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ENERGY-ENTROPY-CONSISTENT TIME INTEGRATION FOR NONLINEAR THERMO-VISCOELASTIC CONTINUA

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Abstract. This paper deals with an energy-entropy and momentum consistent time integration of a single thermo-viscoelastic continuum. The developed ETC time integrator is based on a time discrete spatially weak finite element formulation, but fulfills the same balance laws as the underlying five differential equations. Namely, in addition to the balances of linear momentum, angular momentum and entropy, also the balances of total energy and Lyapunov function are fulfilled. The spatially weak formulation is obtained by integration by parts. Where the resulting virtual stress power term is well-known, the virtual entropy production by conduction of heat is not so often applied, but necessary for entropy consistency. The time discretisation is based (*i*) on the midpoint rule and (*ii*) on non-standard time discrete differential operators due to Oscar Gonzalez. This time integrator is a further development of the TC integrator of Ignacio Romero.

1 INTRODUCTION

In this paper, we present a so-called structure-preserving time integrator, which preserve physical structures of solution spaces of time evolution equations as ODE, PDE and DAE. Examples of structures are geometric constraints, conservation laws for energy or linear and angular momentum as well as balance laws for entropy and Lya-

PUNOV functions. We distinguish between finite difference and finite element methods in time. Existing finite difference methods are symplectic methods [1, 2], energy-momentum time stepping schemes [3], energy-dissipative schemes [4], variational integrators [5] and energy-entropy consistent (TC) integrators [6]. These time stepping schemes are usually second-order accurate. In order to reach a higher-order accuracy, GALERKIN's method may be applied. There are higher-order accurate symplectic methods [7], GALERKIN-based energy-momentum methods [8], GALERKIN-based energy dissipative methods [9], GALERKIN-based variational integrators [10]. Here, we present a finite difference scheme.

2 PROBLEM DEFINITION

We consider the motion $\boldsymbol{\varphi}$ of a single continuum $\mathcal{B}$ (see Fig. 1 and [11]). Total deformations are described by the deformation gradient $\boldsymbol{F} = \nabla\boldsymbol{\varphi}$ and the right Cauchy-Green tensor $\boldsymbol{C} = \boldsymbol{F}^T\boldsymbol{F}$. Viscous deformations with respect to the intermediate configuration $\mathcal{V}_i$ are measured by the internal variable $\boldsymbol{C}_i = \boldsymbol{F}_i^T\boldsymbol{F}_i$. Being in motion in the ambient space with the temperature Θ_∞, the continuum possesses a linear momentum $\boldsymbol{p} = \rho_0\boldsymbol{V}$, a temperature $\Theta = \theta \circ \boldsymbol{\varphi}$ and an entropy $s = Js_c \circ \boldsymbol{\varphi}$. The body is loaded by volume loads

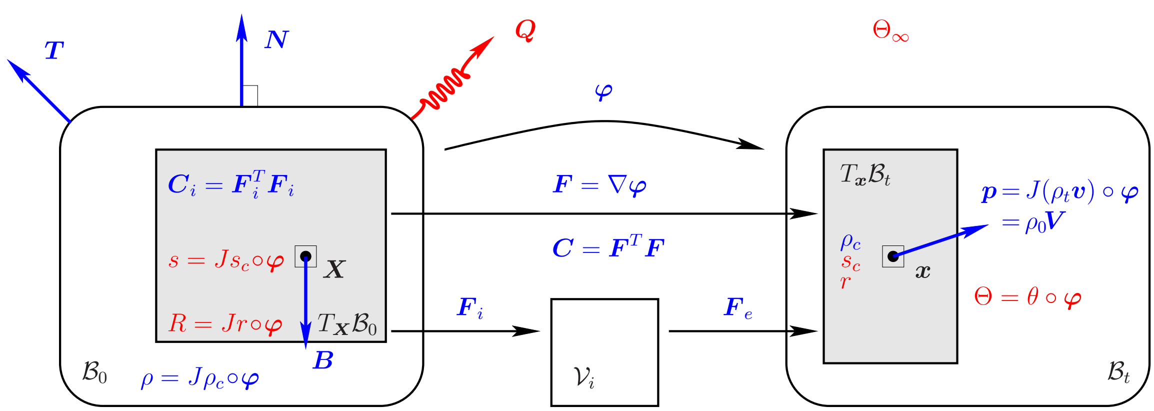

Figure 1: Motion of a single continuum.

$\boldsymbol{B}$ and R and boundary loads $\boldsymbol{T}$ and $\boldsymbol{Q}$. The dynamical state of the body $\mathcal{B}$ is described by the total energy $H = K + E$ consisting of the energies

$$K = \int_{\mathcal{B}_0} k(\boldsymbol{p})\,\mathrm{d}V = \int_{\mathcal{B}_0} \frac{1}{\rho}\boldsymbol{p}\cdot\boldsymbol{p}\,\mathrm{d}V \qquad \text{and} \qquad E = \int_{\mathcal{B}_0} e(\boldsymbol{C}, s, \boldsymbol{C}_i)\,\mathrm{d}V \tag{1}$$

The stability of this state is indicated by the LYAPUNOV function $V = H - \Theta_\infty S$, where

$$S = \int_{\mathcal{B}_0} s\,\mathrm{d}V \qquad \text{and} \qquad \boldsymbol{P} = 2\,\boldsymbol{F}\,\frac{\delta E}{\delta \boldsymbol{C}} \tag{2}$$

denotes the total entropy and the first PIOLA-KIRCHHOFF stress tensor, respectively. The latter depend on the given internal energy density $e = e^{\text{ela}}(\boldsymbol{C}) + e^{\text{the}}(\boldsymbol{C}, s) + e^{\text{vis}}(\boldsymbol{C}, \boldsymbol{C}_i)$. Here, the notation $\delta(\bullet)/\delta(\bullet)$ indicates the derivative of functionals. The heat conduction provides FOURIER's law $\boldsymbol{Q} = -\kappa\, J\, \boldsymbol{C}^{-1}\nabla\Theta$. The non-negative total dissipation

$$D^{\text{tot}} = D^{\text{cdu}} + D^{\text{vis}} = \underbrace{-\frac{1}{\Theta}\,\boldsymbol{Q}\cdot\nabla\Theta}_{\geq 0}\ \underbrace{-\frac{\delta E}{\delta \boldsymbol{C}_i} : \frac{\partial \boldsymbol{C}_i}{\partial t}}_{\geq 0} \geq 0 \tag{3}$$

emanates from the heat flux $\boldsymbol{Q}$ and the internal variable $\boldsymbol{C}_i$. The latter is determined by the time evolution equation

$$\frac{\partial \boldsymbol{C}_i}{\partial t} = -\bar{\mathbb{V}}^{-1}(\boldsymbol{C}_i) : \frac{\delta E}{\delta \boldsymbol{C}_i} \tag{4}$$

where

$$\bar{\mathbb{V}}^{-1}(\boldsymbol{C}_i) = \boldsymbol{C}_i\,\mathbb{V}^{-1}\boldsymbol{C}_i \qquad\qquad \mathbb{V}^{-1} = \frac{1}{2V^{\text{dev}}}\,\mathbb{I}^{\text{dev}^T} + \frac{1}{n_{\text{dim}}V^{\text{vol}}}\,\mathbb{I}^{\text{vol}} \tag{5}$$

leading to a positive-definite quadratic form with respect to the stress tensor $\delta E/\delta \boldsymbol{C}_i$.

3 THE STRONG FORMS

In this section, we recall the local differential equations or strong forms of the considered problem and show their physical structure.

3.1 The derivation from the balances of linear momentum and entropy

We obtain two local equations of motion from the balance of linear momentum

$$\int_{\mathcal{B}_0} \frac{\partial \boldsymbol{p}}{\partial t}\,\mathrm{d}V = \int_{\mathcal{B}_0} \boldsymbol{B}\,\mathrm{d}V + \int_{\partial\mathcal{B}_0} \boldsymbol{T}\,\mathrm{d}A \qquad \text{with } \boldsymbol{T} = \boldsymbol{P}\boldsymbol{N} \tag{6}$$

by introducing the linear momentum $\boldsymbol{p}$ as independent variable by means of the LEGENDRE transform of the material velocity $\boldsymbol{V} = \partial\boldsymbol{\varphi}/\partial t$. Thus, we obtain

$$\frac{\partial \boldsymbol{p}}{\partial t} = \mathrm{Div}\boldsymbol{P} + \boldsymbol{B} \qquad\qquad \frac{\partial \boldsymbol{\varphi}}{\partial t} = \frac{1}{\rho}\,\boldsymbol{p} \equiv \frac{\delta H}{\delta \boldsymbol{p}} \tag{7}$$

Analogously, we consider two heat conduction equations. The first strong form is the local balance of entropy emanating from the entropy inequality principle

$$\int_{\mathcal{B}_0} \frac{D^{\text{tot}}}{\Theta}\,\mathrm{d}V = \int_{\mathcal{B}_0} \left[\frac{\partial s}{\partial t} - \frac{R}{\Theta}\right]\mathrm{d}V + \int_{\partial\mathcal{B}_0} \frac{1}{\Theta}\,\boldsymbol{Q}\cdot\boldsymbol{N}\,\mathrm{d}A \geq 0 \tag{8}$$

and the second is the LEGENDRE transform between temperature and entropy. In this way, we introduce the temperature also as an independent field, and obtain the two equations

$$\frac{\partial s}{\partial t} = \frac{1}{\Theta}\left[D^{\text{vis}} + R - \mathrm{Div}\boldsymbol{Q}\right] \qquad\qquad \Theta = \frac{\partial e}{\partial s} \equiv \frac{\delta H}{\delta s} \tag{9}$$

But the last heat conduction equation is not a HAMILTONIAN state equation, due to the lack of a time differential operator on the left side.

3.2 The fulfillment of the balances of angular momentum and energy

The above strong forms also fulfill the balances of angular momentum, total energy and Lyapunov function. The balance of angular momentum

$$\int_{\mathcal{B}_0} [\boldsymbol{\varphi} - \boldsymbol{x}_0] \times \frac{\partial \boldsymbol{p}}{\partial t} \, \mathrm{d}V \underbrace{=}_{\text{Eq. (7)}} \int_{\mathcal{B}_0} [\boldsymbol{\varphi} - \boldsymbol{x}_0] \times \boldsymbol{B} \, \mathrm{d}V + \int_{\partial\mathcal{B}_0} [\boldsymbol{\varphi} - \boldsymbol{x}_0] \times \boldsymbol{T} \, \mathrm{d}A \tag{10}$$

is defined with respect to the reference point $\boldsymbol{x}_0 = \text{const.}$. Here, we have to taken into account the symmetry of the tensor $\boldsymbol{PF}$. The balance of total energy

$$\frac{\partial H}{\partial t} = P^{\text{mec}} + P^{\text{the}} \tag{11}$$

results from adding the balance of mechanical and thermal energy. Thereby, the equations of motion lead to the balance of mechanical energy

$$\int_{\mathcal{B}_0} \Big[\underbrace{\frac{\delta H}{\delta \boldsymbol{p}} \cdot \frac{\partial \boldsymbol{p}}{\partial t}}_{\partial k/\partial t} + \underbrace{\frac{\delta H}{\delta \boldsymbol{F}} : \frac{\partial \boldsymbol{F}}{\partial t}}_{p^{\text{int}}} \Big] \mathrm{d}V \underbrace{=}_{\text{Eq. (7)}} \underbrace{\int_{\mathcal{B}_0} \frac{\partial \boldsymbol{\varphi}}{\partial t} \cdot \boldsymbol{B} \, \mathrm{d}V + \int_{\partial\mathcal{B}_0} \frac{\partial \boldsymbol{\varphi}}{\partial t} \cdot \boldsymbol{T} \, \mathrm{d}A}_{P^{\text{mec}}} \tag{12}$$

balancing kinetic power and stress power with external mechanical power. The heat conduction equations lead to the balance of thermal energy

$$\int_{\mathcal{B}_0} \Big[\underbrace{\frac{\delta H}{\delta s} \frac{\partial s}{\partial t}}_{p^{\text{ent}}} + \underbrace{\frac{\delta H}{\delta \boldsymbol{C}_i} : \frac{\partial \boldsymbol{C}_i}{\partial t}}_{-D^{\text{vis}}} \Big] \mathrm{d}V \underbrace{=}_{\text{Eq. (9)}} \underbrace{\int_{\mathcal{B}_0} R \, \mathrm{d}V - \int_{\partial\mathcal{B}_0} \boldsymbol{Q} \cdot \boldsymbol{N} \, \mathrm{d}A}_{P^{\text{the}}} \tag{13}$$

balancing entropy power and viscous dissipation with external thermal power. The balance of Lyapunov function, given by

$$\frac{\partial V}{\partial t} \equiv \underbrace{\frac{\partial H}{\partial t}}_{\text{Eq. (11)}} - \Theta_\infty \int_{\mathcal{B}_0} \underbrace{\frac{\partial s}{\partial t}}_{\text{Eq. (9)}} \, \mathrm{d}V \tag{14}$$

results from the balance of total energy and entropy and provides the stability estimate

$$\frac{\partial V}{\partial t} \;=\; -\int_{\mathcal{B}_0} \frac{\Theta_\infty}{\Theta} D^{\text{tot}} \, \mathrm{d}V \leq 0 \tag{15}$$

without mechanical and thermal loads, but with temporally constant thermal and mechanical Dirichlet boundary.

4 THE TIME-CONTINUOUS SPATIALLY WEAK FORMULATION

In this section, we derive a spatially weak formulation, which is the basis for a finite element method in space. Thereby, we take into account the aim of the exact fulfillment of all above summarized balance laws with standard finite elements.

4.1 The derivation from the strong forms

By integration by parts, we obtain the well-known weak form

$$\int_{\mathcal{B}_0}\left[\delta\boldsymbol{\varphi}\cdot\frac{\partial\boldsymbol{p}}{\partial t}+\nabla(\delta\boldsymbol{\varphi}):\frac{\delta H}{\delta\boldsymbol{F}}\right]\mathrm{d}V=\int_{\mathcal{B}_0}\delta\boldsymbol{\varphi}\cdot\boldsymbol{B}\,\mathrm{d}V+\int_{\partial\mathcal{B}_0}\delta\boldsymbol{\varphi}\cdot\boldsymbol{T}\,\mathrm{d}A \tag{16}$$

of the first equation of motion with the well-known virtual stress power, and

$$\int_{\mathcal{B}_0}\delta\boldsymbol{p}\cdot\left[\frac{\partial\boldsymbol{\varphi}}{\partial t}-\frac{\delta H}{\delta\boldsymbol{p}}\right]\mathrm{d}V=0 \tag{17}$$

as the weak form of the second equation of motion. The integration by parts

$$-\int_{\mathcal{B}_0}\frac{\delta\Theta}{\Theta}\,\mathrm{Div}\boldsymbol{Q}\,\mathrm{d}V=\int_{\mathcal{B}_0}\nabla\left(\frac{\delta\Theta}{\Theta}\right)\cdot\boldsymbol{Q}\,\mathrm{d}V-\int_{\partial\mathcal{B}_0}\frac{\delta\Theta}{\Theta}\,\boldsymbol{Q}\cdot\boldsymbol{N}\,\mathrm{d}A \tag{18}$$

of the heat flux leads to the weak form of the first heat conduction equation, given by

$$\begin{aligned}\int_{\mathcal{B}_0}\left[\delta\Theta\,\frac{\partial s}{\partial t}+\frac{\delta\Theta}{\Theta}\,\underbrace{\frac{\delta H}{\delta\boldsymbol{C}_i}:\frac{\partial\boldsymbol{C}_i}{\partial t}}_{-D^{\mathrm{vis}}}\right]\mathrm{d}V \;=\; &\int_{\mathcal{B}_0}\left[\frac{\delta\Theta}{\Theta}\,R+\nabla\left(\frac{\delta\Theta}{\Theta}\right)\cdot\boldsymbol{Q}\right]\mathrm{d}V\\ &-\int_{\partial\mathcal{B}_0}\frac{\delta\Theta}{\Theta}\,\boldsymbol{Q}\cdot\boldsymbol{N}\,\mathrm{d}A\end{aligned} \tag{19}$$

This weak form is not so often applied, but necessary for entropy consistency. The weak second equation of heat conduction represents the weak constitutive equation

$$\int_{\mathcal{B}_0}\delta s\left[\Theta-\frac{\delta H}{\delta s}\right]\mathrm{d}V=0 \tag{20}$$

which is comparable with a part of the first variation of a Hu-Washizu functional [12].

4.2 The fulfillment of all balance laws of continuum mechanics

First, we choose a constant test function $\delta\boldsymbol{\varphi}(\boldsymbol{X},t)=\boldsymbol{c}=\text{const.}$ in the first weak equation of motion, and arrive at the balance of linear momentum

$$\boldsymbol{c}\cdot\underbrace{\left[\int_{\mathcal{B}_0}\left[\frac{\partial\boldsymbol{p}}{\partial t}-\boldsymbol{B}\right]\mathrm{d}V-\int_{\partial\mathcal{B}_0}\boldsymbol{T}\,\mathrm{d}A\right]}_{\text{Eq. (6)}}=0 \tag{21}$$

Then, we choose the test functions $\delta\boldsymbol{\varphi}(\boldsymbol{X},t)=\boldsymbol{c}\times[\boldsymbol{\varphi}(\boldsymbol{X},t)-\boldsymbol{x}_0]$ and $\delta\boldsymbol{p}(\boldsymbol{X},t)=\boldsymbol{c}\times\boldsymbol{p}(\boldsymbol{X},t)$ in the equations of motion. In this way, we obtain the balance of angular momentum

$$\boldsymbol{c}\cdot\underbrace{\left[\int_{\mathcal{B}_0}[\boldsymbol{\varphi}-\boldsymbol{x}_0]\times\left[\frac{\partial\boldsymbol{p}}{\partial t}-\boldsymbol{B}\right]\mathrm{d}V-\int_{\partial\mathcal{B}_0}[\boldsymbol{\varphi}-\boldsymbol{x}_0]\times\boldsymbol{T}\,\mathrm{d}A\right]}_{\text{Eq. (10)}}=0 \tag{22}$$

by bearing in mind the symmetry of the tensor $\boldsymbol{PF}$. The constant test function $\delta\Theta(\boldsymbol{X},t) = \Theta_\infty = \text{const.}$ in the first weak heat conduction equation leads to the balance of entropy

$$\underbrace{\Theta_\infty \left[\int_{\mathcal{B}_0} \left[\frac{\partial s}{\partial t} - \frac{D^{\text{vis}} + R}{\Theta} - \overbrace{\nabla\left(\frac{1}{\Theta}\right) \cdot \boldsymbol{Q}}^{D^{\text{cdu}}/\Theta}\right] \mathrm{d}V + \int_{\partial\mathcal{B}_0} \frac{1}{\Theta} \boldsymbol{Q} \cdot \boldsymbol{N} \, \mathrm{d}A\right]}_{\text{Eq. (8)}} = 0 \tag{23}$$

emanating from the entropy inequality principle with $D^{\text{tot}} \geq 0$. Furthermore, the test functions $\delta\boldsymbol{\varphi}(\boldsymbol{X},t) = \partial\boldsymbol{\varphi}(\boldsymbol{X},t)/\partial t$ and $\delta\boldsymbol{p}(\boldsymbol{X},t) = \partial\boldsymbol{p}(\boldsymbol{X},t)/\partial t$ lead to the balance of mechanical energy

$$\underbrace{\int_{\mathcal{B}_0} \Bigg[\overbrace{\frac{\delta H}{\delta \boldsymbol{p}} \cdot \frac{\partial \boldsymbol{p}}{\partial t}}^{\partial k/\partial t} + \overbrace{\frac{\delta H}{\delta \boldsymbol{F}} : \frac{\partial \boldsymbol{F}}{\partial t}}^{p^{\text{int}}}\Bigg] \mathrm{d}V = \overbrace{\int_{\mathcal{B}_0} \frac{\partial \boldsymbol{\varphi}}{\partial t} \cdot \boldsymbol{B} \, \mathrm{d}V + \int_{\partial\mathcal{B}_0} \frac{\partial \boldsymbol{\varphi}}{\partial t} \cdot \boldsymbol{T} \, \mathrm{d}A}^{P^{\text{mec}}}}_{\text{Eq. (12)}} \tag{24}$$

Next, we consider the test functions $\delta\Theta(\boldsymbol{X},t) = \Theta(\boldsymbol{X},t)$ and $\delta s(\boldsymbol{X},t) = \partial s(\boldsymbol{X},t)/\partial t$. This leads to the balance of thermal energy, given by

$$\underbrace{\int_{\mathcal{B}_0} \Bigg[\overbrace{\frac{\delta H}{\delta s} \frac{\partial s}{\partial t}}^{p^{\text{ent}}} + \overbrace{\frac{\delta H}{\delta \boldsymbol{C}_i} : \frac{\partial \boldsymbol{C}_i}{\partial t}}^{-D^{\text{vis}}}\Bigg] \mathrm{d}V = \overbrace{\int_{\mathcal{B}_0} R \, \mathrm{d}V - \int_{\partial\mathcal{B}_0} \boldsymbol{Q} \cdot \boldsymbol{N} \, \mathrm{d}A}^{P^{\text{the}}}}_{\text{Eq. (13)}} \tag{25}$$

Addition of Eq. (24) and (25) then leads to the balance of total energy

$$\underbrace{\frac{\partial H}{\partial t} = \int_{\mathcal{B}_0} \left[\frac{\partial \boldsymbol{\varphi}}{\partial t} \cdot \boldsymbol{B} + R\right] \mathrm{d}V + \int_{\partial\mathcal{B}_0} \left[\frac{\partial \boldsymbol{\varphi}}{\partial t} \cdot \boldsymbol{T} - \boldsymbol{Q} \cdot \boldsymbol{N}\right] \mathrm{d}A}_{\text{Eq. (11)}} \tag{26}$$

The balance of LYAPUNOV function is obtained in two ways. The first do not exploit the balance of total energy and entropy, and is therefore also accessible for other schemes. Here we choose the test functions $\delta\Theta(\boldsymbol{X},t) = \Theta(\boldsymbol{X},t) - \Theta_\infty$ and $\delta s(\boldsymbol{X},t) = \partial s(\boldsymbol{X},t)/\partial t$ as well as add the balance of mechanical energy [8]. We prefer to take the second way, given by

$$\frac{\partial V}{\partial t} = \underbrace{\frac{\partial H}{\partial t}}_{\text{Eq. (26)}} - \underbrace{\Theta_\infty \int_{\mathcal{B}_0} \frac{\partial s}{\partial t} \, \mathrm{d}V}_{\text{Eq. (23)}} \tag{27}$$

This corresponds to the procedure in Eq. (14) used for the strong forms.

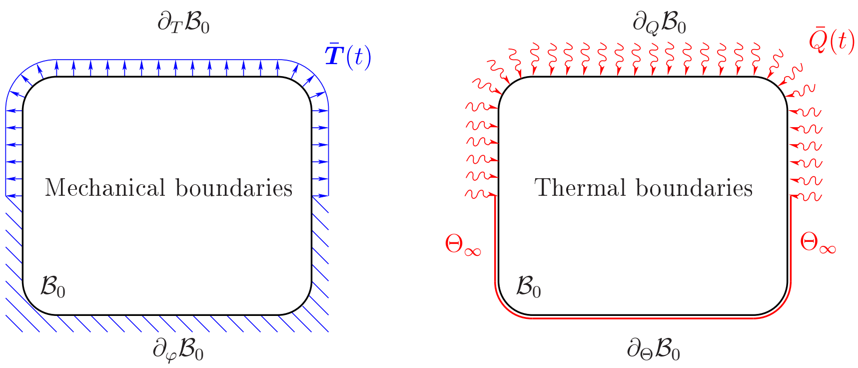

Figure 2: The considered boundary conditions in the simulations.

4.3 The considered boundary conditions

We prescribe vanishing displacements on the DIRICHLET boundary $\partial_\varphi\mathcal{B}_0$, and a transient traction $\bar{\boldsymbol{T}}(t)$ on the NEUMANN boundary $\partial_T\mathcal{B}_0$ (see Fig. 2). On the mechanical DIRICHLET boundary, we exploit the vanishing test function, such that

$$\int_{\partial\mathcal{B}_0} \delta\boldsymbol{\varphi}\cdot\boldsymbol{T}\,\mathrm{d}A = \int_{\partial_\varphi\mathcal{B}_0} \underbrace{\delta\boldsymbol{\varphi}}_{=:0}\cdot\boldsymbol{T}\,\mathrm{d}A + \int_{\partial_T\mathcal{B}_0} \delta\boldsymbol{\varphi}\cdot\bar{\boldsymbol{T}}(t)\,\mathrm{d}A = \int_{\partial_T\mathcal{B}_0} \delta\boldsymbol{\varphi}\cdot\bar{\boldsymbol{T}}(t)\,\mathrm{d}A \tag{28}$$

Then, we prescribe the ambient temperature Θ_∞ on the DIRICHLET boundary $\partial_\Theta\mathcal{B}_0$, and an inward normal heat flux $\bar{Q}(t)$ on the NEUMANN boundary $\partial_Q\mathcal{B}_0$ (see Fig. 2). On the thermal DIRICHLET boundary, we apply the LAGRANGE multiplier technique [13] for determining the outward normal entropy flux. Therefore, the boundary integral reads

$$\int_{\partial\mathcal{B}_0} \frac{\delta\Theta}{\Theta}\boldsymbol{Q}\cdot\boldsymbol{N}\,\mathrm{d}A = \int_{\partial_\Theta\mathcal{B}_0} \delta\Theta\,\lambda_\Theta\,\mathrm{d}A - \int_{\partial_Q\mathcal{B}_0} \frac{\delta\Theta}{\Theta}\,\bar{Q}(t)\,\mathrm{d}A \tag{29}$$

and leads with the constraint

$$\int_{\partial_\Theta\mathcal{B}_0} \delta\lambda_\Theta\,[\Theta-\Theta_\infty]\,\mathrm{d}A = 0 \tag{30}$$

to the temperature Θ_∞ at the finite element nodes on the thermal DIRICHLET boundary $\partial_\Theta\mathcal{B}_0$. The LAGRANGE multiplier λ_Θ denotes the outward normal entropy flux of $\partial_\Theta\mathcal{B}_0$.

5 THE TIME-DISCRETE SPATIALLY WEAK FORMULATION

After deriving the spatially weak forms, we consider now their time discretisation by an integration rule and time-discrete differential operators.

5.1 The ETC integrator

The ETC integrator is represented by a time-discrete form of all evolution equations, which preserve the balance laws of continuum mechanics in a discrete sence. We restrict us to second-order accuracy and apply the midpoint rule for integrating the weak forms. In order to reach exact fulfillment of the fundamental theorem of calculus in a discrete sence, we apply the second-order accurate time-discrete differential operators $\Delta(\bullet)/\Delta(\bullet)$ and $\Delta^P(\bullet)/\Delta(\bullet)$ [3]. Consequently, for a single-variable function as the kinetic energy and the state variables, we use the second order accurate time-discrete operator

$$\frac{\Delta \boldsymbol{f}}{\Delta \boldsymbol{z}} = \frac{\partial \boldsymbol{f}(\boldsymbol{z}_{n+\frac{1}{2}})}{\partial \boldsymbol{z}} + \frac{\boldsymbol{f}(\boldsymbol{z}_{n+1}) - \boldsymbol{f}(\boldsymbol{z}_n) - \dfrac{\partial \boldsymbol{f}(\boldsymbol{z}_{n+\frac{1}{2}})}{\partial \boldsymbol{z}} \odot [\boldsymbol{z}_{n+1} - \boldsymbol{z}_n]}{[\boldsymbol{z}_{n+1} - \boldsymbol{z}_n] \odot [\boldsymbol{z}_{n+1} - \boldsymbol{z}_n]} [\boldsymbol{z}_{n+1} - \boldsymbol{z}_n] \tag{31}$$

for the functions $\boldsymbol{f} \in \{k, s, \boldsymbol{p}, \boldsymbol{\varphi}, \boldsymbol{C}_i\}$ with arguments $\boldsymbol{z} \in \{t, s, \boldsymbol{p}, \boldsymbol{C}, \boldsymbol{C}_i\}$. The corresponding inner products are denoted by $\odot \in \{\ , \cdot, :\}$. This formula includes

$$\begin{aligned} &\text{Special case 1:}\quad \text{Scalar-valued } \boldsymbol{z}: && \frac{\Delta \boldsymbol{f}}{\Delta t} = \frac{\boldsymbol{f}(\boldsymbol{z}_{n+1}) - \boldsymbol{f}(\boldsymbol{z}_n)}{t_{n+1} - t_n} \\ &\text{Special case 2:}\quad \text{Quadratic } \boldsymbol{f}: && \frac{\Delta k}{\Delta \boldsymbol{p}} = \frac{\partial k(\boldsymbol{p}_{n+\frac{1}{2}})}{\partial \boldsymbol{p}} \equiv \frac{1}{\rho} \boldsymbol{p}_{n+\frac{1}{2}} \end{aligned} \tag{32}$$

For the total energy as multi-variable functional, we use the second-order accurate partitioned discrete derivatives

$$\begin{aligned} \frac{\Delta^P H}{\Delta \boldsymbol{p}} &= \frac{\Delta k}{\Delta \boldsymbol{p}} \quad \text{with} \quad k(\boldsymbol{p}) \quad \text{and} \quad e(\boldsymbol{C}, s, \boldsymbol{C}_i) \\ \frac{\Delta^P H}{\Delta \boldsymbol{F}} &= \boldsymbol{F}_{n+\frac{1}{2}} \left[\left.\frac{\Delta e}{\Delta \boldsymbol{C}}\right|_{s_n, \boldsymbol{C}_{i_n}} + \left.\frac{\Delta e}{\Delta \boldsymbol{C}}\right|_{s_{n+1}, \boldsymbol{C}_{i_{n+1}}} \right] \\ \frac{\Delta^P H}{\Delta s} &= \frac{1}{2} \left[\left.\frac{\Delta e}{\Delta s}\right|_{\boldsymbol{C}_n, \boldsymbol{C}_{i_{n+1}}} + \left.\frac{\Delta e}{\Delta s}\right|_{\boldsymbol{C}_{n+1}, \boldsymbol{C}_{i_n}} \right] \\ \frac{\Delta^P H}{\Delta \boldsymbol{C}_i} &= \frac{1}{2} \left[\left.\frac{\Delta e}{\Delta \boldsymbol{C}_i}\right|_{\boldsymbol{C}_n, s_n} + \left.\frac{\Delta e}{\Delta \boldsymbol{C}_i}\right|_{\boldsymbol{C}_{n+1}, s_{n+1}} \right] \end{aligned} \tag{33}$$

In this way, we approximate $\boldsymbol{\varphi}$, $\boldsymbol{p}$, s and $\boldsymbol{C}_i$ globally continuous over the considered time interval $[0, T]$, and perform a midpoint evaluation $(\bullet)_{n+1/2} = [(\bullet)_n + (\bullet)_{n+1}]/2$ of these state variables. The test functions $\delta\boldsymbol{p}_{n+1}$ and $\delta\boldsymbol{\varphi}_{n+1}$ are constant over the time step and admit interelement discontinuities. We obtain the time-discrete weak forms

$$\begin{aligned} &\int_{\mathcal{B}_0} \delta \boldsymbol{p}_{n+1} \cdot \left[\frac{\Delta \boldsymbol{\varphi}}{\Delta t} - \frac{\Delta^P H}{\Delta \boldsymbol{p}} \right] \mathrm{d}V = 0 \\ &\int_{\mathcal{B}_0} \left[\delta \boldsymbol{\varphi}_{n+1} \cdot \frac{\Delta \boldsymbol{p}}{\Delta t} + \nabla(\delta \boldsymbol{\varphi}_{n+1}) : \frac{\Delta^P H}{\Delta \boldsymbol{F}} \right] \mathrm{d}V = \int_{\mathcal{B}_0} \delta \boldsymbol{\varphi}_{n+1} \cdot \boldsymbol{B}_{\frac{1}{2}} \, \mathrm{d}V + \int_{\partial_T \mathcal{B}_0} \delta \boldsymbol{\varphi}_{n+1} \cdot \bar{\boldsymbol{T}}_{\frac{1}{2}} \, \mathrm{d}A \end{aligned} \tag{34}$$

The transient loads are evaluated at the midpoint of the time step, which indicate the index 1/2. The time-discrete weak form of the heat conduction equations are given by

$$\int_{\mathcal{B}_0} \delta s_{n+1} \cdot \left[\Theta_{n+1} - \frac{\Delta^P H}{\Delta s}\right] \mathrm{d}V = 0 \tag{35}$$

and

$$\begin{aligned}\int_{\mathcal{B}_0}\left[\delta\Theta_{n+1}\frac{\Delta s}{\Delta t} + \frac{\delta\Theta_{n+1}}{\Theta_{n+1}}\frac{\Delta^P H}{\Delta \boldsymbol{C}_i} : \frac{\Delta \boldsymbol{C}_i}{\Delta t}\right]\mathrm{d}V \;=\; &\int_{\mathcal{B}_0}\left[\nabla\left(\frac{\delta\Theta_{n+1}}{\Theta_{n+1}}\right)\cdot \boldsymbol{Q}_{\frac{1}{2}} + \frac{\delta\Theta_{n+1}}{\Theta_{n+1}} R_{\frac{1}{2}}\right]\mathrm{d}V \\ &- \int_{\partial_\Theta\mathcal{B}_0}\delta\Theta_{n+1}\,\lambda_{n+1}\,\mathrm{d}A + \int_{\partial_Q\mathcal{B}_0}\frac{\delta\Theta_{n+1}}{\Theta_{n+1}}\,\bar{Q}_{\frac{1}{2}}\,\mathrm{d}A\end{aligned} \tag{36}$$

Note that both the temperature Θ_{n+1} and the test function $\delta\Theta_{n+1}$ are constant over the time step. This approximation is perfectly compatible with the ideas that thermal displacements, defined by $\Theta = \partial\alpha/\partial t$ [14], are continuous as the motion $\boldsymbol{\varphi}$. The time evolutions of the internal variable and the thermal DIRICHLET boundary nodes are determined by the time-discrete equations

$$\frac{\Delta \boldsymbol{C}_i}{\Delta t} + \bar{\mathbb{V}}^{-1}(\boldsymbol{C}_{i_{n+\frac{1}{2}}}) : \frac{\Delta^P H}{\Delta \boldsymbol{C}_i} \;=\; 0 \qquad \int_{\partial_\Theta\mathcal{B}_0}\delta\lambda_{n+1}\left[\Theta_{n+1} - \Theta_\infty\right]\mathrm{d}A \;=\; 0 \tag{37}$$

According to [7], the LAGRANGE multiplier is also constant over the time step. Note that this is also perfectly compatible with the temperature approximation, because the LAGRANGE multiplier coincides with an entropy flux.

5.2 The fulfillment of time-discrete balance laws of continuum mechanics

The time discrete balance of linear momentum is obtained by $\delta\boldsymbol{\varphi}_{n+1}(\boldsymbol{X}) = \boldsymbol{c} = \text{const.}$, and takes the form

$$\boldsymbol{c}\cdot\underbrace{\left[\int_{\mathcal{B}_0}\left[\frac{\Delta\boldsymbol{p}}{\Delta t} - \boldsymbol{B}_{\frac{1}{2}}\right]\mathrm{d}V - \int_{\partial_T\mathcal{B}_0}\bar{\boldsymbol{T}}_{\frac{1}{2}}\,\mathrm{d}A\right]}_{\text{Time discrete balance of linear momentum}} = 0 \tag{38}$$

Then, we choose $\delta\boldsymbol{\varphi}_{n+1}(\boldsymbol{X}) = \boldsymbol{c}\times\left[\boldsymbol{\varphi}_{n+1/2}(\boldsymbol{X}) - \boldsymbol{x}_0\right]$ and $\delta\boldsymbol{p}_{n+1}(\boldsymbol{X}) = \boldsymbol{c}\times\boldsymbol{p}_{n+1/2}(\boldsymbol{X})$. The time-discrete balance of angular momentum is then given by

$$\boldsymbol{c}\cdot\underbrace{\left[\int_{\mathcal{B}_0}\left[\boldsymbol{\varphi}_{n+\frac{1}{2}} - \boldsymbol{x}_0\right]\times\left[\frac{\Delta\boldsymbol{p}}{\Delta t} - \boldsymbol{B}_{\frac{1}{2}}\right]\mathrm{d}V - \int_{\partial_T\mathcal{B}_0}\left[\boldsymbol{\varphi}_{n+\frac{1}{2}} - \boldsymbol{x}_0\right]\times\bar{\boldsymbol{T}}_{\frac{1}{2}}\,\mathrm{d}A\right]}_{\text{Time discrete balance of angular momentum}} = 0 \tag{39}$$

The time discrete balance of entropy is obtained by the test function $\delta\Theta_{n+1}(\boldsymbol{X}) = \Theta_\infty =$ const., and takes the form

$$\Theta_\infty \underbrace{\left[\int_{\mathcal{B}_0}\left[\frac{\Delta s}{\Delta t} - \frac{D^{\text{tot}}_{\frac{1}{2}} + R_{\frac{1}{2}}}{\Theta_{n+1}}\right.\mathrm{d}V + \int_{\partial_\Theta\mathcal{B}_0}\lambda_{n+1}\,\mathrm{d}A - \int_{\partial_Q\mathcal{B}_0}\frac{\bar{Q}_{\frac{1}{2}}}{\Theta_{n+1}}\,\mathrm{d}A\right]}_{\text{Time discrete entropy inequality principle with } D^{\text{tot}}_{\frac{1}{2}} \geq 0} = 0 \tag{40}$$

Now, we choose $\delta\boldsymbol{\varphi}_{n+1}(\boldsymbol{X}) = \Delta\boldsymbol{\varphi}(\boldsymbol{X})/\Delta t$ and $\delta\boldsymbol{p}_{n+1}(\boldsymbol{X}) = \Delta\boldsymbol{p}(\boldsymbol{X})/\Delta t$. In this way, we obtain the time discrete balance of mechanical energy

$$\underbrace{\frac{\Delta K}{\Delta t} + \frac{1}{2}\left[\left.\frac{\Delta E}{\Delta t}\right|_{s_n,\boldsymbol{C}_{i_n}} + \left.\frac{\Delta E}{\Delta t}\right|_{s_{n+1},\boldsymbol{C}_{i_{n+1}}}\right] = \int_{\mathcal{B}_0}\frac{\Delta\boldsymbol{\varphi}}{\Delta t}\cdot\boldsymbol{B}_{\frac{1}{2}}\,\mathrm{d}V + \int_{\partial_T\mathcal{B}_0}\frac{\Delta\boldsymbol{\varphi}}{\Delta t}\cdot\bar{\boldsymbol{T}}_{\frac{1}{2}}\,\mathrm{d}A}_{\text{Time discrete balance of mechanical energy}} \tag{41}$$

Then, by choosing $\delta\Theta_{n+1}(\boldsymbol{X}) = \Theta_{n+1}(\boldsymbol{X})$, $\delta s_{n+1}(\boldsymbol{X}) = \Delta s(\boldsymbol{X})/\Delta t$ and $\delta\lambda_{n+1}(\boldsymbol{X}) = \lambda_{n+1}(\boldsymbol{X})$, we arrive at the time discrete balance of thermal energy

$$\underbrace{\begin{aligned}&\frac{1}{2}\left[\left.\frac{\Delta E}{\Delta t}\right|_{\boldsymbol{C}_n,\boldsymbol{C}_{i_{n+1}}} + \left.\frac{\Delta E}{\Delta t}\right|_{\boldsymbol{C}_{n+1},\boldsymbol{C}_{i_n}} + \left.\frac{\Delta E}{\Delta t}\right|_{\boldsymbol{C}_n,s_n} + \left.\frac{\Delta E}{\Delta t}\right|_{\boldsymbol{C}_{n+1},s_{n+1}}\right]\\ &= \int_{\mathcal{B}_0} R_{\frac{1}{2}}\,\mathrm{d}V - \Theta_\infty\int_{\partial_\Theta\mathcal{B}_0}\lambda_{n+1}\,\mathrm{d}A + \int_{\partial_Q\mathcal{B}_0}\bar{Q}_{\frac{1}{2}}\,\mathrm{d}A\end{aligned}}_{\text{Time discrete balance of thermal energy}} \tag{42}$$

The time discrete balance of total energy is again obtained simply by adding the time discrete balance of mechanical and thermal energy. We arrive at the relation

$$\underbrace{\frac{\Delta H}{\Delta t} = \int_{\mathcal{B}_0}\left[\frac{\Delta\boldsymbol{\varphi}}{\Delta t}\cdot\boldsymbol{B}_{\frac{1}{2}} + R_{\frac{1}{2}}\right]\mathrm{d}V + \int_{\partial_T\mathcal{B}_0}\frac{\Delta\boldsymbol{\varphi}}{\Delta t}\cdot\bar{\boldsymbol{T}}_{\frac{1}{2}}\,\mathrm{d}A - \Theta_\infty\int_{\partial_\Theta\mathcal{B}_0}\lambda_{n+1}\,\mathrm{d}A + \int_{\partial_Q\mathcal{B}_0}\bar{Q}_{\frac{1}{2}}\,\mathrm{d}A}_{\text{Time discrete balance of total energy}} \tag{43}$$

The time discrete LYAPUNOV balance is again obtained in two ways. First by choosing $\delta\Theta_{n+1}(\boldsymbol{X}) = \Theta_{n+1}(\boldsymbol{X}) - \Theta_\infty$, $\delta s_{n+1}(\boldsymbol{X}) = \Delta s(\boldsymbol{X})/\Delta t$, $\delta\lambda_{n+1}(\boldsymbol{X}) = \lambda_{n+1}(\boldsymbol{X})$ and adding the time discrete balance of mechanical energy. Second by subtracting the time discrete balances of total energy and entropy, which means

$$\frac{\Delta V}{\Delta t} = \underbrace{\frac{\Delta H}{\Delta t}}_{\text{Time discrete balance of total energy}} - \underbrace{\Theta_\infty\int_{\mathcal{B}_0}\frac{\Delta s}{\Delta t}\,\mathrm{d}V}_{\text{Time discrete balance of entropy}} \tag{44}$$

which also eliminates the LAGRANGE multiplier.

6 NUMERICAL EXAMPLE

As numerical example, we consider a disc, which is bound between two plates (mechanical DIRICHLET boundary $\partial_\varphi \mathcal{B}_0$), and partly uninsulated (thermal DIRICHLET boundary $\partial_\Theta \mathcal{B}_0$ (see Fig. 6). The motion is initiated by an initial velocity field, and the heat conduction is forced by the thermal DIRICHLET boundary. For a small time step size, the midpoint rule and the ETC integrator compute practically the same results: The ring cools down to ambient temperature. But for a large time step size, the midpoint rule reveals its limited stability region. The midpoint rule tends to hour-glassing in the displacements and waves in the temperature distribution in the radial direction. This is contrary to the ETC integrator.

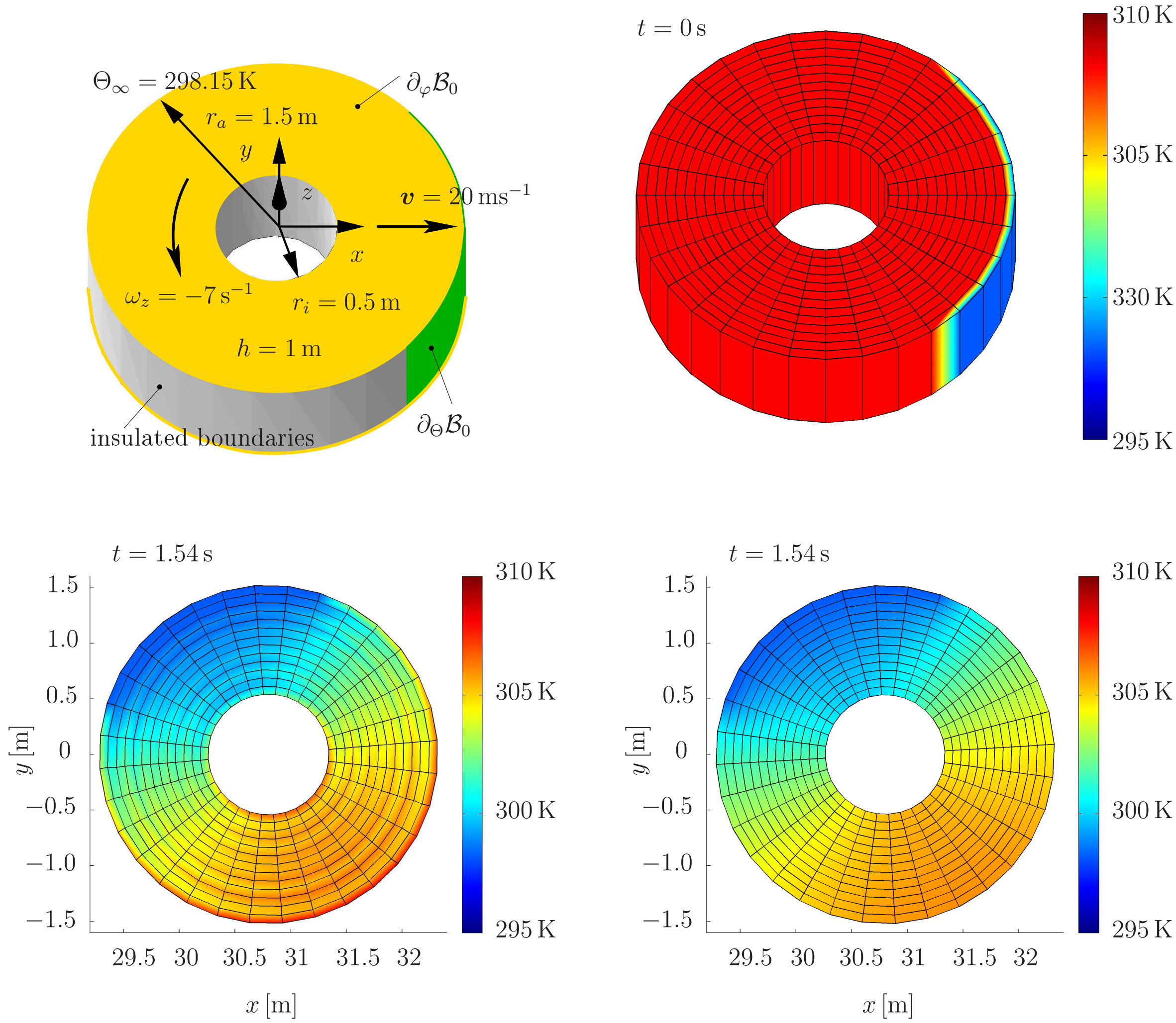

Figure 3: Rail-bound partly uninsulated disc.

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