \quad \int_T \int_{B_0} \left[ \frac{1}{2} S_A - \frac{\partial \Psi}{\partial C_A} \right] : \delta \mathbf{C}_A \, dV \, dt = 0
\]

\[
\int_T \int_{B_0} \left[ \dot{\mathbf{C}} - \dot{\mathbf{j}} \right] \delta \mathbf{p} \, dV \, dt = 0 \quad \int_T \int_{B_0} \left[ \dot{\mathbf{p}} - \frac{\partial \Psi}{\partial \mathbf{J}} \right] \delta \dot{\mathbf{j}} \, dV \, dt = 0
\]

\[
\int_T \int_{B_0} \left[ \dot{\mathbf{H}} - \text{cof}[\mathbf{C}] \right] : \delta \mathbf{B} \, dV \, dt = 0 \quad \int_T \int_{B_0} \left[ \mathbf{B} - \frac{\partial \Psi}{\partial \mathbf{H}} \right] : \delta \dot{\mathbf{H}} \, dV \, dt = 0
\]

\[
\int_T \int_{B_0} \left[ \dot{\mathbf{H}}_A - \text{cof}[\mathbf{C}] \right] : \delta \mathbf{B}_A \, dV \, dt = 0 \quad \int_T \int_{B_0} \left[ \mathbf{B}_A - \frac{\partial \Psi}{\partial \mathbf{H}_A} \right] : \delta \dot{\mathbf{H}}_A \, dV \, dt = 0
\]

As second Piola-Kirchhoff stress tensor, we obtain
\[
\mathbf{S} = 2 \frac{\partial \Psi}{\partial \mathbf{C}} + 2 \mathbf{B} : \frac{\partial \text{cof}[\mathbf{C}]}{\partial \mathbf{C}} + \dot{\mathbf{p}} J^{-1} \text{cof}[\mathbf{C}] + S_A + 2 \mathbf{B}_A : \frac{\partial \text{cof}[\mathbf{C}]}{\partial \mathbf{C}} + \dot{\mathbf{p}}_A J^{-1} \text{cof}[\mathbf{C}] \] (24)

All quantities are approximated with Lagrangian shape functions in space (see Reference [4, 7]) and time (see Reference [7]). All existing integrals are solved with the corresponding Gaussian quadrature rule. We eliminate \(\mathbf{p}\) and \(\eta\) and condense out the resulting formulation at the element level to a displacement and temperature formulation (see Reference [2]). Therefore, all mixed fields except \(\mathbf{q}\) and \(\Theta\) are discontinuous at the boundaries of spatial elements.
4 NUMERICAL EXAMPLES

As numerical example serves the well-known Cook’s cantilever beam with a quadratic distribution of an in-plane load on the Neumann boundary. Two different fibers are used for this example. On the one side a fiber \((F_1, (a_1^0)^T = [1 1 1])\) for mechanical reinforcement of the matrix, but with an equally low thermal conductivity. On the other side, a fiber \((F_2, (a_1^0)^T = [1 1 0])\) with a very high thermal conductivity, but a low stiffness. The energy functions are given by

\[
\Psi_{iso}^M = \frac{\epsilon_1}{2} (tr[C])^2 + \frac{\epsilon_2}{2} (tr[cof[C]])^2 - \epsilon_3 \ln(J) \\
\Psi_{vol}^M = \epsilon_4 \ln(J) \\
\Psi_{ela}^{F_1} = \epsilon_6 \left( \frac{1}{\epsilon_7 + 1} (tr[C M_1])^{\epsilon_7+1} + \frac{1}{\epsilon_8 + 1} (tr[cof[C] M_1])^{\epsilon_8+1} + \frac{1}{\epsilon_9} \det[C]^{-\epsilon_9} \right) \\
\Psi_{ela}^{F_2} = \frac{\epsilon_{10}}{2} (tr[C M_2] - 1)^2 \\
\Psi_{cap}^X = c_0^X (1 - \Theta_\infty) c_1^X (\Theta - \Theta_\infty - \Theta \ln \left( \frac{\Theta}{\Theta_\infty} \right)) - \frac{1}{2} c_0^X c_1^X (\Theta - \Theta_\infty)^2
\]

and the prescribed simulation parameters, shown in Tab. 1. Geometry, configuration and fiber direction \((a_1^0)^T = [1 1 1]\) of cooks cantilever beam are shown in Fig. 1. We compare the mixed finite elements up to cubic order and analyze the spatial convergence for some combinations of polynomial degrees in space of the independent quantities and the effect on the thermo-mechanical coupling. In the second step, we analyze the option of directional heat conduction using the fibers. The element title starts with H for hexahedral element and is followed by the element type and the information about the polynomial degrees of all quantities (see Table 2). Fig. 2 shows the convergence of the \(y\)-coordinate and the stress \(\sigma_{VM}\) of some elements. These element selection is based on the results from Reference [5] and is a selection of the best elements of each element type. They show the same behavior for the spatial convergence. CoCoA elements with a low polynomial degree for the quantities of the anisotropic part have the highest convergence rate, followed by the
CoFEM elements and the standard elements. Also, the HCoSKA1000 element represents a special case and has a very high convergence rate of the $y$-coordinate for a linear element. Nevertheless, you can see a strong oscillation in the convergence rate of $\sigma_{VM}$.

This also has a direct effect on the computing time. Fig. 3 shows the same curves over the computational time. The high convergence rate saves at least one order of magnitude in computational time, because coarse meshes are sufficient for accurate solutions in space. This plays all the more a role for thermo-mechanical systems, since here not only the degrees of freedom increase by a third, also the symmetry of the tangents matrix is lost.

Furthermore, Figs. 4, 5 and 6 show the deformed elements together with the v. Mises equivalence stress $\sigma_{VM}$ at different discretization levels. Here you can also see, that the CoCoA and SKA elements show a very good convergence and with $n_{el} = 256$ they provide nearly the same solution as with $n_{el} = 4000$. All elements show the asymmetric bending caused by the fiber as well as the typical stress curve (tensile and compressive stress, neutral fiber). Fig. 7 shows that the different solutions in the displacement have a corresponding effect on the thermo-mechanical coupling. While no temperature change can be seen in the standard elements, it is clearly visible for the mixed elements (especially on the Dirichlet boundary). However, it is not possible to say which solution is the optimal one, further tests have to be performed.

In the next step, we add the second fiber ($F_2$) and a linear start temperature distribution as shown in Fig. 9. Because of the high conductivity of the second fiber, the temperature in cook’s cantilever beam is distributed much faster (see Fig. 10).

At least we check the conservation properties on the example of the HSCoCoA210000 element with two fibers (see Fig. 8). For instance, the angular momentum ($\mathbf{L}$) is preserved, as the theory for Galerkin-based time integrators with Gaussian quadrature predicts. But, over the entire simulation period, we get a significant error in the energy ($E$). This was to be expected, because we do not use an energy momentum scheme to preserve the energy balance.

Figure 3: Convergence of the $y$-coordinate on point A and the v. Mises equivalence stress $\sigma_{VM}$ on point B for the parameters shown in Table 1 and fiber $F_1$. 
Figure 4: Deformed configuration $B_i$ and v. Mises equivalent stress $\sigma_{VM}$ for the parameters shown in Table 1 and fiber $F_1$ for $t = 1$. Cook's cantilever beam with $n_{el} = 32$ spatial finite elements.

Figure 5: Deformed configuration $B_i$ and v. Mises equivalent stress $\sigma_{VM}$ for the parameters shown in Table 1 and fiber $F_1$ for $t = 1$. Cook's cantilever beam with $n_{el} = 256$ spatial finite elements.

Figure 6: Deformed configuration $B_i$ and v. Mises equivalent stress $\sigma_{VM}$ for the parameters shown in Table 1 and fiber $F_1$ for $t = 1$. Cook's cantilever beam with $n_{el} = 4000$ spatial finite elements.
Figure 7: Deformed configuration $B_t$ and temperature $\Theta$ for the parameters shown in Table 1 and fiber $F_1$ for $t = 1$. Cook’s cantilever beam with $n_{el} = 4000$ spatial finite elements.

Figure 8: Conservation properties of the HSCoCoA210000 element for the parameters shown in Table 1 for $n_{el} = 256$ and fibers $F_1$ and $F_2$. 
Figure 9: Temperature distribution and fiber direction \((a_2^0)^T = [1 \ 1 \ 0]\) of cooks cantilever beam.

Figure 10: Deformed configuration \(B_t\) and temperature \(\Theta\) for the parameters shown in Figure 1 for \(n_\text{el} = 256\) and fibers \(F_1\) and \(F_2\) of Cook’s cantilever beam.
5 CONCLUSIONS

We were able to show that the excellent performance of the mixed elements is still preserved in a thermo-mechanical context. This especially has very good effects on the computing time. Furthermore we have the possibility to determine the mechanical and thermal properties of our model separately by using different fibers. In the next step, we extend this formulation to an energy conserving time integrator and implement thermal Dirichlet and Neumann boundary conditions.

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REFERENCES


THERMO-MECHANICALLY COUPLED FLUID STRUCTURE INTERACTION FOR THERMAL BUCKLING

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Abstract. Experiments have shown that aerothermodynamical loads on thin-walled structures lead under certain constraints to plastic deformation and buckling. The aim of the research is the accurate prediction of thermal buckling behaviour for metallic panels under the before mentioned conditions. In this article the material modelling for thermo-elastoplastic material behaviour is introduced which incorporates non-linear kinematic and isotropic hardening. As a non-linear temperature dependence of mechanical material parameters is included in the model, a special temperature and deformation dependence of the heat capacity is used. This material model is implemented as a user material in Abaqus and coupled with the fluid solver TAU. As the coupling tool for the fluid-structure interaction ifls is used. The results show the expected behaviour and the experimental results of displacement and temperature are reflected in the simulation.

1 INTRODUCTION

Experiments have shown that aerothermodynamical loads induced by high enthalpy flow on thin metallic panels in combination with unavoidable constrains for the movement of the structure might lead to undesirably localized plastic deformation and buckling phenomena. In the considered supersonic flow at Mach numbers of Ma = 7.62, the buckling of panels into the stream flow creates shocks and expansion areas which significantly impact the efficiency. In this work the fluid structure interaction between the panel and the flow are shown. The effects of the panel buckling on the flow is shown in Fig. 1. First investigations to thermal buckling were conducted in [12, 1]. The panel buckling is investigated experimentally in a wind tunnel for 120s, where deformation and temperature are measured over time [2]. The panel heats up due to aerothermodynamical loads, pushes against the surrounding frame and buckles into the flow.
An important part of the structural model is the description of the material behaviour. This requires a fully thermomechanical coupled viscoplastic model including large deformations [5]. Therefore a realistic description of the highly temperature- and rate-dependent material behaviour of the structure must be considered. Besides convection and heat radiation, the temperature dependence of the mechanical material behavior as well as the deformation dependence in conduction and capacity terms have to be included in the thermomechanical coupling. For that an extended thermomechanical model is used which takes non-linear thermal evolution into account [9]. This is achieved by defining material parameters which are nonlinearly dependent on the temperature [13, 8]. Therefore, a thermodynamically consistent model of finite thermo-plasticity with non-linear kinematic hardening and isotropic hardening for large deformations is chosen, which is based on [14]. The Helmholtz energy includes nonlinear functions of the temperature and the isothermal energy, which decomposes into an elastic, a kinematic and an isotropic hardening part. This user material is implemented in Abaqus as a material subroutine (UMAT). For the fluid simulation a steady state is assumed as the deformation is rather slow: 12 mm in 60 s. The fluid-structure interaction coupling tool ifls is provided by the Institute of Aircraft Design and Lightweight Structures (IFL) at TU Braunschweig, which was implemented and extended by [7, 4]. For the fluid computation, TAU from the German Aerospace Center (DLR) is used. The fluid-structure interaction focuses on the choice of an equilibrium iteration method, the time integration and the data transfer between grids.
2 Mechanical model

We assume an multiplicative split of the deformation gradient in an elastic and a plastic part \( F = F_e F_p \) and another split of the plastic part in an elastic and inelastic, motivated by the findings of [6]. The right Cauchy-Green tensor is given by \( C = F^T F \), the elastic part \( C_e = F_e^T F_e \) and the plastic part \( C_{pe} \) of the right Cauchy-Green tensor respectively. The following Helmholtz free energy is proposed, which includes thermal expansion and temperature dependence of the material parameters [9]:

\[
\Psi = \frac{\Theta}{\Theta_0} \Psi_0 - \Lambda(\Theta) \alpha(\Theta)(\theta - \theta_0)(J - 1)
\]  

(1)

Whereas \( \Lambda(\Theta) \) is the temperature dependent Lame constant, \( \alpha(\Theta) \) the temperature dependent thermal expansion coefficient, \( \theta \) the temperature, \( \theta_0 \) is the reference temperature, \( J \) is given as \( \det F \) and \( \Psi_0 \) is additively split into an elastic part, an isotropic hardening part and an kinematic hardening part. For the elastic part a standard Neo-Hooke form is chosen. The isotropic part is a von-Voce-type function and the kinematic part is chosen according to [14, 3]:

\[
\Psi_e = -\frac{\mu(\Theta)}{2} (\text{tr} C_e - 3) - \mu(\Theta) \ln \left( \sqrt{\det C_e} \right) + \frac{\Lambda(\Theta)}{4} (\det C_e - 1 - 2\ln(\det C_e))
\]

(2)

\[
\Psi_{iso} = - H(\Theta) \left( \kappa + \frac{e^{-\beta(\Theta)\kappa}}{\beta(\Theta)} - 1 \right)
\]

(3)

\[
\Psi_{kin} = - \frac{c(\Theta)}{2} (\text{tr} C_{pe} - 3) - c(\Theta) \ln \left( \sqrt{\det C_{pe}} \right)
\]

(4)

Whereas \( \mu(\Theta) \) is the shear modulus, \( \kappa \) is the isotropic hardening variable, \( H(\Theta) \) and \( \beta(\Theta) \) are material parameters for the isotropic hardening part, \( c(\Theta) \) and \( b(\Theta) \) material parameters for the nonlinear kinematic hardening part. All material parameters are temperature dependent. To fulfill the second law of thermodynamics the proposed Helmholtz free energy is inserted into the Clausius-Duhem-inequality

\[
-\dot{\Psi} + S \cdot \frac{1}{2} \dot{C} > 0
\]

(5)

whereas \( S \) is the second Piola-Kirchhoff stress tensor. It yields

\[
\left( S - 2F_p^{-1} \frac{\partial \Psi}{\partial C_e} F_e^{-T} \right) \cdot \frac{1}{2} \dot{C} + (M - \chi) \cdot d_p + M_{kin} d_{pi} - \frac{\partial \Psi}{\partial \kappa} \dot{\kappa} > 0
\]

(6)

For arbitrary \( \dot{C}, d_p, d_{pi}, \) and \( \dot{\kappa} \), the second Piola Kirchhoff stress tensor is

\[
S = 2F_p^{-1} \frac{\partial \Psi}{\partial C_e} F_e^{-T}
\]

(7)
The remaining dissipation inequality yields
\[(M - \chi) \cdot d_p + M_{\text{kin}} d_p_i - \frac{\partial \Psi}{\partial \kappa} \dot{\kappa} > 0\] (8)
whereas the two symmetric Mandel stress tensors
\[M = 2C_e \frac{\partial \Psi}{\partial C_e}, \quad M_{\text{kin}} = 2C_{pe} \frac{\partial \Psi}{\partial C_{pe}}\] (9)
and the back stress and drag stress tensor is given by
\[\chi = 2F_{pe} \frac{\partial \Psi}{\partial C_{pe}} \mathbf{F}_{pe}, \quad R = -\frac{\partial \Psi}{\partial \kappa}\] (10)
The evolution equation are chosen that they fulfill the dissipation inequality
\[d_p = \dot{\lambda} \frac{\partial \Psi}{\partial M}, \quad d_p_i = \dot{\lambda} b(\Theta) M_{\text{kin}}^D, \quad \kappa = \sqrt{\frac{2}{3}} \dot{\lambda}\] (11)
A von-Mises yield function is chosen:
\[\Phi = ||M^D - \chi^D|| - \sqrt{\frac{2}{3}} (\sigma_y(\Theta) - R)\] (12)
with the drag stress derived to \(R = -H(\Theta)(1 - e^{-\beta(\Theta)\kappa})\). As the equations are all in different configurations, they are transfered to reference configuration as due to the symmetric quantities the system of equations reduces to 14.

3 Fluid calculation

The freestream conditions, which have been also used for the experiments [2] are given table 3. The fluid calculation is preformed with the program \textit{TAU} from the German Aerospace Center (DLR). For the fluid simulation a Reynolds-Average-Navier-Stokes (RANS) is used. For the spatial discretization is the AUSMDV-Upwind method used and for the time intergration a pseudo 3rd-order Runge-Kutta method. In Fig. 2 the fluid grid is shown with refinement at the shock interface of the detached bow shock and the boundary layer. The region at the isentropic compression at the beginning of the deformed panel is not yet refined. A more detailed investigations is needed.

| Ma_{\infty} | 7.62 |
| T_{\infty} | 463.7 K |
| p_{\infty} | 52 Pa |
| Pr | 0.72 |
| \gamma | 1.462 |
| R | 346 J/(kg K) |

\textit{Table 1: Freestream conditions [2]}
For the fluid-structure interaction the code ifls from the Institute of Aircraft Design and Lightweight Structures (IFL) at TU Braunschweig is used. It provides a coupling domain for several structural and fluid solvers, e.g. Abaqus FEA and TAU. As the structural deformation is rather slow an equilibrium state for fluid and solid can be assumed in each time step. For the equilibrium iteration method the Dirichlet-Neumann method is used. The Dirichlet problem is solved in the fluid calculation, where the temperature $\tilde{\Theta}$ and the displacement $\tilde{u}$ is held fixed at the domain surfaces. The Neumann problem is solved in the structural computation, where the heat flux $q$ and the pressure $p$ are applied to the domain surfaces. For the transfer of the state quantities a Lagrange multiplier is used for non-conforming meshes. For the time integration an iterative staggered procedure is used. The coupling scheme is schematically shown in Fig. 3. The thermal and mechanical computation of the structural is not yet fully coupled. The heat flux and pressure are applied to a thermal computation in a first step, in which temperature boundary conditions for a mechanical structural computation are calculated. This is used to calculate the thermal
expansion in the second structural computation. The state quantities $\tilde{q}$, $\tilde{p}$, $\tilde{\Theta}$, $\tilde{u}$ refer to the fluid mesh. The values $q$, $p$, $\Theta$, $u$ refer to the solid grid, respectively.

5 Structural model

For the thermal solid computation a standard *Abaqus* heat transfer and radiation model was used. For the mechanical solid computation the above introduced material model was incorporated as a user material routine (UMAT) in *Abaqus* for shell elements. The mechanical model is shown in 4. The clamped support for the structural part are indicated only at the edges but apply to all nodes except the panel. The thermal boundary conditions are as follows: the bottom is fixed at $T = 200^\circ C$ and from the top the heat flux is given from the fluid computation. For the panel shell elements (S4) are used. For the frame (green) and isolation (white) volume elements (C3D8) are used. The material of the panel and frame is Incoloy 800HT and for the isolation Schupp Ultra Board 1850/500 by Schupp Industriekeramik is used. Material parameters are taken from [11, 2]. The panel is discretized by 234 elements and five integration points are used over the thickness. The bending radius is discretized by 4 elements in circumference direction.
6 Results

6.1 Solid

For the displacement and temperature results the same coordinate positions for the measurement are used. The coordinates are given in Tab. 6.1 and lay on the centerline of the panel in flow direction. The comparison between the experimental and simulation results of the displacement are shown in 6. The maximum displacement in z-direction is 13.26 mm for the simulation and 11.8 mm for the experiment. This correlates to an error of 12.4%. The buckling form is similar. The maximum buckling position of the simulation is positioned more to the center of the panel. This correlates to the results of the temperature distribution. The point of the maximum temperature in the simulation is positioned more to the middle. This is shown in Fig. 6, where the temperature in the front is underestimated and overestimated in the middle. In the structural calculation the rounded nose, which can be seen in the fluid model is not modeled. As as isolation is located between the rounded nose and the frame, it should not have a big influence on the temperature distribution and displacement of the model but will be investigated in future works.

6.2 Fluid

The results from the fluid calculation are shown for the Mach number in Fig. 7 and for the $c_p$-distribution in Fig. 8 for the times $t = 0$ s, $t = 30$ s, $t = 60$ s and $t = 120$ s. At $t = 0$ s the panel has not yet started to buckle into the stream, therefore the undisturbed flow field is shown. A detached bow shock is located at the round node. At $t = 30$ s the panel had began to buckle into the flow and a isentropic compression region is formed at the beginning of the panel as the deformation is not convex. This leads to an expansion of the nose shock when the isentropic compression interacts with the bow shock. From
the highest buckling point a Prandtl-Meyer expansion begins, where the fluid accelerates and pressure decreases. At $t = 60$ s, the shock expands more until $t = 120$ s, where the maximum amplitude is reached.

7 Conclusion

A thermo-elastoplastic material model with non-linear isotropic and kinematic hardening for finite strains and with temperature dependent material parameters was introduced. This material model was implemented as a material user subroutine in Abaqus and coupled with the fluid solver TAU. The coupling domain was provided by ifls which is a coupling tool for thermal-mechanical fluid-structure interaction. The comparison of temperature and displacement between simulation and experiment shows good agreement. The boundary conditions from the experiments must be incorporated in more detail for fluid and solid, e.g. a threedimensional flow around the panel and chemical non-equilibrium for the fluid and adapted mechanical and thermal boundary conditions for the structural computation.

8 Acknowledgements

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Figure 7: Mach number at $t = 0$ s (top left), $t = 30$ s (top right), $t = 60$ s (bottom left) and $t = 120$ s (bottom right); max=7.6

Figure 8: $c_p$ distribution at $t = 0$ s (top left), $t = 30$ s (top right), $t = 60$ s (bottom left) and $t = 120$ s (bottom right); max=1.8
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