

# Adaptive Modeling and Simulation 2015

Edited by:  
F. Chinesta, P. Díez, L. Chamoin





**Adaptive Modeling  
and Simulation 2015  
“ADMOS 2015”**



# Adaptive Modeling and Simulation 2015

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on Adaptive Modeling and Simulation (ADMOS 2015)  
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# PREFACE

This book contains the Abstracts of the papers presented at ADMOS 2015, the seventh International Conference on Adaptive Modeling and Simulation, held at École Centrale de Nantes, France, from June 7 to 10, 2015.

In silico experiments that consist in building a virtual reality with numerical models are growing faster than the classical in vivo, in vitro or in situ versions. However, the numerical result is frequently suspicious of lack of realism. The inception of this suspicion is twofold because one may presume that 1) the underlying mathematical model is exaggeratedly simplifying reality and 2) the numerical solver providing an approximate solution is questionable, for instance using a too coarse discretization.

ADMOS 2015 is dealing with the tools that allow qualifying these two presumptions and preventing the mismatching between in silico and in situ tests. Moreover, attention is also paid to the methodologies allowing to efficiently improving the quality of the numerical models (mesh and model adaptivity) and to bringing modeling as closer as possible to reality. Frequently, this requires also accounting for the techniques quantifying the intrinsic uncertainty of the system that has to be modeled.

The objective of the ADMOS 2015 conference is to provide a forum for presenting and discussing the current state-of-the-art achievements on Adaptive Modeling and Simulation, including theoretical models, numerical methods, algorithmic strategies and challenging engineering applications.

This book collects the contributions presented by the participants in the conference, which address a wide range of topics in adaptive modeling, from the classical theoretical aspects and numerical techniques to cutting edge problems and formulations, such as the determination of guaranteed error bounds and adaptive strategies for non-linear, transient or coupled problems, the application of adaptive techniques to reduced order models, the use of goal-oriented anisotropic error estimators and remeshing, as well as the application of adaptive techniques in the stochastic framework.

Advanced numerical techniques are also considered, for example XFEM, Discrete Galerkin, Meshless and Domain Decomposition, as well as the more classical methods. The domain of the applications covers a wide range of problems, from the traditional areas of structural and fluid mechanics, to quantum mechanics or biomechanics, with scales ranging from the nanoparticles, via the mesoscopic level, to those of industrial structures and civil engineering constructions, all studied with a focus on the main goal of adaptivity, seeking reliable and cost efficient modeling.

This book includes abstracts sent directly by the authors, and the editors cannot accept responsibility for any inaccuracies, comments and opinions contained in the text. The organizers would like to take this opportunity to thank all the authors for submitting their contributions.

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## **PLENARY LECTURES**



## Physics dependent de-featuring, is it a prerequisite for mesh generation?

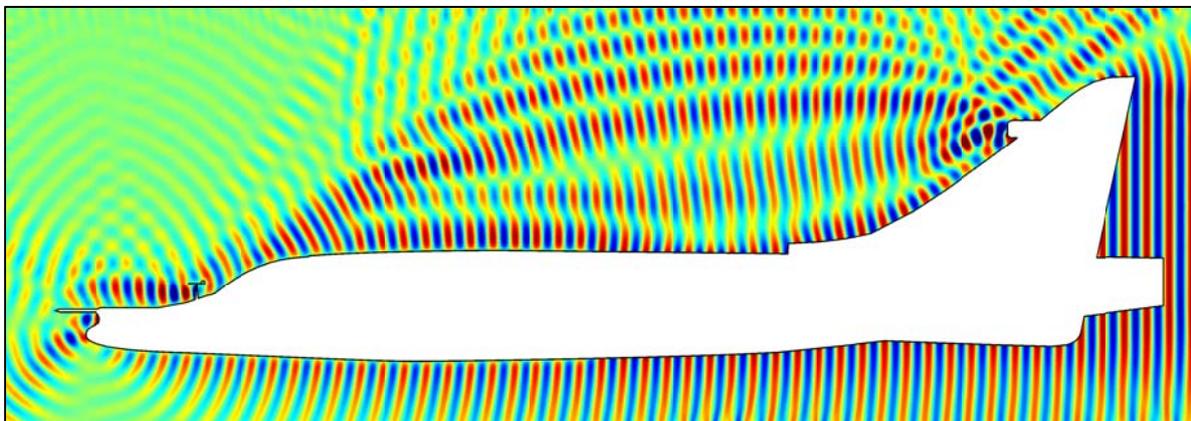
Oubay Hassan and Ruben Sevilla

The use of numerical simulation as a design tool in engineering is nowadays routinely practiced. The initial stage of the simulation process is the generation of an appropriate mesh that is designed to capture the required physics. Mesh generation algorithms require water tight geometries as a starting point. Many automatic software have been developed in the last decades that are capable of ensuring water tightness with a minimum user interventions. However, when dealing with complex objects that contains multi-scale features it is often necessary to manually remove small features which are in the ‘expert’ opinion of the analyst will not have a measurable effect on the solution of the physical system under consideration.

The major drawback of this de-featuring stage is the requirement for manual interaction with CAD systems or geometry cleaning tools. Furthermore, the de-featuring has to be repeated for every physical system that is required to be considered in the design, i.e fluid dynamics, electromagnetics, acoustics, heat and radiation, structure mechanics, etc. In addition, the de-featuring is often dependent on the level of approximation considered for the simulation of the physical system, i.e Euler, Reynolds average or LES in the case of fluid dynamics. In the case of electromagnetics and acoustics simulations, the de-featuring is dependent on every frequency of the required range the designer has to consider.

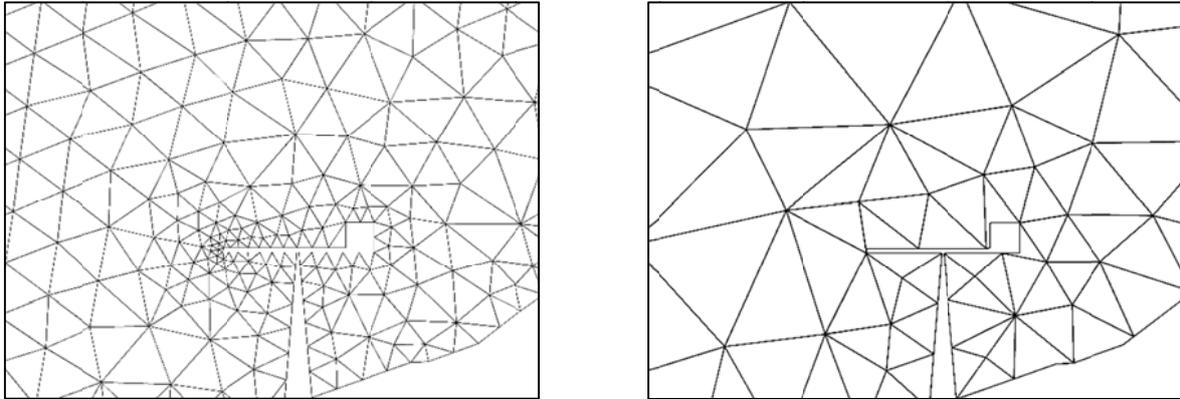
In this presentation we propose an automatic unstructured mesh generation technique using a variant of the advancing front method whereby mesh fronts coincident with the NURBS boundary match the exact geometric definition from CAD independently on the element size. The method allows the possibility to have elements much larger than small geometric features, reducing the overall number of elements required and removing the need for physic dependent de-featuring. The method used to extend the generation technique to high order meshes, based on the approach presented in [1], will also be presented. The presentation will highlight the use of NURBS-Enhanced Finite Element Method [2] to incorporate the resulting meshes within Finite Element codes. Finally, examples will be shown to demonstrate the effectiveness of the proposed method.

The example in Figure 1 shows the simulation of the scattering on an electromagnetic wave by a complex geometry containing small features. In a traditional FE framework, this simulation requires either de-featuring of the geometry or the use of extremely refined meshes if small geometric features are relevant for the correct prediction of the physics.



*Figure 1. Scattering of an electromagnetic wave by a complex geometric configuration containing small geometric features.*

Figure 2 shows the mesh required to simulate the problem using tradition FE (left) and the meshes that can be generated using the proposed approach (right). It can be observed that the size of the elements is completely independent on the geometric complexity and the size of small features.



**Figure 2.** Mesh produced with a standard FE mesh generator (left) showing the required mesh refinement to capture small geometric features and mesh produced with the new approach (right) showing coarse elements capturing complex boundary geometric features.

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## ABSTRACT

HiMod is a model reduction technique to describe phenomena with a dominant dynamics, possibly featuring local relevant transverse components, like for blood flow in arteries, water in rivers, oil in pipes. In particular, HiMod obtains surrogate models by resorting to a different discretization of the full problem along the main and the transverse dynamics, respectively. Originally, the mainstream is tackled by affine finite elements while modal approximation solves the transverse directions [1]. The rationale is that relatively few modes are enough to capture the transverse dynamics of interest with an overall reduction of computational costs. Numerical results show that the approach is versatile and effective, possibly coupled with modal/nodal adaptivity in the transverse/axial direction, respectively [2]. In this presentation, we focus on the most recent advances in the HiMod setting:

1. HiMod modeling of fluids in pipes;
2. extension of the HiMod approach to a parameter-dependent setting;
3. generalization of the HiMod procedure to curved domains.

As for the first item, we have recently generalized the HiMod reduction procedure to 3D cylindrical domains and to the Stokes equations. Blood flow modeling in arteries is the reference application. Selection of the modal basis is crucial in this context. We need a modal basis that automatically includes the boundary conditions assigned on the lateral surface (the wall of the arteries), not necessarily homogeneous Dirichlet data (in view of fluid-structure interaction problems). To tackle the possible dependence of the HiMod approximation on a set of parameters, we propose a new methodology, called HiPOD. We aim at merging the reliability of a HiMod approximation with the computational efficiency characterizing the well-known Proper Orthogonal Decomposition (POD). In particular, we propose two different approaches; the first one is based on a standard POD projection; the second one adopts a two-level POD procedure based on interpolation. In the first case the problem is parametrized by problem coefficients and boundary data, in the latter one we focus on the problem coefficients only.

Concerning the third item, we have recently combined the HiMod reduction technique with the IsoGeometric Analysis (IGA), simply by replacing the finite element discretization along the mainstream with an isogeometric approximation. The IGA intrinsic formulation allows a simpler and more effective geometrical modeling when curved domains are considered. In particular, with a view to practical bioengineering applications, centerlines of the arteries are obtained in a straightforward way via splines or NURBS.

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## The Multiscale Challenges in Modeling Fracture of Metals

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Energy dissipation by dislocation plasticity in metals provides the resistance against crack growth that makes metals tough engineering materials. However, homogenized plasticity constitutive laws must fail at a singular crack tip, one consequence of which is that the conditions for crack growth are typically calibrated using experimental data rather than computed from fundamental mechanics. This issue, along with the size-dependence of plasticity and the need to address chemical aspects of fracture, dictates that plasticity and fracture be studied at smaller scales – from the dislocation level down to the atomistic and quantum levels. The severe challenges in simultaneously capturing the macroscopic plasticity and the nanoscale behavior at the crack tip, and doing so on time scales appropriate to real materials, are first discussed. Emerging multiscale methods for addressing some of these challenges are presented, including the Coupled Atomistic/Discrete-Dislocation (CADD) model, its extension to Quantum Mechanics, its extension from plane strain to full 3d problems, and the Coupled Discrete-Dislocation/Crystal-Plasticity model, which taken together bridge from quantum to continuum scales of plasticity. Examples of successes are shown and limitations identified. Relevant to MATHICSE interests, these advanced multiscale methods, i.e. those that go beyond the basic coupling of atomistics to a hyperelastic continuum (e.g. the Quasicontinuum model), are highly algorithmic, or recipe-based. The coupling is accomplished through ideas akin to domain decomposition but, because the different domains have different constitutive descriptions, the “boundary conditions” at the domain interfaces are non-standard and often non-local. Thus, while these methods preserve important fundamental physics and mechanics with demonstrated high and often controllable accuracy, putting such methods on a firm mathematical foundation appears to be very difficult. However, finding alternative new methods that are derived from a more-formal structure is also a huge challenge because the loss of degrees of freedom (electrons, atoms, dislocations) with increasing scale of description precludes the development of, for instance, a single energy functional from which the mechanics would emerge naturally.

## **GENERAL CONTRIBUTIONS**



# CONVERGENT ERROR-CONTROLLED MESH ADAPTATION

## - ADMOS 2015 -

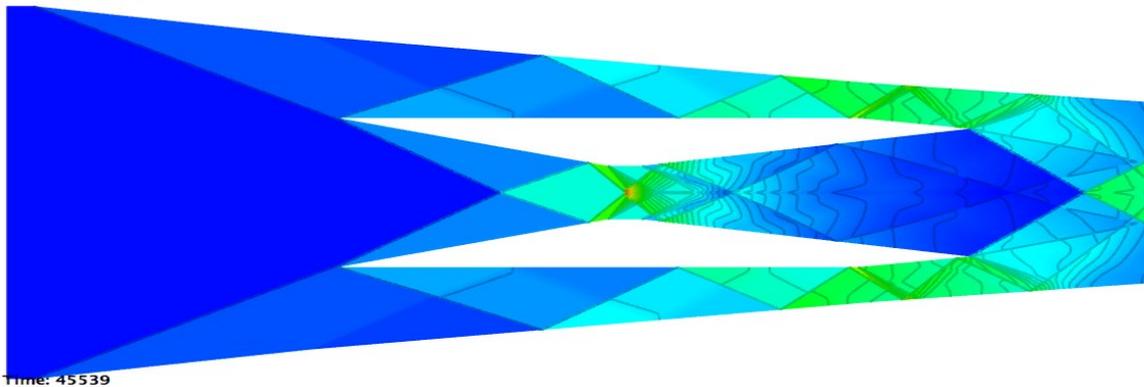
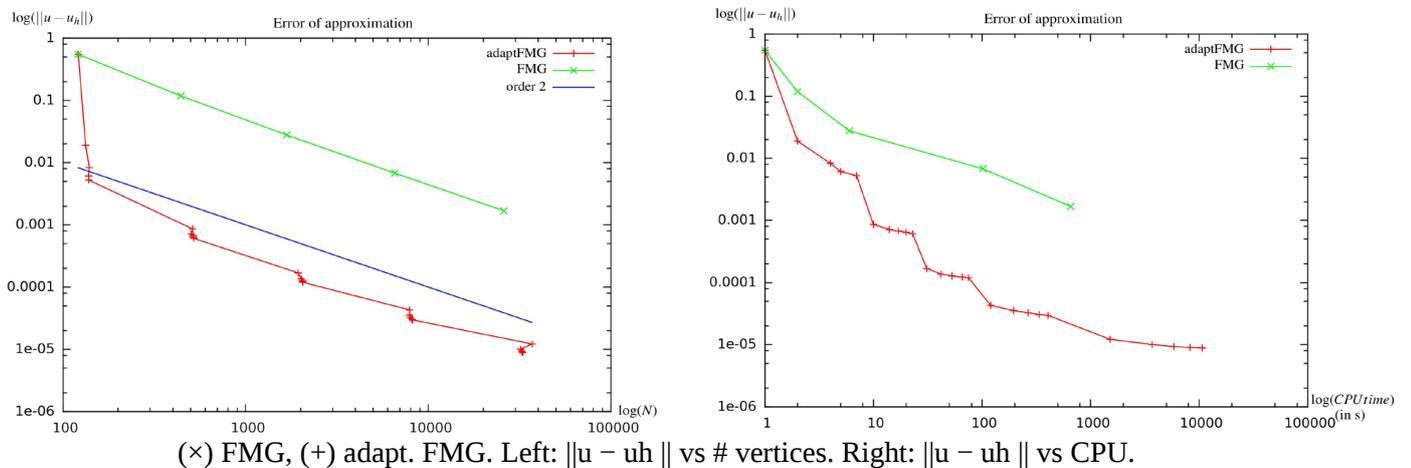
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The proposed communication will address the following question: *Find an approximate solution such that the approximation error norm in L2 is less than a prescribed  $\varepsilon$ .* And indeed we are interested by a small complexity in terms of floats. Answering to this assumes that the algorithm involves a mechanism increasing mesh size. No innovation from this side, the outer loop will be a nested iteration with new 2D meshes four times richer (in terms of vertices) than the previous ones. Decision to continue relies on a corrector. For efficiency the nested iteration is combined with a multigrid (MG) resolution, which will be the most inner loop. The MG cycling also stops on an evaluation of the L2 error estimate. In between, the intermediate loop is a mesh adaptation loop. A novel formulation allows looking for the metric parametrization which minimizes the L2 norm of approximation error. This approach relies on the association of an *adjoint state*, a *corrector field*, and a *local error*, the sensitivity of which with respect to the metric is computed. The calculation of a *boundary layer* with an error of 0.1% is obtained in 10 seconds of adapted FMG, 1000 of FMG. The extension to Euler flows is illustrated with the *scramjet* flow of second figure (second-order convergence is obtained). Extension to Navier-Stokes is on-going.



# Automatic Patient Specific Simulation of Trabecular Bone by using $h$ -Adapted Meshes with Cartesian Grid Finite Element Method

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## ABSTRACT

In this paper we present a methodology to perform elasticity analyses of trabecular bone from human wrist micro CT scans, with the final purpose of providing data which can be used, together with other measures, to develop new diagnostic tools to improve the characterisation of bone quality and its structural behaviour.

This analysis is carried out by using a version of the Cartesian grid Finite Element Method (*cgFEM*) for medical images. As in image based methods, which assign one element to each voxel, *cgFEM* takes advantage of the fact that both the mesh and the image have compatible Cartesian structures in order to create the FE model from the image, in an automatic way, without any intermediate step. In contrast to the image based methods, *cgFEM* can keep the number of degrees of freedom relatively low, by using an efficient  $h$ -adaptive process to adapt the mesh to the heterogeneity of the image.

$H$ -adaptivity allows *cgFEM* to capture the borders of the bodies represented in the medical images without the necessity of creating them explicitly as in the usual geometry based methods. As a consequence, it does not require the cumbersome, often manual, process of creating intermediate geometrical models from the bitmap which are usually one of the most expensive stages in patient specific simulations.

Here, in particular, we show results of trabecular bone overall stiffness tensor evaluation obtained by using *cgFEM* in a homogenisation procedure.

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# Anisotropic Error Estimates for Adapted Dynamic Meshes

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## ABSTRACT

The simulation of real-life problems, with complex moving geometries evolving in unsteady flows in three dimensions, still remains a challenge. To reduce the CPU time of these simulations while preserving their accuracy, anisotropic metric-based mesh adaptation, which has already proved its efficiency for steady problems, appears as a salutary perspective. However, its extension to the unsteady moving mesh case is far from straightforward.

The problematic is that the multiscale mesh adaptation described in [1] only controls spatial errors. But, in the context of time-dependent problems, temporal errors must be controlled as well. In this study, we do not account for time discretization errors but we propose a space-time analysis of the spatial error in unsteady simulations. From this analysis, we design a global iterative fixed-point adaptation algorithm. In this algorithm, the time interval of the simulation is divided in sub-intervals, keep the same adapted mesh for each time sub-interval. These meshes are generated using hessian metrics averaged on the sub-intervals.

This analysis is first performed for unsteady simulations with fixed geometries, then the case of moving meshes is considered. In that case, moving boundaries induce a displacement of the whole mesh to keep a good mesh quality (see [2]). The error estimate is modified to take into account the movement of the mesh. Given a sensor function at time  $t^{k+1}$  and displacement field  $d$  between  $t^k$  and  $t^{k+1}$ , we express an ALE metric field at time  $t^k$ , from which a mesh at time  $t^k$  is generated, which, once moved with displacement  $d$ , will be adapted to the sensor at time  $t^{k+1}$ . The case of linear [3] and quadratic displacements will be considered. The resulting ALE metric allows us to modify the fixed-point unsteady adaption algorithm to take into account the mesh movement, and to couple it with a moving mesh algorithm [2] and an ALE flow solver.

Finally, several 3D examples of moving-mesh unsteady adaptation will be given and analyzed.

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# Improved Conformal Adaptation for Hexahedral Meshes

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## ABSTRACT

To improve the quality of the results of a numerical simulation with a finite element method, mesh refinement is an effective solution. Various techniques have been implemented for many years. In the h-refinement method, the first point consists in selecting some meshes of the domain which are too large. These meshes are divided by cutting their edges. This division produces new meshes of the same category: the division of triangles produces triangles, the division of hexahedra produces hexahedra, etc.

The connection between two zones with different levels of refinement must be taken into account if the numerical method needs a conformal mesh for the resolution: in this case, a node cannot be isolated at the middle of an edge. If the mesh is made of triangle or tetrahedra, this connection can be implemented with specific triangles or tetrahedra. But if the initial mesh is made of quadrangles or hexahedra, the solution is not simple. It cannot be achieved with quadrangles or hexahedra.

In a first attempt, for every hexahedron at the interface between the zones with different levels of refinement a solution was proposed [1, 2]. A quadrangular face could be intact, regularly split or only one of its edges is cut. In this case, the quadrangle is split into 3 triangles. That rule induces 4 situations for the hexahedron and it is cut, using pyramids and tetrahedra.

This technique is effective and allows mesh adaptation. Nevertheless, there is a drawback: in some circumstances, the refinement could spread a lot. The improvement was found by authorizing the splitting of 2 edges of a quadrangle, defining a new refinement of it with 3 quadrangles. Based on this new rule, 47 new patterns are designed to achieve the splitting of the hexahedron. Doing that, the refinement is improved: a conformal mesh is produced and the number of created meshes and nodes is as low as possible.

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# A priori goal-based error estimation and anisotropic adaptive mesh control applied to compressible viscous flows

- ADMOS 2015 -

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## ABSTRACT

A basic feature in finite-element method (FEM) is the initial choice of an interpolation for the unknown and the building of an integration which keeps the exactness of the discretisation for a solution identical to its interpolation. A priori estimates exploits easily the central role of interpolation in FEM. We concentrate on goal-oriented a priori estimates used as refinement criterion for anisotropic mesh refinement. The proposed communication gathers new estimates for the two following basic models, the advection model (a) and the Laplace equation (L).

$$W_t^a + \nabla^* \cdot (\mathbf{V}W^a) = 0 ; \quad -\nabla^* \cdot \nabla W^L = f \quad (+ \text{initial and boundary conditions}).$$

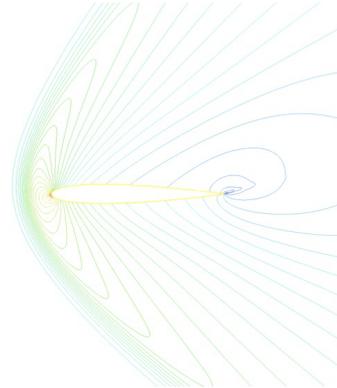
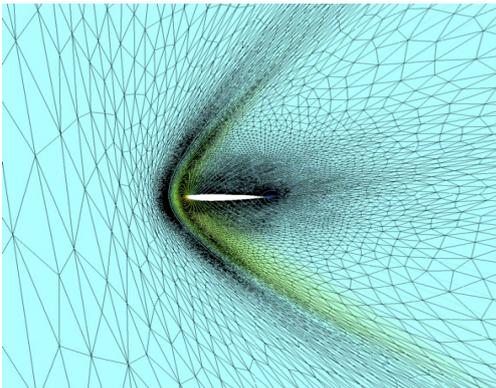
Let  $j = (g, W)$  be a functional. Adjoint state  $W^*$  is the solution of:

$$-W_t^{a,*} - \mathbf{V} \cdot \nabla W^{a,*} = g ; \quad -\nabla^* \cdot \nabla W^{L,*} = g \quad (+ \text{final and boundary conditions}).$$

For both cases we get an estimate expressed in terms of interpolation errors  $\Pi_h W - W$  weighted by derivatives of the adjoint state  $W^*$ :

$$\begin{aligned} |(g, W_h^a - \Pi_h W^a)| &\leq \|K_1(W^{a,*}, \mathbf{V})\| \|\Pi_h W^a - W^a\| \\ |(g, W_h^L - \Pi_h W^L)| &\leq \|K_2(W^{L,*})\| \|\Pi_h W^a - W^a\| \end{aligned}$$

The extension of this analysis to the model of Fluid Mechanics for compressible gas can be done in terms of interpolation errors of algebraic functions of the the unknown. An optimal mesh is then generated by solving an optimisation system whose solution is an optimal metric that minimises the a priori error estimate. Demonstrative results for steady and unsteady viscous flows will be shown, a sample is illustrated above for the laminar supersonic flow (Mach 2., angle of attack  $10^\circ$ , Reynolds 106) around a NACA0012 airfoil.



# Can adaptive mesh refinement produce grid-independent solutions for complex flows?

- ADMOS 2015 -

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## ABSTRACT

One of the trends in computational fluid dynamics today is the use of the ever-increasing computational resources for the high-fidelity simulation of more and more complex flows. For example, simulations are performed for realistic geometries such as ships with their propellers and appendices. Flow separation, vortex shedding and breakup are simulated in detail. Finally, multiphysics computations such as fluid-structure interaction or the modelling of cavitation become more and more common.

The results of such simulations depend heavily on the physical models being used, such as the turbulence model in the Reynolds-averaged Navier-Stokes (RANS) equations. In many cases, such models are being applied in situations which are far more complex than the ones for which they were developed and which may be outside their range of validity. Research of physical modelling for today's realistic simulations is therefore of prime importance.

A complication for this study is the inevitable appearance of numerical errors. To accurately assess the precision of a physical model, we need to know a numerical solution in which the numerical errors are small with respect to the physical ones: a solution that is close to grid convergence. In simple cases, it may be possible for an experienced user to generate reasonable meshes by hand which provide sufficiently small numerical errors. However, for complex flows it is impossible to know beforehand what mesh size is needed where, in order to obtain grid convergence. Adaptive grid refinement is therefore the ideal technique to master the numerical error.

In this paper, we pose the question whether grid refinement can be used in such a way as to guarantee that the solution of a complex flow problem is grid-independent. The work is based on the ISIS-CFD unstructured finite-volume incompressible RANS solver developed by ECN-CNRS [1], which contains an integrated anisotropic grid refinement technique [2].

As a reference, a two-dimensional airfoil flow is simulated on a series of ever finer adapted meshes; these results are compared with simulations on different fine meshes in order to understand if a converging series of adapted meshes truly leads to mesh-independence. The findings of this initial case will then be applied to the simulation of the three-dimensional vortical wakes behind ships in sideslip condition.

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# Adaptive remeshing for industrial unsteady CFD

- ADMOS 2015 -

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## ABSTRACT

FLUSEPA is an advanced simulation tool which performs a large panel of aerodynamic studies. It is the unstructured finite-volume solver developed by Airbus Defence & Space to calculate compressible, multidimensional, unsteady, viscous and reactive flows around bodies in relative motion. The numerical strategy in FLUSEPA is designed for highly compressible flow and keeps its accuracy regardless of the grid. According the desired accuracy, a second-order accurate shock-capturing scheme is generally used for RANS and URANS simulations and a fourth order accurate vortex-centred scheme is used for hybrid RANS/LES simulations[1].

In this paper we introduce an adaptive meshing approach to accurately represent unsteady flows in FLUSEPA. The meshing strategy is based on a multi-overlapping grid intersection which is conservative and allows to quickly and properly mesh 3D complex geometries. It can be seen as a CHIMERA strategy without interpolation. Each part of the bodies is meshed independently and immersed in background grids. This technique will be largely described for it differs from the commonly used interpolation-based CHIMERA methods.

The adaptive mesh construction is based on a simple 2-1 balanced octree approach. Different criteria for refinement will be tested: one relying on the Ducros[2] sensor, another is a basic hessian and the last one is based on the resolved kinetic energy. The aim of this study is to obtain a versatile module for industrial applications combining different criteria. The test case is a transonic turbulent flow around a square cylinder at a Mach number of 0.9 and Reynolds number of  $4.10^5$  based on the experimental conditions of Nakagawa[3]. Computations are carried out using a CFL of 0.8 and on a Cartesian grid. The study will be focused on the interaction between the von Karman eddy street and the shock wave.

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# Anisotropic mesh adaptation for brittle fractures applied to a generalized Ambrosio-Tortorelli model

- ADMOS 2015 -

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## ABSTRACT

The Francfort-Marigo model of quasi-static brittle fracture [1] is a very accurate model, but requires minimizing a highly irregular energy functional. However, this functional can be approximated by a suitable regularization, whose solution converges to the one of the original model. One example of such approximation is given by the Ambrosio-Tortorelli functional. The crack is identified by a smooth phase-field, instead of a lower-dimensional set, as in the case of the Francfort-Marigo model. The minimization of the new functional can be obtained by solving elliptic boundary value problems via a finite element method. The numerical approximation of these variational problems, however, is not trivial, since the employment of a very fine uniform mesh throughout the whole domain turns out not to be computationally affordable in most cases, even in two dimensions. A more efficient approach can be based on the employment of an adapted mesh driven, e.g., via an a posteriori error estimator, in order to refine the grid in a suitable way, typically, only in a thin neighborhood of the crack path (see, e.g., [2]).

In [3,4,5], an anisotropic error estimator and a new minimization algorithm are proposed and applied to the classical Ambrosio-Tortorelli approximation, in the case of both anti-plane and plane-strain isotropic linear elasticity. Several numerical tests assess the reliability of the whole adaptation procedure. The employment of an anisotropic grid allows one to considerably reduce the number of mesh elements in comparison with other (isotropic) adaptation techniques, and thus to save on the overall computational cost.

In this communication, we extend the approach presented in [3,4,5] to the generalized Ambrosio-Tortorelli model considered in [6]. In this model, the basic Ambrosio-Tortorelli functional is modified in order to deal with several types of brittle materials.

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# Adaptive Strategies For Viscous Simulations

- ADMOS 2015 -

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## ABSTRACT

Capturing accurately the whole flow field around a complex geometry remains a challenge for viscous turbulent simulations. The use of quasi-structured boundary layer meshes is required in near-wall regions because of the dramatic variation in the normal direction of some variables such as the velocity.

The scope of this paper is to address this issue from a meshing point of view. We first propose to review the standard approaches [1,4] devised to generate boundary layers meshes: moving mesh methods consisting in moving the front layer in an existing volume mesh, local remeshing methods where patterns are inserted in an existing volume mesh.

We then extend these approaches to devise three mesh adaptation strategies around complex geometries: (i) a fully unstructured approach based on a boundary layer metric, (ii) a mixed approach where the boundary layer mesh is re-generated at each iteration in the mesh adaptation loop, and (iii) a metric-aligned approach, where a single mesh operator is used for both the near-wall regions and the rest of the domain.

The (2D and 3D) test cases considered are a transonic bump, a transonic RAE2822 airfoil, an M6 wing, a geometry from the drag prediction workshop (DLRF6), and a shock/boundary layer interaction. Comparisons of all the approaches are made in terms of robustness, compliance with anisotropic mesh adaptation, CPU time, and compliance with experimental data.

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# Automatic geometric transformations over the input domain to produce a better mesh with an Octree-based technique.

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## ABSTRACT

The Octree [1] technique is one of the most popular methods to produce hex-dominant meshes. It starts by computing the Bounding Box (Bbox) of the input domain; an hexahedron that will define the root Octant. Then, this Octant is recursively split into new Octants until a given constraint is fulfilled.

The Octree is not sensitive to some aspects of the input mesh. For instance if the input is a surface mesh defining a cube with 12 triangles or it is the same cube defined by 1000 triangles, this should not produce any difference in the output. Probably it will only take more time. However if we now consider a cube perfectly aligned with the reference axes and the same cube slightly rotated in one of the axes, the output will certainly be different.

One natural solution to overcome this issue would be to apply geometric transformations over the input domain in order to align it with the reference axes. Then execute the meshing algorithm and finally, apply the reverse transformations to the output mesh.

The most important application of this work is in the medical field. Many simulations must be performed on patient-specific meshes. Consider the following workflow: acquire medical images, achieve proper segmentation, build a surface model and finally build a volume mesh for simulation with a numerical method.

Now, it is clear that most of soft and hard tissues do not count with dominant directions. However, if we consider the problem of mesh adaptation, where the idea is to concentrate more nodes in a given region important for the simulation, our algorithm could be very useful. For instance, consider the simulation of brain tumor resection. It is clear that more precision is needed in the region of the tumor. Normally the Octree can be modified to refine more the elements over this region and leave a coarse mesh elsewhere. This Region of Interest (RoI) is defined regularly with a cube that intersects the brain. Now we can apply the transformations to align the cube defining the RoI with reference axes. Apply the same transformations to the brain surface mesh and then, generate a mesh with the Octree. Finally, apply inverse transformations to the output mesh and start the simulation.

In this work we show how this simple idea can drastically reduce overall amount of nodes in the mesh, while still conserving an important precision in the RoI. We consider these geometric transformations are another small step, yet very important, towards real-time simulation of surgeries.

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# Camarón: A visualization tool for the quality inspection of polyhedral meshes

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## ABSTRACT

The numerical simulation of complex objects requires a good quality domain discretization (mesh). In 2D, meshes are usually composed of triangles and/or quadrilaterals and, in less frequent cases, of convex polygons. In 3D, meshes are usually composed of tetrahedra and/or hexahedra. In case of mixed element meshes, pyramids, prisms and other convex polyhedra might also be included. What is a good quality mesh depends on the problem to be solved and the chosen numerical method. Different quality criteria have been defined such as minimum (dihedral) angle greater than-, maximum (dihedral) angle less than-, and aspect ratio less than- a threshold value, among others, and used to control the refinement and improvement process of a mesh.

Because of geometry restrictions or point density requirements, it is very often that not all mesh elements fulfill the quality criteria required by the user. It would be very useful to know where bad elements are located in order to try to improve them. That is why a visualization tool that allows the user to inspect a mesh before a simulation is run can be very useful to prevent simulation problems.

There are several open-source visualization tools, but they are mostly oriented to visualize meshes composed of only one element type and are associated to a mesh generator. For example, TetView [1] is related to the tetrahedral mesh generator TetGen [1] and it is able to visualize tetrahedral meshes. GeomView was specially designed for the visualization of surface meshes composed of any polygonal cell. A tool that integrates mesh generation and visualization is MeshLab [2]. It is oriented to the generation, repairing and processing of 3D triangular meshes. None of them allows a user the interactive evaluation of the mesh quality and only Meshlab handles several input/output file formats.

In this paper, we present the design and implementation of an open-source portable and extensible visualization tool for large polygonal and polyhedral meshes. The surface meshes can be triangular, quadrilateral or mixed-element meshes composed of any polygonal cell. The 3D meshes can be tetrahedral, hexahedral or mixed-element meshes composed of any polyhedral cell. The current implementation allows: (1) input/output formats such that OFF, PLY, M3d, Ansys, TRI and visf, among others. Visf is an extension of the OFF format to handle meshes of general polyhedra. (2) Several rendering strategies: flat, glass and Phong shading. (3) Several quality criteria are available: Minimum and maximum (dihedral) angle, aspect ratio and volume, among others, (4) Elements can be selected according to some quality criteria or if they intersect a user specified primitive such as a sphere, cuboid or plane, and (5) Element quality statistics. The tool was implemented in c++ using OpenGL with shaders. Several examples were used to compare the performance and memory usage among Camarón, GeomView, TetView and MeshLab. Our current implementation is, in most of the cases, faster than the others, but with a greater memory cost. We will also discuss design and implementation issues.

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# THE APPLICATION OF MULTI-SCALE AND ADAPTIVE SIMULATION METHODS TO TIDAL ENERGY SYSTEMS

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## ABSTRACT

Generating energy from clean renewable sources is clearly attractive for a number of reasons. In stark contrast to other further developed and exploited resources such as wind, tidal-based energy conversion has the crucial benefit of being entirely predictable. However, a new tidal-energy-based industry will only flourish if the development of large installations, such as turbine arrays comprising 100s of individual devices, can be shown to be both economically viable and to have a minimal impact on the environment. This new industry is currently in its early stages where no major projects have yet been developed, although many have been approved and are in various stages of planning. Sophisticated numerical simulation methods are vitally important to support resource analysis, array design, and the optimisation of financial profits while minimising environmental impacts.

Since the installation of large numbers of energy converters can fundamentally change the nature of the resource, fully-coupled simulations of the large-scale resource including the presence of arrays of turbines is required. In addition, individual turbines need to be either resolved or parameterised in order to accurately represent the turbulent turbine-wake-turbine interactions which are crucial for the purpose of individual turbine micro-siting as a component of array design analysis and optimisation. This results in the requirement for simulations that resolve spatial scales in the horizontal greater than 100 km to represent the tidal resource, and down to sub-metre scale to resolve turbines and their turbulent wakes: i.e. scales varying by at least five orders of magnitude. Also, depth-averaged dynamics can be considered in the far-field, whilst fully three-dimensional dynamics should be considered at the smallest scales. This is therefore a truly multi-scale, timely and challenging engineering problem which requires the design of highly efficient numerical techniques, especially given that multiple flow calculations will be required as part of array optimisation strategies.

In this presentation we will describe the approaches we have taken to tackle this multi-scale problem, including the use of unstructured mesh generation, anisotropic mesh adaptivity, and gradient-based optimisation algorithms. Applications of the developed technology to idealised as well as real-world case studies will be presented. Future topics such as the inclusion of uncertainty, and multi-rate time-stepping may also be discussed.

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# Efficient 3D Finite Element Analysis based on Cartesian grids considering exact CAD geometries

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## ABSTRACT

This contribution proposes a 3D immersed boundary method, based on Cartesian grids, modified to improve the accuracy along the boundary and the efficiency during the resolution.

On the one hand, the embedded domain will be defined by its CAD boundary representation with NURBS or T-Splines, instead of using an approximated faceted representation. The exact boundary representation of the embedded domain allows overcoming the major drawback of existing immersed methods that is the inaccurate representation of the physical domain. A novel approach to perform the numerical integration taking into consideration the exact representation of the physical domain is presented and its accuracy and performance evaluated using numerical tests.

On the other hand, and now from the analysis point of view, we propose to use a Nested Domain Decomposition (NDD) reordering technique. When a direct solver is used to solve a system of equations a previous reordering is usually used in order to improve the performance of the solver. Usually this reordering is obtained via an optimization process which not always obtains the best reordering for the system of equations. In our case, the NDD is based on the Cartesian grid structure, intimately related to the mesh topology, thus providing an optimal reordering. This reordering will yield in a significant reduction of the computational cost associated to the resolution of the system of equations.

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# A Study of Anisotropic Mesh Adaptation through High-Dimensional Embeddings

Franco Dassi      Hang Si      Simona Perotto

November 10, 2014

## Abstract

In [2, 1] the authors provide a new re-meshing technique based on a higher dimensional embedding to get a curvature adapted anisotropic surface mesh. In this work we extend this new technique to anisotropic mesh adaptation of two dimensional function  $f : \mathbb{R}^2 \rightarrow \mathbb{R}$ . We propose a new embedding map  $\Phi : \mathbb{R}^2 \rightarrow \mathbb{R}^4$  that it is able to incorporate the directional features of the function  $f$  we are interpolating. Then we provide a series of standard mesh modification that optimizes the mesh in the  $\mathbb{R}^2$  and uses an embedding space in  $\mathbb{R}^4$  to evaluate mesh size and quality. The result is a triangular anisotropic mesh whose triangles are stretched according to the features of the function  $f$ . The reliability and robustness of the proposed method is illustrated through various examples.

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# Application of an Automatic h-Adaptive Refinement Algorithm in a Second Order Immersed Boundary Code

## VII International Conference on ADAPTIVE MODELING AND SIMULATION - ADMOS 2015

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### ABSTRACT

An automatic adaptive refinement algorithm is an important technique to reduce the computation time while increasing the local accuracy of the numerical simulation. For this goal, the Residual Least Squares (RLS) error estimator has been developed in the Author's own code SOL [1-4], which is suitable for h-adaptive algorithms on unstructured grids.

When applying a h-adaptive algorithm for the case with a complex geometry (curved boundary), special attention is required in order to maintain the grid curvature. For this cases the adaptive grid is dependent of the initial unstructured grid which must be provide by the user or by a grid generator, also keeping a good grid quality is an important issue, during the adaptive refinement.

For this case, an alternative approach is to use an immersed boundary [5] or a cut cell [6] based method, which does not require an initial grid shape, just the domain size must be defined. An immersed boundary has been implemented in the SOL code based on a conservative cut cell approach which maintains the grid quality and the local second order error decay is guarantee by using a least squares method to correct the velocity nearby the complex geometry.

The main objective of the work is to validate the joint techniques of the h-refinement and immersed boundary. The article consists in three parts: the first one shows an example of the adaptive algorithm and error estimator, the second one is the verification of the proposed immersed boundary method based in a conservative cut and the document concludes with an application of an automatic adaptive refinement of the flow around cylinder using the developed immersed boundary method.

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# **High order anisotropic adaptive meshing by generalisation of the length distribution tensor paradigm**

**- ADMOS 2015 -**

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## **ABSTRACT**

Anisotropic mesh adaptation techniques have been shown to be very efficient in the last decade with very convincing applications. In modern anisotropic Finite Element, the element stretching can attain very high level as 1 for 1000 to 10000 when capturing boundary layers. The gain in terms of mesh points versus a uniform mesh is thus about 1000 to 10000 and it has been proven by certain applications for which anisotropic mesh adaptation is the only successful known solution. These techniques are well understood and fully developed for P1 simplex element. Until now, the gain in terms of mesh entities was so huge that it allowed compensating low order element. The new available supercomputers showing more than thousand cores enable to run computations on meshes of several million of nodes and it changes this point of view. The over cost of constructing a higher order mesh is gaining in position to be compensated by using high order element and higher convergence.

High order meshes mean building curved element. In this paper, we propose an extension and generalization of the tensor approach and the associated edge based error first introduced in [1]. The novelty of this extension is that it gives a clue for a straightforward construction of curved edges as a consequence of minimizing the interpolation error. We will show that effectively high order approximation give rise to Riemannian geometries in which optimal meshes have curved edges and providing an explicit way of construction.

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# Curved meshing for high Reynolds flows solved using high order framework.

- ADMOS 2015 -

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## ABSTRACT

In this work, we are interested in the mesh generation problem for simulation of compressible fluids using high order schemes. For this kind of simulation, it is well-known [1] that the subparametric discretization used for geometry's representation (usually piecewise-linear) may lead to errors dominating errors related to the variable field discretization. To solve this problem, we need to generate curved meshes with the same order of the numerical schemes. That means curved elements are essential for approximations of order more than three. As the mesh curvature is a non local property, an element cannot be curved without controlling the neighboring ones.

Our strategy to generate curved meshes [2] is the following: we start with an initial straight mesh and we consider it as an elastic solid. We impose a displacement on the mesh boundaries in order to fit them with the curved geometry. Then we solve linear elasticity equations in order to propagate the boundary curvature inside the mesh. The validity of the final curved volumic mesh is obtained thanks to linear elasticity equation and some properties of Bezier curves/surfaces.

We applied this algorithm to the generation of several simplicial curved meshes both in 2D and 3D. In particular, we are able to generate curved meshes for several turbulent test cases such a M6 wing (Figure 1) and a RAE airfoil.

To illustrate the work, we performed some isogeometric numerical results for compressible fluid dynamics and we compared them with the results provided by the same scheme on a piecewise-linear mesh.

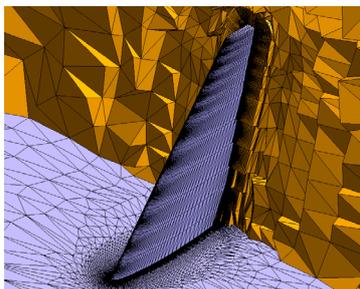


Figure 1: Curved mesh of a M6 Wing

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# Geometrical Accuracy and Numerical Properties of High-Order Meshes

- ADMOS 2015 -

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## ABSTRACT

In the computational physics community, a consensus is forming on the superior efficiency of high-order numerical schemes for problems with high resolution requirements. However, many contributions show that a linear discretization of the geometrical model can limit the accuracy of high-order methods. Thus, it becomes necessary to develop robust and efficient methods for curvilinear mesh generation and adaptation.

In a previous work [1], a method for generating valid high-order meshes has been presented. The meshing procedure starts with a mesh that is straight-sided everywhere in the domain, except on the boundary, where high-order nodes are placed on the real geometry. An optimization procedure is used to untangle the invalid elements that often appear in the vicinity of curved boundaries, while preserving the original mesh as much as possible.

In this talk, we focus on the problem of estimating and controlling the geometrical accuracy of high-order meshes as well as their impact on the stability and accuracy of the simulation.

The geometrical accuracy of curvilinear meshes can be estimated by measuring a distance between a mesh boundary and the corresponding geometrical model entity. Distance measures defined in the literature, namely the Hausdorff and the Fréchet distances, rely on a solid mathematical basis. However, they are complex to implement, and their computational cost is prohibitive in the present context, even in an approximate form. We present an alternative estimate for the geometrical error, that is simple and computationally efficient enough to be used in 2D and 3D applications.

The curvilinear character of high-order meshes also impacts the performance of the numerical scheme. In most Finite Element methods, the functional space of approximation locally defined on a reference element is affected by curved elements in physical space, which may lead to a degraded accuracy [2]. The conditioning of the spatial discretization is also influenced, with possibly negative consequences on the maximum time step that can be used with explicit time integration schemes [1]. We put these effects in evidence and identify Jacobian-based measures that quantify them.

Finally, we describe how the existing mesh optimization procedure can be adapted to take into account the geometrical error or the numerical effects of the mesh. We illustrate the benefits of this method with several examples.

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# High-order Mesh Untangling and Smoothing Using the Hierarchical Smoother

- ADMOS 2015 -

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## ABSTRACT

In the last years, high-order methods are emerging to simulate physical phenomena in applied sciences and engineering. However, these kind of methods rely on a high-order discretization. One of the most used methods to generate a high-order mesh is the *a posteriori* approach. First, a linear mesh that contains the required features for the simulation is generated. Then, the interpolation degree of the mesh is increased, and the additional nodes are inserted. However, when the high-order nodes are inserted, low-quality or inverted elements may appear if high-curved surfaces are present in the geometry. Thus, mesh untangling and smoothing is a key step of the meshing process to obtain valid high-order discretizations. Usually, the smoothing process is performed in two steps, as shown in [1,2]. First, the boundary nodes are moved by taking into account the quality of the boundary elements. Then, the quality of the maximal dimension elements is optimized by moving the position of the inner nodes. However, the boundary nodes position may constrain the quality of the whole mesh. Thus, we propose a novel framework in which we only consider the quality of the maximal dimension elements [3]. To this end, we minimize an objective function defined as the distortion of the maximal dimension elements, by moving the position of the inner nodes, as well as the position in the parametric space of the face and edge nodes. Although the objective function is defined globally, for implementation purposes, we propose to perform a node-by-node relocation process by using a non-linear Gauss-Seidel approach. That is, we first move the edge nodes, then the face nodes, and finally the inner nodes, until convergence is achieved.

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## DIRECT NUMERICAL SIMULATION FROM 3D IMAGING

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**Key Words:** *Finite elements, 3D Imaging, 3D X-Ray Tomography, Mathematical Morphology, Image Processing, Mesh Generation and Adaptation*

In the last decade, the finite element method has shown to be a powerful and accurate computational tool to deal with material behavior and fluid-structure interaction simulations, with the increase on the computational power through the use of grids or cloud computing. On the other hand, numerical description of the researched objects with the improvement of imaging techniques, like X-Ray tomography (micro or nano) is very interesting, since it accesses the heterogeneity of the different phases with a definition and quality that may be very important. In the literature, the classical method to generate finite element meshes from images (2D or 3D) is based on a three-step processes: segmentation, for the identification of the different phases in the image; construction of a surface mesh for each phase, representing its boundary; construction of one or several volume meshes on which the specific properties of each phase can be defined.

In this paper, we propose an efficient way to build directly the volume finite element representation of the multiphase domains using an “image immersion” method, by skipping the Marching Cubes’ step. Before mapping the image values in the mesh, we apply mathematical morphology treatments to the image, such as segmentation, distance to the interfaces function construction, and etc. Then, the treated image values are mapped in the coarse initial mesh by direct interpolation, providing the distance field distribution on the mesh. An appropriate error estimator built from this distance is used to compute a metrics field that our topological mesher will consider to adapt the mesh [1]. Finally, we have implemented a reinitialization procedure that, coupled to the automatic anisotropic mesh adaptation algorithm, allows the smoothing of the interpolated distance, but also the built-up of a smooth and regularized Heaviside function of this distance, which is actually a phase function. Meshes obtained using these techniques are well adapted for monolithic based methods (one mesh containing all the phases, each represented by an implicit - phase - function, like in classical diffuse interface methods). Furthermore, mesh adaptation provides nodal enrichment near phases “boundaries or interfaces”, which will allow results to converge towards a “sharp-interface” solution.

Computations on such meshes will illustrate the relevance of our methodology. Firstly, we will show general cases of multiphase flows on common 2D pictures, all these 2D pictures can be taken from Paint, Camera, and even Smartphone. Secondly, for the 3D cases, the 3D images contain a huge number of fibers. Flows are calculated using a stabilized mixed finite element method, obtained through discretization of the Navier-Stokes equations and by imposing the rigid body motion.

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# GEOGRAM: A Library of Geometric Algorithms

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We present a set of geometric algorithms for grid generation. The implementation of the algorithms is available in the public GEOGRAM [1] library (BSD Open-Source License). The set of algorithms comprises :

- ◊ Robust geometric predicates, using adaptive precision floating point arithmetics [2] simulation of simplicity [3] to handle the corner cases, and arithmetic filters [4] to early detect and quickly handle the easy cases;
- ◊ Geometric search data structures, including Kd-Trees (for nearest neighbors queries) and Axis-Aligned BBox Trees (for mesh intersection);
- ◊ Delaunay triangulation and power diagrams in 3d;
- ◊ Restricted Voronoi Diagram in arbitrary dimension.

The design of the library follows a minimalistic principle, combined with the algorithmic state of the art, inspired by [5]. Compared with CGAL, our implementation is significantly more memory efficient, sometimes faster, much easier to understand (no generic programming), at the cost of being less generic/dynamic. All the algorithms are parallelized using an abstract model that supports pthreads, OpenMP and Windows threads. In addition, the library has no dependancy and is easy to compile on any platform that has IEEE754 floating point arithmetics (Linux, Mac, Windows, Android, ...). The library was used to implement a solver for Optimal Transport [6]

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# Flow computations on urban environments built from 3D dense point clouds or triangulations using anisotropic adaptation and implicit functions

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## ABSTRACT

3D scanning and mapping are useful in several applications and, in particular, for urban outdoor environment modelling. These models can be used, for example, in flow computations for pollutant dispersion studies, thermal impacts or crowd massive displacements. These simulators and models need to be based on real data and new methods to create samples are based on very dense acquisition systems, which may be satellite for regional scales or mobile laser scanners for local ones. In the last case, models are composed of very dense point clouds, which produce more and more data, as a result of the accuracy wanted by the users. Most often, surfaces represented by this point-cloud are triangulated (after segmentation), but do not allow a direct computation on this model.

In this context, we propose an original technique to build numerical finite element models issuing from dense point-cloud acquisitions or their triangulated version. In fact, a 3D anisotropic adapted mesh is generated, by computing an implicit function that is related to the distance on each point to the point-cloud or to the triangulation, and by minimizing the associated interpolation error. Hence, reduction of the size of the stored data can be accomplished, while preserving the detail.

Applications on urban environments illustrate our approach, by performing both mesh generation and adaptation, but also flow computation on these 3D meshes.

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# Impact of mesh adaptivity on the interpretation of transport processes in porous media

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## ABSTRACT

An accurate modeling of solute transport processes in the subsurface is a crucial issue with a view to several engineering applications. These include groundwater vulnerability assessment and modeling of hydrocarbon reservoirs. All the available modeling options encompass the definition of effective transport parameters, which are essentially representative of the porous medium and of the geometry at hand. The estimation of these parameters is typically performed within model calibration schemes, which require an iterated numerical approximation of the selected model with a consequent computational burden.

In this contribution, we provide a space-time grid adaptation procedure to improve the accuracy of the numerical simulation of solute transport in porous media, while containing the computational costs. We rely on a simple model for transport processes, based on the standard Advection Dispersion Equation (ADE). In particular, we focus on the interpretation of non-reactive transport experiments in homogeneous and heterogeneous porous media through model calibration. In contrast to a numerical approximation based on a fixed space-time discretization, our approach is grounded on a joint automatic selection of the spatial grid and of the time step to capture the main space-time system dynamics. Spatial mesh adaptation is driven by an anisotropic recovery-based error estimator [1,2], which enables us to properly select the size, shape and orientation of the mesh elements. The adaptation of the time step is performed through an *ad-hoc* local reconstruction of the temporal derivative of the solution via a recovery-based approach [3].

The impact of the proposed adaptation strategy on the capability to provide reliable estimates of the key parameters of an ADE model is assessed with reference to experimental solute breakthrough data measured after the injection of a non reactive tracer in a porous system. Model calibration is performed in a Maximum Likelihood (ML) framework upon relying on the representation of the ADE solution through a generalized Polynomial Chaos Expansion (gPCE). The results obtained show that the proposed anisotropic space-time grid adaptation leads to ML parameter estimates and to model results of markedly improved quality when compared to classical inversion approaches based on a uniform space-time discretization.

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# Prediction of Ventricular Boundary Evolution in Hydrocephalic Brain via a Combined Level Set and Adaptive Finite Element Mesh Warping Method

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## ABSTRACT

Hydrocephalus is a serious neurological disorder caused by abnormalities in cerebrospinal fluid (CSF) flow, resulting in large brain deformations and neuronal damage. Treatments drain the excess CSF from the ventricles either via a CSF shunt or an endoscopic third ventriculostomy. However, patients' response to these treatments is poor. Mathematical models of hydrocephalus mechanics could aid neurosurgeons in hydrocephalus treatment planning. Current models and corresponding computational simulations of hydrocephalus are still in their infancy, despite this being a disease with serious long-term implications.

We propose a novel geometric computational approach for tracking the evolution of hydrocephalic brain tissue – ventricular CSF interface via the level set method and an adaptive mesh warping technique. In our previous work [1], we evolved the ventricular boundary in 2D CT images which required a backtracking line search for obtaining valid intermediate meshes for use with FEMWARP, a finite element-based mesh warping method. In [2], we automatically evolved the ventricular boundary deformation for 2D CT images via the level set method. To help surgeons determine where to implant a shunt, we also computed the brain ventricle volume evolution for 3D MR images using FEMWARP.

In this work, we generalize the results from [1,2] and incorporate adaptive mesh refinement following mesh deformation. Based on the use of the solution gradient of the PDE in the mesh warping approach as an enrichment indicator, the mesh is refined where the solution gradient is large and is coarsened where it is small. We present computational simulations of the onset and treatment of pediatric hydrocephalus based on 2D CT images which demonstrate the success of our combined level set/adaptive finite element-based mesh warping approach.

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# On explicit error estimates for the elastic wave propagation in heterogeneous media

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## ABSTRACT

This work deals with explicit *a posteriori* error estimates for elastic wave propagation in heterogeneous media. Based on some previous works on acoustic problems ([1]), the proposed explicit error estimator is derived in a non-natural  $L^\infty$  norm.

Two main ideas are developed: the second-order elastodynamic equation is transformed firstly to a first-order hyperbolic system ([2], [3]); and the residual method of *a posteriori* error estimates is exploited with a series of field reconstructions in time and in space ([4], [5]). These reconstructions are performed with respect to different regularities required by corresponding ingredients of the estimator. The effectivity of the estimator on uniform meshes and adaptive meshes is studied numerically. The numerical results indicate that the error estimator gives a good estimation to the true error and that it is asymptotically exact as the computational effort grows. Improvements for the reconstruction in time and in space are proposed.

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## Verification for eigenvalue problems

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### ABSTRACT

In this paper, the approach proposed by Ladevèze and Pelle in 1989 [1] for deriving computable, sharp and guaranteed lower bounds for eigenvalues is revisited. The key lies in a static quotient where a load space and a corresponding statically admissible stress space are introduced. The difficulty is on the computation of strict lower bound of the first nonzero eigenvalues. There are two additional eigenvalue problems to be solved. The first one is global and one computes only the first eigenvalue; the second one is defined over the element and then local.

The goal of this work is twofold. First, we would like to make easier the implementation of these additional problems which are not classical [2-6]. The second aim is to get sharper the computed lower bound.

Our answer introduced here is a multiscale approach, the smaller scale being used for the computation of the additional problems. It is developed in this paper for  $P_1$ -triangle elements.

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# Adaptive space time finite element methods for dynamic nonlinear thermomechanical coupled problems

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## ABSTRACT

In this contribution, we consider nonlinear thermomechanical coupled problems of the following type: Find a displacement field and a temperature distribution, which fulfil the equation of motion with a temperature dependent stress field and the heat equation including a heat source depending on the displacement. The continuous model is discretized with a space time Petrov Galerkin method using continuous and piecewise d-linear basis functions in space and time, which can be reduced to a time stepping scheme due to the discontinuous piecewise constant temporal test functions, see for instance [1]. The coupled system is solved by a staggered scheme. The aim is to control the discretization error as well as the error in the solution scheme in a nonlinear goal functional. To this end, we use the dual weighted residual (DWR) method. In detail, we combine the ideas from [1] for goal oriented error estimation in nonlinear time dependent problems and from [2] for balancing discretization and numerical error in static problems. The discretization error is measured by the usual DWR techniques discussed for time dependent problems, e. g., in [1], while the numerical error is estimated by testing the residuum with the discrete dual solution, cf. [2]. However, the error estimator can only be evaluated after solving the complete primal and dual problem. Thus, we have to design a special solution algorithm. The main idea is to solve the primal problem doing only one step of the staggered solution scheme in each time step. Then the discretization and the numerical error is estimated. If the numerical error is dominant, an additional loop over all time steps including one step of the staggered scheme is executed. Otherwise, the mesh is adaptively refined. By this approach, we can reduce the numerical effort for the accurate solving of thermomechanical problems by adopting the solution scheme to the special needs of the underlying problem and the chosen goal functional.

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# Adaptive Finite Element Simulation of Multi-Physics Turbulent Flow with Applications in Aerodynamics

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## ABSTRACT

The error magnitude and the order of accuracy of a new unsteady Variational MultiScale (VMS) solver are examined. Indeed, while vast majority of industrial simulations today are restricted to only computing a statistical average of the flow field, we propose in this work the simulation of unsteady turbulent flows using finite element methods with residual based stabilization to solve the Navier-Stokes equations. The basic idea is to consider that the unknowns can be split in two components, coarse and fine [1], corresponding to different scales or levels of resolution. Compared to early Large Eddy Simulation approaches (LES) where small scales are explicitly solved introducing a Smagorinsky-type dissipative term, the proposed VMS acts here as an implicit Large Eddy Simulation (ILES) technique by solving first the fine scales, then by tracking them in time and finally by replacing their effect into the large scales taking into account their nonlinearity. As a result, an important fraction of the degrees of freedom are used for the small resolved scales whereas consistency is retained in the large resolved scales only. We show that the new solver gains also efficiency and robustness by incorporating dynamic anisotropic mesh adaptation [2] and increases accuracy by including a new a posteriori error estimator that deals with boundary layers and flow detachments. Therefore, several test cases and confrontation with literature are proposed. The massively parallel simulations and comparisons with experimental results of flows past complex 3D industrial geometries such as a drone will be presented.

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# Complementarity in structural dynamics: A new procedure for bounding eigenfrequencies

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## ABSTRACT

Pairs of approximations of complementary nature, one being compatible and the other equilibrated, are commonly used for the determination of bounds of the exact solution of elastic problems. The main advantage of the application of this approach is that, provided the fundamental conditions are respected, a strict bound of the error is obtained and, therefore, an interval containing the exact solution can be computed.

In modern applications the compatible approximation is typically computed using a displacement based finite element model, while the equilibrated one may be either recovered from the weak form of equilibrium present in the finite element solution or computed from a complementary, stress based, finite element model. Furthermore the quality of the solutions and of its bounds is greatly influenced by the quality of the approximations, i.e. when both are good (close to the exact one) a sharp bound is obtained, whereas bad approximations lead to very large intervals.

While the formulation of compatible finite element models for the dynamic analysis of structures is covered in most textbooks, its complementary models, strictly enforcing dynamic equilibrium, which were developed from the 1970's by Tabarrok [1] are not so well known. Furthermore the application of pairs of eigensolutions for the determination of bounds of the eigenfrequencies, as formulated by Ladevèze [2], never gained a widespread application.

In this communication we will discuss the application of a new approach, based on two complementary models, wherein, instead of solving two separate eigenvalue problems, both finite element models are combined. Preliminary results indicate that from the solution of this combined model it is possible to obtain bounds of the structural eigenfrequencies.

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**ADAPTIVE MODELING AND NUMERICAL APPROXIMATION FOR  
A SIMPLE EXAMPLE OF MULTISCALE HYPERBOLIC  
RELAXATION SYSTEM**

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**ABSTRACT**

The present work considers the mathematical and numerical analysis of a new adaptive goal-oriented strategy based on local *hpm* discontinuous Galerkin (DG) method (*h* for grid, *p* for accuracy of shape function and *m* for model). In order to perform an exhaustive analysis, we consider steady-state solutions to the one-dimensional linear hyperbolic system with multiple relaxation times  $\varepsilon(x)$ :

$$\begin{aligned}\partial_t u^\varepsilon + \partial_x v^\varepsilon &= 0, \quad x \in [0, L], \quad t > 0, \\ \partial_t v^\varepsilon + a^2 \partial_x u^\varepsilon &= \frac{-1}{\varepsilon(x)} (v^\varepsilon - bu^\varepsilon),\end{aligned}\tag{1}$$

with  $L > 0$ ,  $a, b$  given constants satisfying  $0 < |b| < a$  and prescribed initial and boundary conditions [1]. The above system, for which the associated equilibrium equation reads  $\partial_t u + \partial_x bu = 0, t > 0$  (2), may be viewed as a simple model of a hierarchy of PDE systems arranged according to a cascade of relaxation mechanisms. For instance, such relaxation systems are involved in the study of multiphase flows or multiscale coupling problems. In regions where  $\varepsilon$  is small, the numerical approximation of the full system (1) may become very costly and a strategy to overcome this difficulty may consist in approximating the associated steady-state equilibrium equation.

According to the main features of the flow and to the required accuracy of the description, the model, coarse (2) or fine (1), has to be locally adapted for computational efficiency. Then, these different models have to be appropriately coupled at some interfaces [2]. The automatic choice of the appropriate model requires model adaptation procedures [3] where the position of the interface has to be optimized in such a way that in the region where one computes the coarse model, the model error (expressed in term of output functionals) between the fine and coarse models does not exceed some given tolerance. Nevertheless, only an approximation of the adapted model is known in practice, thus the approximation involves both a model and a discretization error [4]. These two kinds of errors have to be localized for the model and numerical adaptation procedure.

The main goal of this work is to understand how the error of our *hpm* DG method depends on the relaxation parameter, the boundary layer effects and the coupling interface layer effects in order to validate our approach. Special emphasis is given to the theoretical (PDE level) study of the modeling error. Numerical experiments will be considered to assess the performances of the present method.

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# Multiscale hybrid methods for time-domain electromagnetics

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## ABSTRACT

In this work, we are interested in the propagation of electromagnetic waves in complex media. More precisely, we would like to study time dependent wave propagation problems with strong multiscale features (possibly in space and time). In this context we would like to contribute in the design of innovative numerical methods particularly well suited to the simulation of such problems. Indeed when a PDE model is approximated via classical finite element type method, it may suffer from a loss of accuracy when the solution presents multiscale features on coarse meshes. To address this issue, we rely on the concept of multiscale basis functions that is one solution to allow for accuracy even on coarse meshes. These basis functions are defined via algebraic relations. Contrary to classical polynomial approximation, they render by themselves a part of the high-contrast features of the problem at hand. Recently, a new family of finite element methods has been introduced in [1]-[2], referred as “Multiscale Hybrid-Mixed methods” (MHM), which is well adapted to the simulation of high-contrast or heterogeneous problems. The underlying approach relies on a two level discretization. Shortly, basis functions computed on a fine (second level) mesh allow for the reconstruction of the solution on a coarse (first level) mesh. Such MHM have been initially designed in the context of stationary problems, such as Darcy flows. In this work, we propose to extend the concept of MHM to time dependent electromagnetic wave propagation problems. The model problem relies on the time dependent Maxwell's equations. The continuity of the electric field is relaxed via the introduction of a Lagrange multiplier. The solutions are expressed on a basis computed at the second level that incorporates the heterogeneity of the problem via the resolution of a PDE. Several schemes are proposed from implicit to explicit time schemes and continuous finite elements to discontinuous ones for the spatial discretization of the local problems at the second level.

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# Goal-oriented error control within non-overlapping domain decomposition methods to solve elliptic problems

- ADMOS 2015 -

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## ABSTRACT

In this work, we are interested in designing an adaptive version of domain decomposition algorithms [1] to control the error on the estimation of quantities of interest [2] for elliptic problems solved by the finite element method. We present (i) an a posteriori error estimator [3] which enables to separate the different sources of error, namely the discretisation error (due to finite element approximation) per subdomain and the algebraic error (due to the iterative domain decomposition technique), and (ii) its extension [4] to goal-oriented error estimation. The estimator is based on the error in constitutive relation [5] and a parallel reconstruction of admissible fields [6] for both the reference and adjoint problems; it gives a guaranteed upper bound that enables to adapt the solver's stopping criterion to the discretization error. Our algorithm enables us to drive parallel computation by an objective of accuracy on quantities of interest while avoiding useless iterations.

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# CONSTITUTIVE RELATION ERROR ESTIMATOR : AN ADMISSIBLE FIELD CONSTRUCTION USING A DOMAIN DECOMPOSITION STRATEGY

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**Key words:** Domain decomposition, Finite elements, Admissible field, Error assessment

**Abstract.** We are interested in error estimate using the constitutive relation error concept. The construction of an admissible fields is a pillar of the method and is revisited in this work using a domain decomposition strategy. An approximation is introduced in the estimate of the error and makes it possible to separate the initial global problem into several local ones (see [1]).

An analysis of the cpu-cost is presented in this work, it shows clearly the interest on large problems. The numerical results also shows that the quality loss introduced by the approximation is widely acceptable in a practical use. Some perspectives to this works will also be presented in the field of non-linear mechanics.

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# Controlling Parallel Adaptive Sparse Grid Collocation Simulations with Chiron

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## ABSTRACT

Nonintrusive UQ methods, roughly describing, use a (expected small) number of runs of a deterministic computational model, each one having as inputs judiciously chosen points of the stochastic input space. Statistics of the outputs are then estimated from the deterministic computations, generating a large amount of data and thus requiring careful management [1]. Using Chiron, a data-centric scientific workflow engine that executes, in parallel, scientific applications, helps to control and manage these data. Chiron uses a dynamic data-centric approach, where scientific workflow algebra handles the parallel workflow execution efficiently. The algebra also standardizes data consumption and production as algebraic operands, with adherence to W3C provenance data model. Provenance is essential for scientific and engineering experiments and ensures that the experiment can be repeated over different conditions. Chiron provides native support for distributed provenance by storing provenance data during the execution of all samples and making it available for querying at runtime. Thus, it is possible to monitor the status of each input point run and availability of results through runtime provenance dataflow queries. Monitoring some specific attributes, results or checking the elapsed time of a given task may indicate that a failure happened. Such information can be used to refine the task (to prevent it from failing again) and resubmit it. Depending on the gathered results, the user may decide to change (or add) parameters corresponding to an input point or to make other decisions regarding the simulation. Finally, note that since each input corresponds to a parallel job assigned to a number of processors, which is in turn also solved in parallel, Chiron handles the execution of several simultaneous jobs, which configures a two-level overall parallel execution scheme. Uncertainty quantification scenarios with adaptive sparse grid collocation are particularly amenable to be steered and controlled by Chiron [2]. They require the ability of adapting the workflow, at runtime, based on user input and dynamic steering, according to error measures (or input thresholds) given by the user. We evaluate our approach using a novel and real large-scale workflow for uncertainty quantification on a 640-core cluster. The results show impressive execution time savings from 2.5 to 24 days, compared to non-iterative workflow execution.

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# Supercomputer Simulation of Gas Flow Properties in Metallic Microchannel

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## ABSTRACT

In our work we consider gas flows into metallic microchannels of technical systems. The gas consists of two components: nitrogen and hydrogen. The material which is often used for microchannels production is nickel and its alloys. The supersonic expansion of gas mixtures is accompanied by several simultaneous non equilibrium processes: mixing of layers, shock waves, heat exchange with walls and etc. We will take into account real geometry for metal (including microtopography) and thermal heating. To investigate such complex problems it is essential to develop adequate numerical technique that implies using stable and robust numerical algorithms and calculations on fine grids by means of high performance computer systems. Parallel computer realization of numerical approach is oriented to using of supercomputers with hybrid architecture. Each node of such supercomputer has several multi-core central processors (CPU) and a few graphics processors (GPU).

We propose multi-scale method for computation of mixture gas flow in metal microchannel. This method integrates macroscopic approach with molecular description of processes near metal walls. Macroscopic approach is based on the quasi-gasdynamic equations for mixture (QGDM) [2]. Microscopic approach is the correction of the flow parameters in Knudsen's layer that is performed by methods of molecular dynamics (MMD). The QGDM system is a generalization of the quasi-gasdynamic equations for one component gas. The quasi-gasdynamic equations are solved numerically on both structured or unstructured grids by finite volumes method. The system of molecular dynamic equations is used as a sub-grid algorithm. The MMD give a chance to get some information about processes on molecular scale, and on times of a few nanoseconds.

The parallel algorithm is based on "domain decomposition" technique and a splitting on physical processes. Gas dynamics is calculated on CPUs units. The computational area is split into sub domains. Parallelization is realized on a grid of the processing units. Molecular dynamic calculations are distributed on GPUs. For MMD parallelization an equal number of particles is sent to each computing unit. According to the algorithm the molecular dynamic calculations do not require exchanges. Splitting on physical processes means that QGD-equations are processed by CPUs and MD is processed by GPUs.

The results of calculations obtained in this paper show that the algorithms give high efficiency when it is implemented on modern hybrid systems with a large number of cores in use.

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# Optimized approximation space for Trefftz-discontinuous Galerkin methods

- ADMOS 2015 -

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## ABSTRACT

Helmholtz equation is classically encountered when modelling waves and vibrations. The numerical approximation of its solution is complex because of the generally small characteristic wavelength and of the potential sign-indefiniteness [1] which imply to use adapted formulations.

The Trefftz-discontinuous Galerkin methods [2] are characterized by the use of exact solutions of the governing equation inside subdomains as shape functions [3]. Therefore they are not subject to the same limitation than Finite Element methods (pollution and dispersion error). However, they lead to an ill conditioned algebraical system caused by a loss of coercivity.

In this presentation, we propose a method to solve the system in a selected approximation subspace where the coercivity and the condition number are controlled, as well as the slight loss of accuracy due to the reduction technique. If needed, that subspace can be used as the coarse level of a multigrid method.

We derive the method on a specific Trefftz-DG method: the Variational Theory of Complex Rays (VTCR) [4]. The accuracy and performance of the proposed solver are demonstrated on a set of numerical examples of acoustic wave propagation.

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# PRACE project results : performing calculations on full Tier0 supercomputers with mesh adaptation and FEM very large linear systems resolution

- ADMOS 2015 -

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## ABSTRACT

In this paper we will present works and results obtained during the one year PRACE project Cim128Ki [1]. This project aims to make computation on full Tier0 supercomputers or at least up to 131,072 cores.

The goal of such a project was to validate the scalability used to develop our application at such a large scale. The development context is a finite element formulation using an implicit scheme in time discretization leading to solve at the end very large linear systems. Another main axe in our strategy is doing mesh adaptation to reduce the size of the space discretization keeping the precision of the simulation unchanged. The main idea behind this to combine the benefits of every numerical technique rather than choosing one neglected others. This has become crucial has the power given by  $10^5$  cores allow us to deal with very large problems containing several billion unknowns.

To illustrate we want to use up to  $10^5$  cores but keeping anisotropic mesh adaptation [2] that could reduce the number of unknowns to solve the problem by a factor  $10^3$ . To purchase in that way of reducing CPU time for larger problems we have implemented a parallel multigrid solver using PETSc framework [3] to reduce the algorithmic complexity for solving linear system and again reduce the number of operations done to solve the system by an other factor  $10^3$ . At the end as we combine all these improvements we are able to reduce the CPU time by a factor  $10^{11}$  to be compare to “only”  $10^5$  if we “only” take full advantage of Tier0 supercomputers.

We will first present improvements done to make us able to use more than  $10^5$  cores where the details become a bottleneck, like using the MPI\_Alltoall function; memory and IO management; but also keeping in mind that the size of local data hosted by a core has the same order of the number of cores used.

Then we will present some parallel performances obtain during this PRACE campaign in term of hard and weak speed-up for the two main CPU consuming steps that are mesh adaptation and linear system resolution. 2d respectively 3d “biggest” runs will also be presented using two different Tier0 supercomputer (Curie : Bullx Intel/InfiniBand with 4GB/core and JuQUEEN IBM BlueGENE/Q with 1GB/core) leading to solve a 100 billion unknowns system respectively 50 billion unknowns using 64,536 cores on Curie and 262,144 cores on JuQUEEN in only some hundreds of seconds.

Finally we will present some more reasonable (using about one thousand cores) but more realistic (using complex and real data given by big 3d tomographic image or complex object) simulations.

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# Verification of reduced-order models for real-time applications with haptic feedback

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## ABSTRACT

Real-time simulation systems equipped with haptic peripherals, like those employed in virtual surgery or industry lay-out design, require feedback rates on the order of 1kHz. Such an impressive requirement for a simulation code, usually including non-linear approaches, has recently been accomplished by model order reduction techniques [1] within the framework of the so-called computational vademecums [2]. These vademecums are in fact a pre-computed solution of a high dimensional parametric problem. This solution is obtained in a very efficient manner through the use of Proper Generalized Decomposition (PGD) and then evaluated (rather than simulated) in real time very efficiently.

In this work a verification strategy has been developed towards an effective use in health and industry of such systems. Error estimation [3] has been accomplished with especial emphasis in one particular quantity of interest, namely, the force transmitted to the haptic peripheral. This force is crucial to provide the user with a realistic sensation in the operation of the simulation system.

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# A posteriori verification of PGD reduced models with application to engineering computation

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## ABSTRACT

Despite the important progress in computer sciences, the cost associated with the resolution of multi-parametric problems can be extremely prohibitive. This is especially important when dealing with problems depending on numerous parameters, as encountered in optimization studies, which are becoming more and more mandatory for the design of new products. Reduced Order Modelling (ROM) is a convenient answer to circumvent this issue, usually called curse of dimensionality. However, a main drawback of ROM is the lack of robust a posteriori error estimators to measure the quality of the approximated solution, even if first advances have been performed [1,2].

This paper extends the a posteriori verification procedure proposed in [3] that enables to control and certify PGD-based model reduction techniques, which are currently the subject of many research activities [4]. This procedure uses the concept of constitutive relation error allowing to get guaranteed global/goal-oriented error estimator taking both discretization and PGD truncation error into account. By splitting the errors sources, it also leads to a natural greedy adaptive strategy, which can be driven in order to optimize the accuracy of PGD approximation [5,6]. We extend it to the cases of geometrical parameters models and PGD separation of space variables [7].

The focus of the talk is on two technical points: (i) construction of equilibrated fields required to compute guaranteed error bounds for those specific cases; (ii) error splitting and adaptive process when performing PGD-based model reduction.

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# Mathematical and numerical study on the parametric sensitivity of a structural dynamic Hyper-reduction

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## ABSTRACT

We consider the Hyper-reduction technique [1], in the framework of parametric structural dynamic problems. Efficient parametric models in hyper-reduction of structural design allow to act towards real time computations. The reduced coordinates are solutions of equations restricted to a subdomain, named the reduced integration domain (RID). Then one **significant question** is: Can we control the accuracy of the reduced-basis and the RID so they can be used *online* to reproduce dynamic solutions, which are different than the ones computed to generate the reduced-basis?

Concerning the mathematical formulation of the Hyper-reduction, we propose a time-continuous Petrov-Galerkin one. This formulation is more general than the Galerkin projection one [2], since we are able to write our hyper-reduced order model through a reduced basis which is not necessarily orthogonal. **We attest** the following assumption on the Hyper-reduction of a structural dynamic problem, in this case: While dynamic solutions are regular via parametric evolution and no bifurcation occurs, then the parametric *online* error relative to the Hyper-reduction by reference reduced elements is also regular with respect to parametric evolution. In particular, a reference hyper-reduction is justified when variations occur within a viscoelastic dynamic problem, for the viscosity parameter. So to answer the preceding question, we show a **mathematical and sharp a priori upper bound** of the parametric *online* error relative to a reference hyper-reduction. We show mathematically that the parametric accuracy of the Hyper-reduction is improved when considering **enriched reduced elements** in association with the reference snapshots expanded by the ones of the parametric derivative of the viscoelastic dynamic solution at the same reference viscosity value [3, 4]. All these findings are generalisations to hyperbolic equations of the ones developed in [4] for parabolic equations in the context of fluid mechanics. Numerical validations of these theoretical results will be shown during the conference for academic applications in structural design.

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# Improving the $k$ -Compressibility in Hyper Reduced Order Models with Moving Sources

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## ABSTRACT

Nowadays, the use of Hyper Reduced Order Models (HROMs) to tackle the high computational complexity of problems found in science and in engineering is becoming an interesting option to reach real-time computations. These methods look for the solution to the problem in subspaces of the solution space of very small dimension by making the hypothesis that the quantities to be hyper-reduced are  $k$ -compressible in a certain basis in the sense that these quantities have at most  $k$  non-zero significant entries when expressed in terms of that basis. In HROMs based on the Proper Orthogonal Decomposition (POD), a first reduction is performed by reducing the dimensionality of the test and trial spaces. It is widely known that in order to significantly reduce the computational complexity of the problem, the cost of assembling the residual and the tangent matrix at each Newton iteration must be reduced [1]. Consequently, a second reduction is accomplished by building approximations to the residual and the tangent matrix from sampling them at very few points of the domain.

In this work, we examine different strategies for addressing hyper-reduction of problems characterised by multiple non-linear contributions. Schemes in which the residual is hyper-reduced as a unit, taking the history of the residual as snapshots for the reconstruction procedure, are usually found in the literature [2]. This strategy is used as a reference technique for comparison in our work. As observed from numerical experiments, poor  $k$ -compressibility and tangent matrix conditioning are obtained when applying this technique for the design of HROMs in the considered problems. In order to improve performance and robustness, it is proposed to separately hyper-reduce each of this non-linear terms. Additionally, the use of moving reference frames is proposed to hyper-reduce cases that involve moving heat sources.

Applications to nonlinear phase change problems with temperature dependent thermophysical properties and welding problems are particularly considered. Through these examples we show the improvement in performance and robustness of the introduced HROMs.

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# ACCURACY ASSESSMENT OF PGD-LATIN METHOD FOR POWER FLOW PROBLEMS IN ELECTRIC GRIDS

- ADMOS 2015 -

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**Keywords:** Electric grids, Proper Generalized Decomposition (PGD), Model Order Reduction, LATIN solver, Error Assessment

## ABSTRACT

A “Smart Grid” is an efficient management of the electricity that uses computer technology in order to achieve a safe and sustainable electricity supply. They promise to improve the efficiency of power grid systems through incorporating of power generation as distributed generation (DG) [1]. The analysis and optimization of smart grids with distributed generators requires performing a large number of power flow simulations, and each of them undergoes solving a nonlinear system of algebraic equations. In practice, the problems to be solved are parameterized. The free parameters (design variables and stochastic dimensions describing the randomness of energy supply and demand) lie in a multidimensional space to be explored.

The application of the Large Time Increment (LATIN) method [2], in this context is proposed as a nonlinear solver extremely well fitted for the particular nonlinear algebraic system to be solved. It is seen as an alternative to other standard approaches (Newton-Raphson, HELM...). Moreover, the LATIN is also combined with a Proper Generalized Decomposition (PGD) solver [3,4], in order to account for the parametric dependence in an explicit manner (location and nominal power of the generators, grid parameters...). The PGD-LATIN solution constitutes a computational vademecum and, accordingly, the exploration of the parametric space in view of solving any optimization problem is reduced to a simple post-processing.

Here, we focus on analyzing the errors committed calculating the system losses using the PGD-LATIN method. The system losses are considered to be the Quantity of Interest (QoI) to be assessed and the corresponding dual problem is readily introduced to make use of the goal-oriented error assessment machinery. Note that here, the error assessment is devised to account for the influence in the computed QoI of the LATIN solver (iterative scheme) and the PGD strategy (truncated separated representation).

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# Effectivity and limits of PGD computational techniques

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## ABSTRACT

Mechanics, like other domains, continues to supply numerous engineering problems that, despite the impressive progress of computational simulation techniques, remain intractable today. RB, POD and PGD model reduction methods are leading to a new generation of high-performance computational tools which provide solutions to engineering problems which are inaccessible to standard codes based on classical and well-established numerical techniques. This is a true breakthrough with a potential gain of several orders of magnitude.

The approach we are considering here is the Proper Generalized Decomposition (PGD) which can be seen as an extension of POD. The main idea consists in calculating the shape functions and the solution itself simultaneously *offline* using an iterative procedure. *A priori*, these shape functions are arbitrary and must satisfy only a variable separation hypothesis, this hypothesis being also at the center of POD and RB reduction methods.

First, the aim of the lecture is to examine the validity of the variable separation hypothesis, which is central in the PGD. For that, we use a benchmark proposed by S. Idelshon which is a unidimensional transient thermal problem with a moving load, the parameter being the velocity of the load. Non-separated shape functions are also studied. The second part of the lecture deals with the different techniques for the computation of PGD approximation. They include a new one based on the “PGD-error indicator” introduced in [2,3]. The reference to quantify the effectivity is the  $H^1$ -SVD of the “exact” solution. Some error estimators are also computed.

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# A “Tuning-free” multi-field reduced basis method with application to multiscale modelling.

- ADMOS 2015 -

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## ABSTRACT

The reduced basis method [1,2] is an increasingly popular reduced order modeling technique for parameterized partial differential equations. In this talk, we will present a new reduced reduced basis method for affinely parametrised elliptic PDEs based on the concept of two-field surrogates [2].

The main idea is to construct separate reduced bases approximations for the primal variable and for the flux of the elliptic PDE. The primal surrogate is constructed in such a way that it satisfies the Dirichlet conditions exactly, while the flux surrogate satisfies the balance equation of this field. In this context, the Constitutive Relation Error permits to compute a certain measure of the exact error that is made when solving these surrogates [3]. We use this error as a guide to construct an efficient reduced basis, through a greedy sampling of the parameter domain.

In a second step, we make this strategy goal-oriented, by minimising the error in the outputs of the reduced model, using the well-known adjoint methodology.

We show that the proposed strategy is significantly more efficient than state-of-the art alternatives in terms of computational costs, for a given level of accuracy. In addition, we show that the goal-oriented setting allows for the algorithm to be “tuning-free”: the only input parameter that is required from the engineer is the tolerance on the output of the computation. Finally, we show that this new reduced basis paradigm is easy to use and implement.

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# Effect of the separated approximation of input data in the accuracy of the resulting PGD solution

- ADMOS 2015 -

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## ABSTRACT

Separated representations are commonly used to avoid the so-called *curse of dimensionality*, that is, an exponential increase in the number of degrees of freedom with the number of dimensions. In order to use separated functions to approximate the solution of some Boundary Value Problem (BVP), the differential operators defining the BVP must be separable. This is the case, for example, of the Proper Generalised Decomposition (PGD). Separability of operators, in practice, requires separability of all the input data. For example, the diffusivity function in the bilinear operator in a Poisson equation must be separable. In the case the original data is not separable, it has to be approximated by a separated *approximation*. This approximation can be obtained by means of a singular value decomposition, proper orthogonal decomposition, higher-order singular value decomposition, or other similar techniques.

Thus, in addition to the classical error sources in the PGD context, namely the PGD truncation and the underlying finite-element discretisation, the error arising from using a separable approximation of the input data is also affecting the PGD solution.

In this work we study the error in the PGD solution due to the separation of the input data. This error is mainly controlled by two factors: i) the mesh of the parametric dimensions and ii) the number of terms involved in the separation of the input data. In the case of a Poisson problem separated in spatial coordinates, the error due to the separation of the diffusivity behaves linearly with the error of the PGD solution.

This source of error is eventually limiting the convergence of the solution because the data resolution establishes a threshold in the accuracy of the final approximation.

# Interpolation of the inverse of parameter dependent operator for preconditioning parametric and stochastic equations.

- ADMOS 2015 -

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## ABSTRACT

When solving partial differential equations with parametrized (or random) coefficients, one usually needs to solve high dimensional problems for a large number of realizations of the coefficients, which is computationally expensive. Model reduction techniques such as the Reduced Basis Method [4] or the Proper Generalized Decomposition [2] are now commonly used for the construction of approximation of the solution of such problems. The idea is to build a subspace on which a projection of the solution can be computed with a low computational cost. From a practical point of view, that subspace is constructed so that it minimizes some norm of the residual associated with the equation. In practice, we observe that a bad condition number of the operator leads to a poor approximation : preconditioning is necessary to achieve efficient model reduction.

There exist in the literature different definitions for the preconditioner. A widely used preconditioner is the inverse of the operator at a given parameter value [4], or the inverse of the mean operator in the context of uncertainty quantification. In [1], the authors propose an analytical interpolation of the inverse of the operator, and show the benefits of using a parameter dependent preconditioner.

We propose here different interpolation methods of the inverse of the operator for the construction of the preconditioner, and compare them. In particular, we show that the interpolation based on the projection of the identity matrix [3] with respect to the Frobenius norm seems to be the most appropriated strategy. In addition, we introduce a greedy algorithm for the construction of the preconditioner: the corresponding set of interpolation points results in a better preconditioner. Finally, numerical examples show that the quality of the model reduction (Reduced Basis or PGD) is significantly better when using the proposed preconditioner.

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# Adomian decomposition method in free vibration of stepped beam with restraint edges and resting on Winkler foundation

- ADMOS 2015 -

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## ABSTRACT

This work deals with free transverse vibration characteristics of an Euler-Bernoulli stepped beam resting on Winkler foundation. The ends of beam are elastically restrained against translation and rotation. A semi-analytical method, Adomian decomposition method, has been used to obtain characteristic equation of the beam. First three natural frequencies have been obtained. The effects of step length, height ratio, breadth ratio, translational and rotational spring stiffness, boundary conditions and foundation parameter have been studied on first three natural frequencies. Natural frequencies have been compared, wherever possible, and a close agreement of results is observed. Numerical results show the accuracy and efficiency of the method for the dynamic analysis of stepped beams resting on foundation. Corresponding mode shapes are also drawn. Frequency of stepped beam with uniform width decreases as the length of first section increases. Frequency of stepped beam having uniform thickness is oscillating. Frequency decreases as the thickness of second section decreases. The existence of foundation increases the values of frequency. The effect of width ratio is not uniform for all the three modes. With the increase in rotational and translational stiffness, frequency increases and becomes constant after certain values of rotational and translational stiffness parameters.

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# A Method of Analytical Decomposition in Analyses of Elastic Structures of Complex Geometry

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## ABSTRACT

The paper addresses the new numerical-analytical method for analyzing two-dimensional linearly elastic heterogeneous structures composed of a number of contiguous rectangles. For each rectangle we can build a common solution in a form of series with indeterminate coefficients. These coefficients are evaluated meeting boundary conditions of the whole structure and conjugation conditions of the contiguous areas.

The analytical method of superposition was used to build a general solution for the orthotropic/isotropic rectangle with arbitrary boundary conditions on its edges. This method was used in [1,2] to evaluate the stress fields in the two-dimensional elastic isotropic rectangle under symmetric loads on its opposite sides. The paper [3] reviewed the progress in the superposition method for the solution of boundary-value problems.

In this paper in accordance with the superposition method the general solutions for the orthotropic and isotropic rectangles are composed of two solutions obtained by the method of initial functions [4,5] in the form of trigonometric series with undetermined coefficients. The process of satisfying the boundary conditions leads to an infinite system of linear algebraic equations to determine the unknown coefficients in the solution. A simple reduction to a finite system is used to obtain a solution.

If a structure may be presented by a number of contiguous rectangles with finite dimensions then we can use general solutions constructed for each of the rectangles and get again an infinite linear algebraic system to determine unknown coefficients in all general solutions [6]. We name this approach a “method of analytical decomposition”. It can be used to analyze as homogeneous as heterogeneous structures.

An application of this method is demonstrated on analyzing the stress and strain state of a rectangle ( $x \in [0, h]$ ,  $y \in [0, a]$ ) loaded on the side  $x=0$  and clamped on two opposite sides ( $y=0, a$ ) with a number of cracks parallel to the axe  $Ox$  in in the neighborhood of the side  $x=h$ .

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# Utilizing Adjoint-based Error Estimates to Adaptively Resolve Response Surface Approximations

- ADMOS 2015 -

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## ABSTRACT

Uncertainty and error are ubiquitous in predictive modeling and simulation due to unknown model parameters and various sources of numerical error. Consequently, there is considerable interest in developing efficient and accurate methods to quantify the uncertainty in quantities of interest from computational models. Monte Carlo techniques are the standard approach to quantify the uncertainty in a computational model. Unfortunately, the number of samples required to accurately estimate certain probabilistic quantities, especially the probability of high-risk, low-probability events, may be prohibitively large for high-fidelity computational models. Many high-fidelity computational models require vast amounts of computational effort and thus the number of model evaluations that can be used to interrogate the uncertainty in the system behavior is limited. Therefore, any approximation of a probabilistic quantity of interest contains both deterministic (discretization) and stochastic (sampling) errors. Producing a reliable estimate of a probabilistic quantity requires that each of these sources of error be reduced to an admissible level. A number of recently developed methods for uncertainty quantification have focused on constructing response surface approximations (RSA) using only a limited number of high-fidelity model evaluations. The fact that a very large number of samples may be efficiently computed using the RSA effectively reduces the statistical component of the error. However, the deterministic component of the error may be quite large for each sample due to the standard sources of discretization error as well as the interpolation of the RSA. The accumulation of these deterministic errors may significantly affect the accuracy of the probabilistic quantity of interest.

In this presentation, we show how adjoint-based techniques can be used to efficiently estimate the error in a quantity of interest computed from a sample of a RSA [1]. We then show how these error estimates can be combined with adaptive sparse grid approximations to provide enhanced convergence, new adaptive strategies, and a means to avoid over-adapting the sparse grid beyond the accuracy of the spatial discretization [2]. Finally, we demonstrate that these a posteriori estimates can also be used to guide adaptive improvement of a RSA with the specific goal of accurately estimating probabilities of events [3].

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# Adaptive methods for efficient sampling in molecular dynamic simulations

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## ABSTRACT

I will present some numerical challenges raised by the simulation of materials at the atomistic level. One of the main difficulties is related to a timescale problem: at the molecular level, the typical timescale is much smaller than the timescale of interest at the macroscopic level. This is related to the fact that the stochastic process which models the evolution of the molecular system is metastable: it remains trapped for very long times in some regions of the phase space (called metastable states). Specific techniques have been devised in order to circumvent these problems, in order to sample efficiently the configurations and the trajectories.

In this presentation, I will focus on the configurational sampling problem. The question is then how to devise efficient sampling technique to sample multimodal measures in high dimension. I will present in particular adaptive biasing techniques which have been proposed in the molecular dynamics community to construct on the fly biasing potential, in order to more efficiently sample the target measure. These techniques can thus be seen as adaptive importance sampling methods.

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# Goal-based adaptive control of stochastic and deterministic errors in compressible CFD

- ADMOS 2015 -

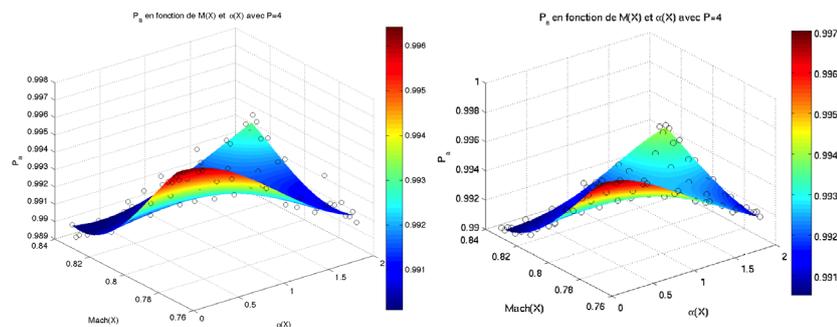
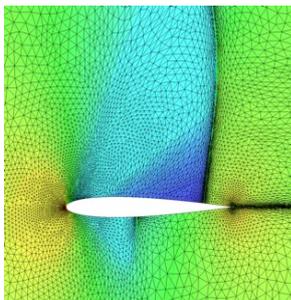
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## ABSTRACT

The purpose of this paper is to control both deterministic discretisation error and stochastic error for compressible CFD simulations when a quantity of interest is targeted. Recent works [2,4] have extended goal-based methodologies to problems with uncertain data, mostly by extending the well-known dual-weighted a posteriori error estimation to the stochastic error. Nevertheless several non-trivial questions remain to be addressed. Our goal is to build a goal-oriented method for anisotropic adaptive control of both deterministic and stochastic errors. An a priori error estimator is used as refinement criterion for anisotropic meshes. Anisotropy in the deterministic space is controlled for a functional of interest via a riemannian metric (hessian) based method (see [1]), while h and h-p refinement will be applied to the stochastic space where an anisotropic refinement criterion based on the local variance is considered (see [3]). Performance of the proposed approach is illustrated on 2D and 3D numerical experiments for shock-dominated flows. We represent the stochastic component of the solution by a piecewise polynomial approximation in a finite probability space. The results obtained in an initial investigation for a transonic flow around a NACA0012 airfoil are shown in the images below: goal-based adapted mesh (left image), stochastic response on uniform meshes (middle image) and stochastic response for adaptive meshes (right image) with uncertain Mach number and angle of attack. The improvement of the stochastic response is visible not only as a decrease of the overall error on the quantity of interest but also by an improvement of the statistics.



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# Fast r-adaptivity for multiple queries of heterogeneous stochastic material fields

- ADMOS 2015 -

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## ABSTRACT

The Monte Carlo approach in stochastic modeling requires multiple queries to numerical (typically finite element) solutions of similar problems. In the case of random material fields, only the material properties vary between different realizations, often representing perturbations of a simple material description around a reference configuration (typically a uniform material field). The different instances of the Monte Carlo sampling are usually computed with the same finite element mesh, which is designed to provide a reasonable accuracy in the case of the average material field. However, this mesh is not accounting for the actual realization of the stochastic material field and therefore it does not obtain the maximum accuracy that could be achieved with the computational resources employed. The possibility of designing a new mesh from scratch for each Monte Carlo realization is not realistic: the computational cost of redesigning the mesh based on the fluctuating material field is unaffordable when the number of Monte Carlo samples increases. Moreover, the perturbations in the material field are not expected to require a drastically different mesh. Note for instance, that the local mesh refinement resolving the patterns in the solution associated with the geometrical features of the domain are kept constant all along the Monte Carlo process. The strategy proposed in this paper consists in modifying for each realization a mesh designed to be efficient in the reference (unperturbed) case. The mesh is then modified following an r-adaptive scheme at each Monte Carlo realization. The mesh adaption is performed on the basis of simple criteria accounting for the actual (perturbed) material field. Note that the r-adaptive approach suits the needs of the current scope (optimal distribution of the computational resources, having set a priori the number of degrees-of-freedom) but does not allow guaranteeing the final accuracy of the results obtained.

# A POSTERIORI ERROR ESTIMATION FOR PARTIAL DIFFERENTIAL EQUATIONS WITH SMALL UNCERTAINTIES

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**Key words:** uncertainty quantification, *a posteriori* error analysis, perturbation method, PDEs with random input

**Abstract.** Partial differential equations (PDEs) are widely used for modelling problems in many fields such as physics, biology or engineering. In general, any problem is affected by a certain level of uncertainty, due to the intrinsic variability of the system or the inability to adequately characterize all the involved input. Nowadays, it is common to include uncertainty in the mathematical models describing such complex systems, using for instance probability theory characterizing the uncertain input by random variables or more generally by random fields.

The purpose of this work is to perform *a priori* and *a posteriori* error analysis for PDEs with random input data. We consider small uncertainties and adopt a perturbation approach expanding the exact (random) solution  $u$  of a given problem up to a certain order as

$$u(\mathbf{x}, \omega) = u_0(\mathbf{x}) + \varepsilon u_1(\mathbf{x}, \omega) + \varepsilon^2 u_2(\mathbf{x}, \omega) + \dots \quad (1)$$

where  $\varepsilon$  is a parameter that controls the amount of randomness in the input data. Uncoupled deterministic problems can be derived to find each term in the expansion, the previous term being needed to compute the next one. Each of these problems can be solved approximately using for instance the finite element method (FEM). We derive *a*

*priori* and *a posteriori* error estimators in various norms for the error between the exact solution and an approximation of a certain order. For instance for the first order approximation, which requires the resolution of only one deterministic problem, we obtain an *a posteriori* error estimator constituted of two computable parts, namely a part due to FE discretization (which depends on the mesh size) and another part due to the uncertainties affecting the input data. This estimator, easy and cheap to compute, can then be used for mesh adaptation to balance the two sources of error.

We apply this method to several classes of problems. We first consider the linear elliptic problem

$$-\operatorname{div}(a(\mathbf{x}, \omega) \nabla u(\mathbf{x}, \omega)) = f(\mathbf{x}) \quad (2)$$

where the random diffusion coefficient  $a$  depends in an affine way on a finite number of independent random variables. The derivation of *a priori* and *a posteriori* error estimates in various norms for the first order approximation  $u \approx u_{0,h}$ , with  $u_{0,h}$  the continuous, piecewise linear finite element approximation of  $u_0$ , is detailed in [1]. The analysis is straightforwardly extended to higher order approximations and to some class of nonlinear problems. We then consider the steady Navier-Stokes equations on randomly perturbed domains and, in particular, the flow past a cylinder with perturbation of the center or the outer shape of the cylinder. A stochastic mapping is introduced which transforms the original problem to PDEs on a deterministic reference domain with random coefficients. Finally, we consider the heat equation with random (Robin) boundary conditions. For this time-dependent problem, the *a posteriori* error estimator contains a third term due to time discretization.

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# Variance reduction in random homogenization : Special Quasirandom Structures

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Joint work with C. Le Bris and F. Legoll (École des Ponts, INRIA)

**June, 7–10 (Nantes)**

In this work, we introduce a variance reduction approach for the homogenization of a random, linear elliptic second order partial differential equation set on a bounded domain in  $\mathbb{R}^d$ . The random diffusion coefficient matrix field  $A(\frac{x}{\varepsilon}, \omega)$  is assumed to be uniformly elliptic, bounded and stationary (“periodic in law”). In the limit when  $\varepsilon \rightarrow 0$ , the solution of the equation converges to that of a homogenized problem of the same form, the coefficient field of which is a deterministic and constant matrix  $A^*$  given by an average involving the so-called corrector function that solves a random auxiliary problem set on the *entire* space.

In practice, the corrector problem is approximated on a bounded domain  $Q_N$  as large as possible. A by-product of this truncation procedure is that the *deterministic* matrix  $A^*$  is approximated by a *random*, apparent homogenized matrix  $A_N^*(\omega)$ . We therefore introduce a variance reduction approach to obtain practical approximations of  $A^*$  with a smaller variance in order to reduce the statistical error. We derive conditions (e.g. exact fraction in a bi-composite) for the selections of finite supercell environments on which we solve the corrector equation.

# Uncertainty Quantification in Porous Media with Multi-Level Monte Carlo

- ADMOS 2015 -

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## ABSTRACT

Geological storage of CO<sub>2</sub> is an attempt at controlling future climate changes. Modelling and simulation of underground CO<sub>2</sub> storage are however subjected to significant sources of geological uncertainties, which requires the use of stochastic approaches. Sources of uncertainties in the CO<sub>2</sub> storage problem can be classified as either geological, physical, or operational uncertainties. Ranking the importance of the model parameters based on their influence can provide a better understanding of the system. Computationally efficient methods for sensitivity analysis, uncertainty quantification, and probability risk assessment are therefore needed. Furthermore, due to the computational complexity of such problems, as even a single deterministic simulation may require parallel high-performance computing, stochastic simulation techniques based on standard Monte Carlo are currently inefficient for these problems. To overcome the prohibitive computational cost of standard Monte Carlo, we propose a Multi-Level Monte Carlo technique to estimate statistical quantities of interest within some prescribed accuracy constraint. We illustrate and verify our proposed approach by a comparison with a Monte Carlo simulation using a common benchmark problem for CO<sub>2</sub> injection. We obtain a significant computational speed-up compared with Monte Carlo.

# Sparse generalized polynomial chaos expansion for non-intrusive uncertainty quantification in aerodynamic computations

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## ABSTRACT

Because of the high complexity of steady-state or transient fluid flow solvers, non-intrusive uncertainty propagation techniques have been developed in aerodynamic simulations for the consideration of random inputs such as the operational conditions or some geometrical data of the profile. Polynomial surrogate models based on dedicated collocation sets or generalized polynomial chaos (gPC) have usually been implemented [1,2], though kriging-based or radial basis function surrogates may also be envisaged [3]. Polynomial representations suffer from the so-called curse of dimensionality when the number of inputs increases since the evaluation of the expansion coefficients becomes intractable in this situation. Sparse quadrature rules may be achieved using the algorithm proposed by Smolyak (see *e.g.* [1] and references therein), but we envisage in this work to use the sparsity of the output signal, or quantity of interest, in trying to circumvent the dimensionality concern. Indeed, sparsity in the gPC basis expansion is expected to be enhanced in higher dimensions, where it is commonly observed that many cross-interactions between the input parameters are actually negligible. This yields only a small fraction of the polynomial coefficients to be significant, hence a sparse signal. In this context the number of samples needed for the synthesis is typically less than the one anticipated by the Shannon sampling theorem. We therefore expect to achieve a successful signal recovery by the techniques known under the terminology of compressed sensing [4], which are reported to be highly efficient for such sparse signals using incoherent random projections for their reconstruction. The procedure shall be illustrated on some basic examples of flow simulations about uncertain profiles, or fluid-structure interaction test cases with uncertain structural parameters.

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**Spectral-based numerical method for Fokker-Planck-Kolmogorov equations in  
infinite dimensional Hilbert spaces.  
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**ABSTRACT**

We propose a numerical method for approximate the solution of a class of infinite dimensional parabolic problems. In particular, for the Fokker-Planck-Kolmogorov (FPK) equations in an infinite dimensional Hilbert space. The FPK equations are partial differential equation that describe the time evolution of the probability density function of the velocity of a particle under the influence of drag forces and random forces, it is a kind of continuity equation for densities. This type of equations have been deeply studied in the last years, see for instance [1], [2], [3], [4] and the references therein.

In a separable infinite-dimensional Hilbert space  $\mathcal{H}$  with inner product  $\langle \cdot, \cdot \rangle_{\mathcal{H}}$  we define a Gaussian measure  $\mu$  with mean zero and nuclear covariance operator  $\Lambda$  with  $Tr(\Lambda) < +\infty$ .

We focus on the stochastic differential equation in  $\mathcal{H}$

$$dX_t = AX_t dt + B(X_t)dt + \sqrt{Q}dW_t, \quad (1)$$

where the operator  $A : \mathcal{D}(A) \subset \mathcal{H} \rightarrow \mathcal{H}$  is the infinitesimal generator of a strongly continuous semigroup  $e^{tA}$  in  $\mathcal{H}$ ,  $Q$  is a bounded operator from another Hilbert space  $\mathcal{U}$  to  $\mathcal{H}$  and  $B : \mathcal{D}(B) \subset \mathcal{H} \rightarrow \mathcal{H}$  is a nonlinear mapping.

The equation (1) can be associated to a Kolmogorov equation in the next way, we define

$$u(t, x) = \mathbb{E}[u_0(X_t^x)], \quad (2)$$

where  $u_0 : \mathcal{H} \rightarrow \mathbb{R}$  and  $X_t^x$  is the solution to (1) with initial conditions  $X_0 = x$  where  $x \in \mathcal{H}$ . Then  $u$  satisfies the Kolmogorov equation:

$$\frac{\partial u}{\partial t} = \frac{1}{2}Tr(QD^2u) + \langle Ax, Du \rangle_{\mathcal{H}} + \langle B(x), Du \rangle_{\mathcal{H}}. \quad (3)$$

We propose a based-spectral numerical method for the Equation (3) in the following way.

$$u(t, x) = \sum_{n \in \mathcal{J}} u_n(t)H_n(x), \quad x \in \mathcal{H}, \quad t \in [0, T], \quad (4)$$

where  $u_n : [0, T] \mapsto \mathbb{R}$  and  $H_n(x)$  are the Hermite functionals which take values on  $\mathcal{H}$ .

After some calculations the Kolmogorov equation becomes

$$\sum_{n \in \mathcal{J}} \dot{u}_n(t)H_n(x) = - \sum_{n \in \mathcal{J}} u_n(t)\lambda_n H_n(x) + \sum_{n \in \mathcal{J}} u_n(t)\langle B(x), D_x H_n(x) \rangle_{\mathcal{H}} \quad (5)$$

By truncation the infinite system (5) we obtain a matrix differential equation and by solving it we fix the functions  $u_n(t)$  and then we set up the numerical solution by using (4).

We test the method for the simple case of a 1-d diffusion and we will present the description of the method and the results for this test case. The future of the research is apply this method to the solution of the stochastic Navier-Stokes equations and study the stability of the method, rate of convergence of the approximations to the theoretical solution.

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# A real time solution reconstruction and material identification with data obtained from measures in combination with the Proper Generalized Decomposition

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## ABSTRACT

Some industrial processes, such as polymer curing, require control algorithms in order to guarantee a certain level of quality for the components that are being processed. These control algorithms work in a real time constraint because they need to modify, on-line, the operating parameters. Additionally, the material parameters, such as the diffusion coefficient, are not necessarily constant along time or, in some situations, they are simply unknown. This makes difficult that existing techniques provide, in real time, enriched information about the process to the control algorithm. In this work we propose a novel approach that makes use of a reduced basis obtained from the multi-parametric solution provided by the Proper Generalized Decomposition [1]. This reduced basis accounts with the explicit dependence of the solution of the parameters. Thus, by only solving a system of equations of the size of the reduced bases, we are able to both, obtain the reconstructed solution and identify the parameters that define it. Additionally, we also augment the method with a technique to place the sensors where best suits to the reduced bases, based on the Discrete Empirical Interpolation Method (DEIM) [2]. Finally we provide an *a priori* error indicator, with upper-bounding properties, useful to evaluate the size of the reduced bases for a certain level of accuracy, and also an *a posteriori* error indicator to control the accuracy of the results.

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# Real-time model updating using modified CRE, Kalman filtering, and PGD-reduced models

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## ABSTRACT

The DDDAS concept has received an increasing interest during the last decade, in particular in the Computational Mechanics community [1]. The main idea is to create a feedback loop between a real system and its numerical model, in order to: (i) control the evolution of the system using model predictions; (ii) update model parameters using data measured on the physical system. A potential application may be structural health monitoring with real-time identification and control of damage evolution in composite materials [2].

In this talk, we focus on the identification step and model updating procedure; this requires solving an inverse problem which is usually *ill-posed*. In order to address this issue, many approaches are possible [3] such as deterministic approaches based on the definition of a cost function with regularization techniques, or stochastic approaches using Bayesian inference.

The approach we propose is based on a coupling between the (stochastic) Kalman filtering [4] and the (deterministic) modified Constitutive Relation Error (mCRE) tool [5]. On the one hand, Kalman filtering enables effective data assimilation and prediction of system evolution from incomplete information; it can be extended to non-linear systems. On the other hand, mCRE is a robust and powerful tool for complex model identification; leaning on energy functionals as well as duality and convexity properties, it has the ability to identify model parameters from highly corrupted data [6]. In order to reach the “real-time” feature of the inverse method, mCRE is here associated with reduced order modelling based on Proper Generalized Decomposition [7,8]. The proposed data assimilation strategy is applied to several mechanical problems with real-time identification/updating of evolving boundary conditions, thermal source localizations, or material parameters.

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# Identification of heterogeneous elastoplastic behaviors using constitutive equation gap method

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## ABSTRACT

Cohesive zones models are commonly used in numerical simulations to take into account the onset and the propagation of microcracks leading to the fracture of materials. Their numerical implementation in finite element schemes is based on embedding surface traction-separation law between two adjacent bulk elements. The traction between two neighboring elements is linked to the corresponding opening by a cohesive relationship.

The objective of the work reported here is to extend the approach developed in [1, 2] to identify the shape and parameters of the cohesive zone models in metal matrix composites with brittle inclusions and adapt this method to the study of initially heterogeneous material (*e.g.* graded metals or ceramics).

To treat these applications where mechanical fields are heterogeneous, local stress fields are to be estimated in addition to conventional kinematic fields to build the energy balance associated with the transformation. Here we propose to estimate these fields by an identification method using kinematic and thermal data from imaging. The proposed method is based on the minimization of a functional associated with the error in constitutive relation (Constitutive equation gap method) [3]. In its classical (mechanical) formulation, this functional depends on two sets of parameters: the stress field and the mechanical material properties (elasticity, plasticity, damage).

We show here that the identification procedure is capable to estimate the stress fields and material properties for elastic and elastoplastic behavior. The method was applied on noisy measured displacement fields to assess its robustness in the case of elastic behavior. The method is now being extended to damageable plasticity. The introduction of a second (calorimetric) term in the functional, related to the heat sources is also examined.

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# Real-Time Object Tracking Based On Sequential Frames

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## ABSTRACT

Although real-time object tracking is not a new problem in research in the field of computer vision, it still remains a problem that continues to receive much attention from researcher. Many approaches have been developed so far and documented in the literature. This presentation is an attempt to propose a new approach for real-time object tracking. Our approach is Fast Silhouette Determination Algorithm (FSD Algorithm), a fast algorithm to find the difference between two sequential frames based on the motion of an object in front of the camera to determine which pixels have changed from one frame to the other. Once the pixels have been identified, noise is eliminated from the data using some morphological operations and noise reduction filtering. The last step of the algorithm is to determine the silhouette based on the contours of the areas that contain a combination of neighboring pixels and calculate the position of the silhouette within the frame. Accordingly, this algorithm allows for tracking multiple types of objects that do not depend on the shape or the color of the object.

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# A study of the sensitivity of a sequential variational data assimilation algorithm to the errors of the input data

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## ABSTRACT

An automated system of air monitoring is being developed in Ust-Kamenogorsk city. This system should be able to model contamination and assess air condition. It contains data assimilation module for chemistry composition measurements. Its data assimilation algorithm is based on variational approach and adjoint problem methods. In the present paper we consider results of sensitivity studies of the data assimilation algorithm for convection-diffusion model to various input data perturbations. Sensitivity study allows to make a conclusion on the relative importance of input variables for the data assimilation algorithm, to identify key variables and identify ones that may be excluded from consideration.

The model of pollutants transport and turbulent diffusion can be expressed in the operator form:

$$\frac{\partial \phi(x, t)}{\partial t} + A(Y)\phi(x, t) = f(x, t) + r(x, t), (x, t) \in D_t$$

$$\phi(x, 0) = \phi_0(x), \quad x \in D$$

Here  $A$  is a "spatial" matrix operator;  $f$  – a priori source functions;  $\phi(x, t)$  - state-function (concentrations);  $\phi_0(x)$  - initial state,  $D_t = D \times [0, t]$ ,  $D$  – spatial domain;  $t \in [0, t]$  - time interval;  $Y$  - vector of model parameters. Control variable for the assimilation is the emission rate  $r$ . Solution of the data assimilation problem is sought as the minimum of target functional combining a norm of control function and a discrepancy between the modeled and measured data [1,2].

Errors may be in the initial data (which is uncertain), in the assimilated measurements data (due to the instrument errors) and also coefficients of chemical transport model may contain errors due to the imperfect numerical modeling of meteorological parameters [3]. In this paper we performed numerical experiments to determine the sensitivity of the data assimilation result to the noise in the observations, as well as the sensitivity to perturbations in meteorological fields (model coefficients).

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# Sparse grid, reduced basis approximation for Bayesian inverse problems

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## ABSTRACT

Bayesian inversion has emerged in recent years as a very effective and versatile methodology for solving inverse problems in, e.g. oil recovery, weather forecasting, medical imaging etc. It amounts to predict, for given noisy observation data of a system output, the solution of the Bayesian inverse problem as the posterior distribution of the unknown system input based on some proper assumption on the prior distribution. The distributed uncertain system input is parametrized by random fields represented by high or possibly infinite dimensional random variables. Bayesian prediction amounts to integration over the parameter space. Numerical quadrature faces the curse of dimensionality.

In order to tackle these challenges, adaptive algorithms play a crucial role. To deal with curse of dimensionality, we explore sparsity of the posterior ([4]) and employ dimension-adaptive interpolation and integration algorithms based on sparse grid ([5,6]). Fidelity-adaptive algorithms based on hierarchical model order reduction techniques, particularly the reduced basis method, from [1,2] are extended to address the large-scale computation as well as the curse of dimensionality. To this end, an efficient and accurate sparse grid, reduced basis algorithm is proposed for computational Bayesian PDE inversion.

The proposed framework allows to solve a large range of PDE-based Bayesian inverse problems. We present its application for inverse scattering problem and demonstrate the superior computational property and identify some further difficulties. Work supported in part under ERC Advance Grant No. 247277.

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# On the predictive capabilities of multiphase Darcy flow models

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## ABSTRACT

Darcy's law is a widely used model and the limit of its validity is fairly well known [1]. When the flow is sufficiently slow and the porosity relatively homogeneous and small, Darcy's law is the homogenized equation arising from the Stokes and Navier-Stokes equations and depends on a single effective parameter (the absolute permeability). However when the model is extended to multiphase flows, the assumptions are much more restrictive and less realistic. Therefore it is often used in conjunction with empirical models (such as relative permeability and capillary pressure curves), derived usually from phenomenological speculations and experimental data fitting.

In this work, we present the results of a Bayesian calibration of a two-phase flow model, using high-fidelity DNS numerical simulation (at the pore-scale) in a realistic porous medium [2]. These reference results have been obtained from a Navier-Stokes solver coupled with an explicit interphase-tracking scheme. The Bayesian inversion is performed on a simplified 1D model in Matlab by using adaptive spectral method [3]. Several data sets are generated and considered to assess the validity of this 1D model.

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# Adaptive Response Surface Approximation Method for Bayesian Inference

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## ABSTRACT

The need for surrogate models and adaptive methods can be best appreciated if one is interested in parameter estimation using a Bayesian calibration procedure for validation purposes [1,2]. We extend our work on error decomposition and adaptive refinement for response surfaces [3] to the development of a surrogate model that can be utilized to estimate the parameters of Reynolds-averaged Navier-Stokes models. The error estimates and adaptive schemes are driven here by a quantity of interest and are thus based on the approximation of an adjoint problem. The desired tolerance in the error of the posterior distribution allows one to establish a threshold for the accuracy of the surrogate model. Particular focus is paid to accurate estimation of evidences to facilitate model selection.

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# A Posteriori Analysis for Nonlinear Eigenvalue Problems, Application to Electronic Structure Calculations

- ADMOS 2015 -

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Work done in collaboration with Eric Cancès, Yvon Maday, Benjamin Stamm and Martin Vohralik.

## ABSTRACT

Many mathematical models aiming at the determination of electronic structures give rise to nonlinear eigenvalue problems whose resolutions require very large computational resources [1]. The complexity of these computations reflects, among others, the chosen discretization and the chosen (possibly iterative) algorithm. The *a posteriori* analysis of such problems enables to reduce the computations involved to solve the problem by first giving a guaranteed upper bound on the total error and second by separating the error components stemming from the different sources and controlling each of them. This makes possible to iteratively fit these discretization parameters leading to small error at low computational cost [3].

We shall first present a full *a posteriori* analysis for a simple but representative one-dimensional Gross-Pitaevskii type equation, in a periodic setting with planewave (Fourier) approximation. The nonlinear discretized problem is solved with a Self-Consistent Field (SCF) algorithm, which consists in solving a linear eigenvalue problem at each step. To start with, we provide a computable upper bound of the energy error. We then separate this bound into two components, one of them depending mainly on the dimension of the discretized space, the other one on the number of iterations done in the SCF algorithm. This enables to adaptatively choose between refining the discretization and performing SCF iterations, as we try to balance the error components. We also illustrate numerically the coherent performances of this *a posteriori* analysis. We then postprocess the approximate solution (eigenvalue and eigenfunction) using a linear perturbation theory based on residual computation [2]. This theoretically and numerically reduces the error significantly both for the eigenvalue and the eigenfunction.

This work is a first step towards an *a posteriori* analysis and postprocess of more complex electronic structure models like Hartree-Fock or Kohn-Sham models. We shall present the first results for the extension of our results in this framework.

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# A discontinuous Galerkin goal-oriented error estimator based on orthogonal discrete dual spaces

- ADMOS 2015 -

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## ABSTRACT

Goal-oriented error estimation [1] has seen increasing interest for adaptive discretizations of engineering problems, as these methods aim to minimize the error in the quantity of interest that motivates the engineering analysis in the first place. However, the main disadvantage of deriving refinement indicators based on goal-oriented error estimators is that an additional “dual problem” needs to be solved, often in higher resolution than the primal problem, comparing badly with the simpler estimators requiring only local operations in terms of the computational cost.

In this work, we aim to reduce the cost of approximating the dual solution. Taking inspiration from the fact that often its interpolation on the primal mesh is subtracted from the approximate dual solution in obtaining localized refinement indicators, we propose to discretize the dual problem using a space orthogonal to the primal discretization space. We assume to start with a discrete dual space that is a strict superset of the primal discretization space and decompose it into coarse and fine parts and only use the fine-scale solution, discarding the coarse problem. We then apply the ideas originating from the variational multiscale framework [2] to take care of the influence of the discarded coarse scales on the finer resolved scales. We prove that under certain conditions the fine-coarse coupling can be chosen to disappear altogether, resulting in a cheap error estimator identical to the conventional and more expensive estimator based on dual discretizations using a refinement of the discrete primal spaces.

We choose to apply these concepts to the discontinuous Galerkin methods [3], leveraging the simplicity of constructing orthogonal bases for discontinuous polynomial spaces. We numerically investigate the quality of the resulting estimator for a 1D convection-diffusion problem with varying Peclet numbers. Our preliminary results indicate that the proposed estimator performs exceptionally in the diffusion-dominated range; however, the dependence on the choice of the projection in splitting the scales and whether or not a coarse scale model is employed appears to be very significant in the advection-dominated regime.

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# An adaptive inexact Uzawa algorithm based on polynomial-degree-robust a posteriori estimates for the Stokes problem

- ADMOS 2015 -

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## ABSTRACT

In this paper, we are interested in designing an adaptive version of the inexact Uzawa algorithm [4] applied to the linear Stokes problem solved by the finite element method. We present an a posteriori error estimate based on the equilibrated flux reconstruction which can distinguish the different error components, namely the discretization error component, the inner algebraic error component, and the outer Uzawa iteration error component. Following the ideas of [1, 3], on each outer Uzawa iteration step and on each inner linear solver iteration step, we prove that our estimate gives a guaranteed upper bound on the overall error as well as a polynomial-degree-robust local efficiency as in [2]. Our adaptive inexact algorithm stops the outer Uzawa iteration or the inner linear algebraic solver iteration when the Uzawa error component or the algebraic solver error component, respectively, do not have a significant influence on the overall error. With our adaptive inexact Uzawa algorithm, the unnecessary iterations on the inner algebraic solver as well as those of the outer Uzawa iteration can be avoided. The developed framework covers all standard conforming and conforming stabilized methods. The implementation into the FreeFem++ programming language [5] is invoked, and two numerical examples showcase the performance of our adaptive strategy.

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# An adaptive scheme for homogenised domains

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## ABSTRACT

In this paper, we extend the concept of modelling error estimation for the homogenisation of elliptic PDEs. In order to do so, we fully acknowledge that the rapid spatial variation of microscopic diffusion constants cannot be known exactly. Therefore, we represent the microscopic diffusion coefficients as a random field. In this context, the accuracy of surrogate models, such as homogenisation schemes, can be quantified by estimating the error in the first moments of the probability density function of a quantity of interest.

We propose a way to bound the error in the two first moments, following and extending the seminal work of [1]. Our derivations rely on the Constitutive Relation Error[2] (CRE), which states that a certain distance between the solutions delivered by the primal and a dual surrogates of the original stochastic problem is equal to some measure of the exact and unaffordable errors. We further assume that these surrogates are deterministic, consistently with the theory of homogenisation. Minimising the CRE in this subset of homogenisation schemes leads us to an optimal surrogate that is closely related to the classical Voigt and Reuss models. This result is used in a goal-oriented setting to establish upper and lower bounds for the first two moments of the quantity of interest.

We show that the method respect the numerical separation of scales, and is therefore affordable and easy to implement, and that it produces useful results as long as the mismatch between the diffusion coefficients of the microstructure remains small. We will propose extensions for the case of high mismatch, by allowing the surrogate solutions to fluctuate in the stochastic domain.

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# A posteriori estimation of modelling error for a building thermal model

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## ABSTRACT

In the past decade, efficient energy use for civil buildings receives big attention, especially through optimal control which is meant to minimize energy consumption and maintain occupant comfort. Different thermal models can be considered in both theoretical and practical use. In our case we focus on a building model in which thermal dynamics of envelopes and zones are described respectively by a parabolic PDE coupled with an ODE (cf. [4]).

For various technical and numerical reasons, model simplification is necessary in practice. In this case, modeling errors should also be taken into account. In our paper, we investigate the impact of the modeling error on some quantity of interest such as the average temperature.

More precisely, we are interested in estimating quantitatively the bounds of the error on the quantities of interest due to model simplification through *a posteriori* error estimators which could be later used to choose the appropriate simplified model for optimal control purpose.

In this paper, we apply and extend the adaptive modeling strategy of elliptic PDEs (cf. [5], [6]) to a building thermal model: parameter homogenization for a single PDE system. For the steady case, the upper and lower bounds between the fine and simplified models are obtained through a dual approach as in the literature. We use the solutions of primal and dual problems associated to the simplified model and the parameters are assumed to be known. For the unsteady case the upper bound is obtained using similar technique.

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# Space-Time Decomposition of A Posteriori Error Estimate for Linear and Nonlinear Parabolic Equations with Semi-Implicit Schemes

- ADMOS 2015 -

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## ABSTRACT

In recent years there has been a growing interest in a particular class of nonlinear parabolic equations known as phase-field models, which is characterised by evolving diffuse interfaces instead of sharp interfaces. These models are energy dissipative and mass conservative. Moreover, these models exhibit alternating fast and slow variations in time and impose severe demands on the resolution of the interface. There are many semi-implicit finite difference time-stepping schemes which inherit these properties at the discrete level [1]. Obviously, to efficiently and accurately simulate these problems, there is a need to employ a posteriori error estimates to drive adaptive mesh refinement and adaptive time-step selection for fully discrete schemes.

In this contribution, we introduce a general space-time adaptive framework for linear and nonlinear parabolic equations, based on a duality-based two-level error estimator [2]. The framework employs semi-implicit time-discretizations combined with Galerkin finite elements in space. According to Verfurth's decomposition [3], we split the global space-time error estimate into a spatial part and a temporal part, and develop an efficient space-time adaptive refinement methodology. A blockwise adaptive approach is one of the key strategies, which has been discussed and developed by Carey et al [4]. Following this idea, we divide the time domain into blocks, and apply the adaptive algorithm for each block. Several numerical experiments are presented to demonstrate the proposed adaptive algorithm.

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# Active learning surrogate models for the conception of systems with multiple failure modes.

- ADMOS 2015 -

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## ABSTRACT

The conception (or risk assessment) of complex mechanical systems has to take into account a series of constraints. Such constraints can be due to certification criteria, performance objectives, cost limitations, and so on. In this context, the role of simulation has kept increasing for the last decades, as it should be able to predict if a given configuration of the system is likely to fulfill these constraints without having to build it and to test it experimentally. In many cases, the computation of these constraints is associated with a series of computer software, whose physics can vary a lot. For instance, in the car industry, the conception of a new vehicle can be subjected to constraints on its size and weight, which are rather easy to compute, but also on its emergency stopping distance, its crash or aerodynamic resistance, which can be much more difficult to evaluate. Thus, several software (structure dynamics, multibody modeling, fluid dynamics software for instance) are generally needed to verify all the constraints.

Numerical methods to identify the limits of such “conception domains”, that is to say domains in which all the constraints are verified, are needed [1]. As the computational costs associated with the constraints can be very different, the question then arises of how to optimize the number of evaluations of each code to minimize the uncertainties about these limits, for a given computational budget.

In this prospect, this paper presents an innovative approach to predict the limits of the considered conception domain, but also to quantify the uncertainty associated with this prediction. Based on an adaptive Gaussian process regression, this method allows us to find iteratively the new code evaluations that will maximize the knowledge about the searched limits at the minimal computational cost.

First, the scientific basis of such an approach will be presented. The efficiency of such a method will then be illustrated on an analytical example.

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# Hybridizable discontinuous Galerkin degree-adaptive computations

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## ABSTRACT

Discontinuous Galerkin methods (DG) are finite element methods that are locally conservative and stable, and allow to achieve high order accuracy. The interest in DG methods has increased in the last years since they proved to be suited for the construction of robust high-order numerical schemes on arbitrary unstructured and non-conforming grids, for a variety of physical phenomena.

The main drawback that has always been claimed for DG methods is the increased number of degrees of freedom (DOF) respect to continuous methods (CG). However, a novel DG approach has been recently proposed that allows to drastically reduce the coupled DOF of the computation seeking for an approximation of the solution that is defined only on the faces of the mesh: the hybridizable discontinuous Galerkin method (HDG). Furthermore, the particular choice of the numerical fluxes driven by the hybridization technique allows to obtain an optimally converging solution not only for the primal unknown but also for its derivative. This characteristic allows to perform a post-process that provides a super-convergent solution.

The discontinuous character of the solution provides an optimal framework for a degree-adaptive technique. Degree-adaptivity further reduces the number of degrees of freedom in the HDG computation by means of degree-refining only where more precision is needed. The post-processed solution of HDG can be used to construct a cheap and reliable error estimator that drives an element by element modification of the approximation degree.

The proposed degree-adaptive HDG method is compared with high-order degree-uniform HDG computation and also high-order CG computation with static condensation of the interior nodes. Two challenging problems are considered for the comparison: a non-homogeneous scattering problem over an unbounded domain and the motion of a viscous incompressible flow.

# Dirichlet boundary conditions in sequences of Cartesian grids using a stabilized Lagrange multipliers technique based on recovered tractions

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## ABSTRACT

The procedures used in the standard FEM to apply the boundary conditions cannot be used within the framework of immersed boundary methods, as in these methods the FE nodes do not generally lay on the boundary. The case of the Neumann boundary conditions is solved taking into account that the elements can be cut by the integration surface not necessarily on element faces, as they do in the standard FEM. However, the case of the Dirichlet boundary conditions is much more complex.

To solve the problem, a common alternative is to use the Lagrange multiplier technique. Nevertheless, it can be difficult to find a compatible discretization of displacements and multipliers that satisfies the *InfSup* condition. In practice, the main problem appears when the number of Lagrange multipliers is too high, which can cause undesired oscillations in the Lagrange multiplier field. This is an open problem, and several approaches based on stabilized methods have been presented recently. The alternative implemented in this work consists of a stabilized Lagrange multiplier method suitable for cases where a sequence of successively *h*-refined hierarchical Cartesian grids meshes [1] is used in the analysis.

In this contribution the stabilization term are the tractions evaluated from the recovered field [2] on the Dirichlet boundary. The solution for each mesh *i* is obtained via an efficient iterative process (the system matrix remains constant through the process) where the recovered tractions are updated in each step [3]. The hierarchical data structure of the Cartesian grids allows to easily and efficiently project the recovered tractions evaluated in mesh *i-1* to the current mesh *i* in order to initialize the iterative process.

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# An adjoint approach to determine the optimal source term for modelling vortex generators

- ADMOS 2015 -

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## ABSTRACT

Vortex generators (VGs) are a commonly used means of passive flow control, often applied on e.g. wind turbines. They introduce streamwise vortical structures that provide mixing of the inner part of a boundary layer, thus adding energy to the flow and thereby reducing the susceptibility to flow separation. The large difference in scale between VGs and the surface of application, however, prohibits direct inclusion of these small structures into numerical meshes. Instead, usually the effect of the VG on the flow is modelled by the addition of a suitable source term to the governing equations, based on an approximate analytical model like e.g. [1]. Although being cheap to evaluate, this approach is insufficient to capture all relevant downstream flow characteristics, especially on the coarse grids usually made use of.

In this contribution we investigate how such a source term modelling approach can be improved. To this end we aim to find the optimal source term distribution in order to represent the characteristics of a given high-fidelity 3D flow field on a low resolution mesh. This high-fidelity solution is obtained using an incompressible RANS simulation on a dense body-fitted mesh with resolved boundary layer on both the surface and the VG, and is assumed to yield the exact result. The accuracy of the source term model can then be assessed by looking at the deviation between the approximate flow field characteristics and the projection of the exact result on the low resolution mesh.

In order to find this optimal source term  $\mathbf{f}^*$  to model the effect of the VG on the flow an inverse approach is used. We solve the constrained optimization problem

$$\mathbf{f}^* = \operatorname{argmin}_{\mathbf{f}} J(\mathbf{u}(\mathbf{f})) \quad \text{with} \quad J(\mathbf{u}) = \int_{\Omega} (\mathbf{u} - \tilde{\mathbf{u}})^2 d\Omega \quad \text{subject to} \quad \mathbf{R}(\mathbf{u}, p, \mathbf{f}) = 0,$$

where the objective function  $J$  consists of the least squares minimization of the difference between the desired and the actual flow field on the domain of interest and  $\mathbf{R}$  represents the set of state equations. This problem is solved using a Lagrange multiplier method, the optimality conditions of which result in a set of adjoint equations that allow calculating the sensitivity of the objective function to changes in the source term. The (continuous) adjoint system is solved simultaneous with the state equations and using the assumption of frozen turbulence.

The knowledge gained from calculating this optimal source term for different situations allows us to identify the weak points in conventional source term models. In a next step, we aim to use this information for the construction of an improved and adaptive source term modelling approach to allow for more efficient and accurate simulations of flows past VG arrays.

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# Goal Oriented Adaptivity and Sensitivity Analysis for Reacting Flows

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## **Abstract**

We discuss the use of the chemistry and transport library *Antioch*, in combination with the *Libmesh* application *GRINS*, to solve adjoints of Low-Mach reacting flows to obtain *a posteriori* error estimates and sensitivity analysis. The implementation is powered by built-in automatic differentiation features added to *Antioch* and *Libmesh*.

## Improving the convergence of bounds for effective elastic parameters of heterogeneous materials

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### ABSTRACT

The aim of this contribution is to improve the bounds for the effective parameters of heterogeneous materials which are calculated by computational homogenisation. To model the behaviour of realistically sized structures whilst accounting explicitly for the microstructure of the material is unfeasible, but also unnecessary in practice as the effect of the heterogeneities is only “felt on average” at the macroscopic scale. Based on this observation, multiscale approaches have been developed to obtain the overall macroscale material properties of materials from the knowledge of their microstructure, and also to gain some insight into the microscopic fields without resorting to a full microscopic description of the macroscopic structure.

Computational homogenisation aims to address the limitations of analytical or semi-analytical homogenisation schemes by using computational power to solve RVE problems [1]. As RVEs for random distributions may be extremely large, the homogenisation is usually performed on smaller domains, called statistical volume elements (SVE) [2]. In order to limit the influence of the boundary conditions on the results of the SVE problems, one may employ periodic or mixed boundary conditions to represent the effect of the environment. Alternatively, using homogeneous Dirichlet and Neumann boundary conditions associated with an ensemble averaging over the SVEs leads to homogenised quantities with controlled accuracy. However, for these bounds to be sharp, the required size of the SVEs may be very large, leading to a prohibitive computational cost. The bounds are slow to converge because of the homogeneous boundary conditions which pollute the accuracy of the fields close to the boundary. In this contribution we derive efficient non-homogeneous boundary conditions for the SVE problems in a manner that will respect the method's bounding properties.

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# A quality criterion for multiresolution computations

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## Abstract

We present a quality criterion for multiresolution computation in order to evaluate the accuracy of a multiresolution computation in comparison with the same computation on the regular finest grid. We show that, with a constant tolerance, the quality decreases with the number of iterations and we propose a new method to avoid this phenomenon, while ensuring CPU time compression with respect to the fine grid computation. Examples are shown on a transport equation as well as compressible Euler equations, where analytical solutions are known.

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## Modeling and Simulation of the Shrink Fit Assembly Behavior under the Influence of Axisymmetric Defect Form

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### ABSTRACT

The technique of assembly by shrink fit is increasingly used today. However, the methodology of parts sizing has not changed for several years. It considers that the contact surfaces of the assembled parts are perfectly smooth. This therefore requires to specify very precisely [1] and using expensive manufacturing processes. To reduce these costs, the study of the influence of form defects on the characteristics of assembly strength is essential. Some recent studies show the advantage of higher resolution models to understand interference-fits joints better. Fontaine and Siala [2] showed that form defects have a significant influence on the local stress state at the contact area. To take into account the effects of stress gradient properly, Lanoue et al. [3] indicate that the mesh must be refined near the interface of the shaft and hub. A convergence study has been performed to reveal this influence.

In this work, we are interested in studying the influence of the defect form on the behavior of the shrink fit assemblies. Diverse finite element simulations were carried out on an axisymmetric. The results obtained by simulations show that the defect form alters the distribution of the Von Mises stress and pressure in the contact interface, as shown in figure 1 below.

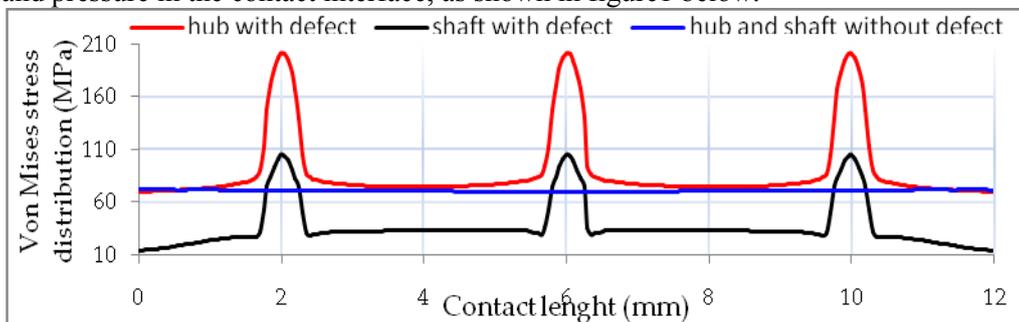


Figure 1: Distribution of Von Mises stresses at the interface of contact for cases with and without defect form

Other results obtained in this work also show that the defect form contributes to resistance of the shrink fit assembly. It can confer it greater strength than without the presence of the defect. On the practical level, taking into account the defect form in the modeling, avoids the use of very costly super finishing means.

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# Parallel Program Complex for Fluid Flows Simulation on Hybrid GPU-Based Computer Systems

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## ABSTRACT

The development of the most powerful modern computer systems based on massively parallel multicore processors with powerful accelerators such as general purpose graphics processing units (GP-GPUs) new opportunities to mathematical modeling. However, the difficulties in the efficient use of such hybrid systems are much greater than those in using conventional high performance computers. The experience shows, that for an effective application it is preferable to apply the algorithms as simple as possible from the logic point of view.

This paper presents further development of a program complex [1], oriented on heterogeneous GPU-based computer systems, which uses the explicit variant of kinetically consistent finite difference schemes based on quasi gas dynamic (QGD) equation system [2, 3]. These schemes belong to the class of kinetic or Boltzmann schemes which are presently often used in the CFD. The use of previous version of our program complex was limited by rectangular grids. Here we present a new version of this program complex, which uses no orthogonal curvilinear structured hexahedral grids. In addition the use of multi block grids is provided. This permits to solve problems with complex geometry by grid adaptation to it.

Usually the explicit schemes impose stringent stability limitations on a time step, especially when the parabolic equations are solved ( $\Delta t \sim h^2$ ) which is not appropriate for fine grids used in HPC calculation. To improve this situation we used the flux relaxation approach proposed in [1].

The results presented in this article, have been obtained on the GPU-based K-100 hybrid cluster which was constructed in KIAM RAS (Moscow, Russia) in cooperation with “KVANT” institute in 2010. Parallel realization is based on the domain decomposition principle. Simulation domain is divided into subdomains – blocks. Each block is processed by one device (GPU or CPU's core). Each device can process one or several blocks serially. Intel C++ language was used for programming. As the communication environment we used shmem (shared memory).

The program complex was tested on a number of test problems such as subsonic and supersonic flows around a circular cylinder, a supersonic flow around truncated pyramid, a simulation of the wind load on a launch vehicle standing on the launch pedestal. A detailed investigation of speed-up and scaling were made for the last test problem. The numerical experiments show that the use of single GPU gives 10 – 16 times acceleration in comparison with single CPU core. Thus the productivity of one node of K-100 system at calculation on GPU was 3 – 4 times higher than on CPUs only. For this reason when block division is not uniform we can distribute blocks between GPUs and CPU-cores so that large blocks will be processed on GPUs and small blocks – on CPU-cores. The results of calculations show good parallelization efficiency up to very large number of parallel nodes in use.

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This ebook contains the abstracts of the papers presented at ADMOS 2015, the seventh International Conference on Adaptive Modeling and Simulation, held at École Centrale de Nantes, France, from June 7 to 10, 2015.

In silico experiments that consist in building a virtual reality with numerical models are growing faster than the classical in vivo, in vitro or in situ versions. However, the numerical result is frequently suspicious of lack of realism. The inception of this suspicion is twofold because one may presume that 1) the underlying mathematical model is exaggeratedly simplifying reality and 2) the numerical solver providing an approximate solution is questionable, for instance using a too coarse discretization.

ADMOS 2015 is dealing with the tools that allow qualifying these two presumptions and preventing the mismatching between in silico and in situ tests. Moreover, attention is also paid to the methodologies allowing to efficiently improving the quality of the numerical models (mesh and model adaptivity) and to bringing modeling as closer as possible to reality. Frequently, this requires also accounting for the techniques quantifying the intrinsic uncertainty of the system that has to be modeled.

