

Dynamic thermo-mechanical coupling in fiber-reinforced bodies simulated by higher- order variational energy-momentum schemes

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Structure-preserving numerical methods for coupled problems

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Motivation, goals and strategy

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Introduction

Variational setting

Continuum model
Variational principle
Euler-Lagrange equations

Discrete setting

Global E-L equations
Local E-L equations
Mechanical energy balance
Total energy balance
Total momenta balances
Total entropy balance

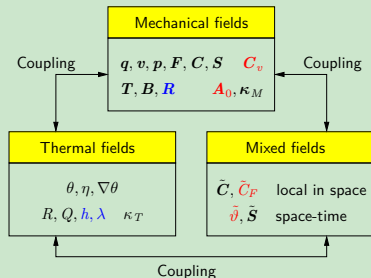
Numerical studies

Summary

Motivation

- 1 Dynamic simulations of fiber-reinforced materials in light-weight structures
- 2 Variational design of energy-momentum schemes on arbitrary coupled fields

Goal 1: energy-momentum schemes for coupled fields



Goal 2: energy-momentum schemes based on variation

- 1 Statics: Multifield principles of virtual work (mixed finite elem.)
- 2 Dynamics: Multifield principles of least action (Hamilton's principle) $\leadsto$ momentum-consistent (VI)
- 3 Dynamics: Multifield principles of virtual power (energy-momentum schemes for coupled fields)

Strategy

(cf. Miehe & Schröder [2001], Armero [2008], Betsch & Janz [2016], Schlögl & Leyendecker [2016])

- 1 Energy-momentum schemes arise as discrete Euler-Lagrange equations

Continuum model of a fiber-reinforced body I

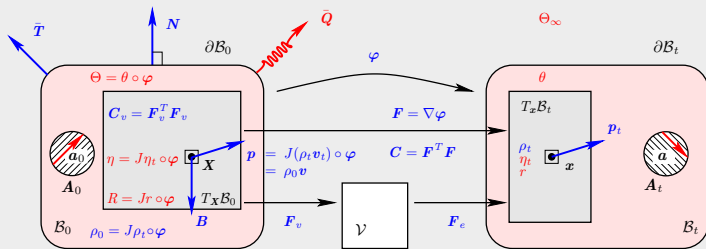
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Continuum model

Transversely isotropic material in motion

(cf. Schröder, Neff & Balzani [2005])



Deformation of fibers and matrix

(cf. Klinkel, Sansour & Wagner [2005])

1 Deformation gradients

$$F_F := a \otimes a_0 = FA_0 \quad a = Fa_0 \quad A_0 := a_0 \otimes a_0$$

2 Right Cauchy-Green tensors

$$\mathbf{C}_F := \mathbf{F}_F^T \mathbf{F}_F := \mathbf{C}_F \mathbf{A}_0 \quad \mathbf{C}_F := \mathbf{C} : \mathbf{A}_0 \equiv \mathbf{I}_4^C \quad \mathbf{C} := \mathbf{F}^T \mathbf{F}$$

3 Isotropic viscoelastic matrix

$$\mathbf{F} = \mathbf{F}_v \mathbf{F}_e \quad \mathbf{C}_v = \mathbf{F}_v^T \mathbf{F}_v \quad \leadsto \text{symmetric internal variable}$$

Continuum model of a fiber-reinforced body II

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Total free energy

- 1 Elastic free energy

$$\Psi^{\text{ela}}(\mathbf{C}, C_F; \mathbf{A}_0) = \hat{\Psi}_M^{\text{ela}}(I_1^C, I_2^C, I_3^C, I_4^C) + \hat{\Psi}_F^{\text{ela}}(C_F)$$

- 2 Thermoelastic free energy

$$\Psi^{\text{the}}(\Theta, \mathbf{C}, C_F) = \hat{\Psi}^{\text{cap}}(\Theta) - n_{\text{dim}} \beta_M (\Theta - \Theta_{\infty}) \hat{\Psi}_M^{\text{vol}}(I_3^C) - 2\sqrt{C_F} \beta_F (\Theta - \Theta_{\infty}) \hat{\Psi}_F^{\text{ela}}(C_F)$$

- 3 Viscoelastic free energy

$$\Psi_M^{\text{vis}}(\Lambda) = \hat{\Psi}_M^{\text{ela}}(I_1^{\Lambda}, I_2^{\Lambda}, I_3^{\Lambda}) \quad \Lambda = \mathbf{C} \mathbf{C}_v^{-1} \quad \mathbf{C}_e = \mathbf{F}_e^T \mathbf{F}_e$$

Total equilibrium and non-equilibrium stress

- 1 Total second Piola-Kirchhoff stress tensor

$$\mathbf{S} := 2 \frac{\partial \hat{\Psi}}{\partial \mathbf{C}} = \mathbf{S}_M^{\text{ela}} + \mathbf{S}_M^{\text{the}} + \mathbf{S}_M^{\text{vis}} + \mathbf{S}_F(\Theta, C_F) \mathbf{A}_0$$

- 2 Viscous evolution equation and non-equilibrium stress tensor

$$\boxed{\mathbf{Y} = \mathbb{V}(\mathbf{C}_v) : \dot{\mathbf{C}}_v} \quad \mathbf{Y} := -\frac{\partial \Psi_M^{\text{vis}}}{\partial \mathbf{C}_v} \quad D^{\text{int}} := \mathbf{Y} : \dot{\mathbf{C}}_v \geq 0$$

$$\mathbb{V}(\mathbf{C}_v) = \frac{1}{4} \left(V_{\text{vol}} - \frac{V_{\text{dev}}}{n_{\text{dim}}} \right) \mathbf{C}_v^{-1} \otimes \mathbf{C}_v^{-1} + \frac{V_{\text{dev}}}{4} \mathbb{I}^{\text{sym}} : \mathbf{C}_v^{-1} \quad (\text{pos.-def.})$$

Basis of the principle of virtual power I

Total energy balance in functional form

$$\dot{T}(\dot{\varphi}, \dot{v}, \dot{p}) + \dot{\Pi}^{\text{ext}}(\dot{\varphi}, \dot{C}_v, \dot{\Theta}, \tilde{\Theta}, R, h, \lambda) + \dot{\Pi}^{\text{int}}(\dot{\varphi}, \dot{C}_v, \dot{\tilde{C}}, \dot{\tilde{C}}_F, S, S_F, \dot{\Theta}, \dot{\eta}, \tilde{\Theta}; \tilde{S}, \tilde{S}_F) = 0$$

Kinetic energy

$$T = \frac{\rho_0}{2} v \cdot v \qquad \mathcal{T} := \int_{\mathcal{B}_0} T \, dV - \int_{\mathcal{B}_0} [v - \dot{\varphi}] \cdot p \, dV$$

Kinetic power functional

$$\dot{T}(\dot{\varphi}, \dot{v}, \dot{p}) := \int_{\mathcal{B}_0} \left[\frac{\partial T}{\partial v} - p \right] \cdot \dot{v} \, dV - \int_{\mathcal{B}_0} \dot{p} \cdot [v - \dot{\varphi}] \, dV + \int_{\mathcal{B}_0} p \cdot \dot{\varphi} \, dV$$

External power functional

(cf. Romero [2010])

$$\begin{aligned} \dot{\Pi}^{\text{ext}} := & - \int_{\mathcal{B}_0} \rho_0 B \cdot \dot{\varphi} \, dV - \int_{\partial_T \mathcal{B}_0} \bar{T} \cdot \dot{\varphi} \, dA - \int_{\partial_\varphi \mathcal{B}_0} R \cdot (\dot{\varphi} - \dot{\bar{\varphi}}) \, dA \\ & + \int_{\mathcal{B}_0} \frac{1}{\bar{\Theta}} \nabla \bar{\Theta} \cdot Q \, dV + \int_{\mathcal{B}_0} \frac{\bar{\Theta}}{\bar{\Theta}} [R + D^{\text{tot}}] \, dV + \int_{\partial_Q \mathcal{B}_0} \frac{\bar{\Theta}}{\bar{\Theta}} \bar{Q} \, dA \\ & + \int_{\partial_\Theta \mathcal{B}_0} \lambda (\bar{\Theta} - \Theta) \, dA - \int_{\partial_h \mathcal{B}_0} h (\dot{\Theta} - \dot{\bar{\Theta}}) \, dA + \frac{1}{2} \int_{\mathcal{B}_0} \dot{C}_v : \mathbb{V}(C_v) : \dot{C}_v \, dV \end{aligned}$$

with $D^{\text{tot}} := D^{\text{int}} + D^{\text{cdv}} = D^{\text{int}} - \frac{1}{\bar{\Theta}} \nabla \Theta \cdot Q$

Basis of the principle of virtual power II

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Fourier's law of transversely isotropic heat conduction

Al-Kinani [2014]

$$\mathbf{q} := -\boldsymbol{\kappa} \mathbf{F}^{-T} \nabla \Theta \quad \boldsymbol{\kappa} := k \mathbf{I} + \frac{k_F - k}{\|\mathbf{a}\|^2} \mathbf{a} \otimes \mathbf{a} \quad \mathbf{Q} := - \left[\frac{k_F - k}{\bar{C}_F} \mathbf{A}_0 + k_0 \mathbf{C}^{-1} \right] \nabla \Theta$$

Internal energy

$$\begin{aligned} \Pi^{\text{int}} := & \int_{\mathcal{B}_0} [\Psi_M(\Theta, \tilde{\mathbf{C}}, \mathbf{C}_v; \mathbf{A}_0) + \Psi_F(\Theta, \tilde{\mathbf{C}}_F; \mathbf{A}_0)] \, dV - \int_{\mathcal{B}_0} \eta [\tilde{\Theta} - \Theta] \, dV \\ & - \frac{1}{2} \int_{\mathcal{B}_0} \mathbf{S}_M : [\tilde{\mathbf{C}} - \mathbf{C}(\varphi)] \, dV - \int_{\mathcal{B}_0} \mathbf{S}_F : [\tilde{\mathbf{C}}_F - \mathbf{C}(\varphi) : \mathbf{A}_0] \, dV \\ & + \frac{1}{2} \int_{\mathcal{B}_0} \tilde{\mathbf{S}} : \tilde{\mathbf{C}} \, dV + \frac{1}{2} \int_{\mathcal{B}_0} \tilde{\mathbf{S}}_F : \tilde{\mathbf{C}}_F \, dV \end{aligned}$$

Internal power functional

$$\begin{aligned} \dot{\Pi}^{\text{int}} := & \frac{1}{2} \int_{\mathcal{B}_0} \left\{ \left[2 \frac{\partial \Psi}{\partial \tilde{\mathbf{C}}} + \tilde{\mathbf{S}} - \mathbf{S} \right] : \dot{\tilde{\mathbf{C}}} + \left[2 \frac{\partial \Psi}{\partial \tilde{\mathbf{C}}_F} + \tilde{\mathbf{S}}_F - \mathbf{S}_F : \mathbf{A}_0 \right] : \dot{\tilde{\mathbf{C}}_F} \right\} \, dV \\ & - \frac{1}{2} \int_{\mathcal{B}_0} \dot{\mathbf{S}} : [\tilde{\mathbf{C}} - \mathbf{C}(\varphi)] \, dV + \frac{1}{2} \int_{\mathcal{B}_0} \mathbf{S} : \dot{\mathbf{C}}(\dot{\varphi}) \, dV + \int_{\mathcal{B}_0} \frac{\partial \Psi}{\partial \mathbf{C}_v} : \dot{\mathbf{C}}_v \, dV \\ & - \frac{1}{2} \int_{\mathcal{B}_0} \dot{\mathbf{S}}_F : [\tilde{\mathbf{C}}_F \mathbf{A}_0 - \mathbf{C}_F(\varphi)] \, dV + \frac{1}{2} \int_{\mathcal{B}_0} \mathbf{S}_F : \dot{\mathbf{C}}_F(\dot{\varphi}) \, dV \\ & + \int_{\mathcal{B}_0} \dot{\eta} (\tilde{\Theta} - \Theta) \, dV + \int_{\mathcal{B}_0} \dot{\Theta} \left[\eta + \frac{\partial \Psi}{\partial \Theta} \right] \, dV + \int_{\mathcal{B}_0} \eta \dot{\Theta} \, dV \end{aligned}$$

Principle of virtual power

(cf. Schröder & Kuhl [2015], Klinkel & Wagner [1997], Hackl [1997])

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Mixed principle of virtual power $\delta_* \dot{\mathcal{H}} = 0$

$$\delta_* \dot{T}(\dot{\varphi}, \dot{v}, \dot{p}) + \delta_* \dot{\Pi}^{\text{ext}}(\dot{\varphi}, \dot{C}_v, \dot{\Theta}, \dot{\bar{\Theta}}, \mathbf{R}, h, \lambda) + \delta_* \dot{\Pi}^{\text{int}}(\dot{\varphi}, \dot{C}_v, \dot{C}, \dot{C}_F, \dot{\Theta}, \dot{\eta}, \dot{\bar{\Theta}}, \mathbf{S}, \mathbf{S}_F; \tilde{\mathbf{S}}, \tilde{S}_F) = 0$$

Virtual kinetic power

$$\delta_* \dot{T}(\dot{u}, \dot{v}, \dot{p}) := \int_{\mathcal{B}_0} \left[\frac{\partial T}{\partial v} - p \right] \cdot \delta_* \dot{v} \, dV - \int_{\mathcal{B}_0} \delta_* \dot{p} \cdot [\mathbf{v} - \dot{\varphi}] \, dV + \int_{\mathcal{B}_0} \dot{p} \cdot \delta_* \dot{\varphi} \, dV$$

Virtual external power

$$\begin{aligned} \delta_* \dot{\Pi}^{\text{ext}} := & - \int_{\mathcal{B}_0} \rho_0 \mathbf{B} \cdot \delta_* \dot{\varphi} \, dV - \int_{\partial_T \mathcal{B}_0} \mathbf{T} \cdot \delta_* \dot{\varphi} \, dA - \int_{\partial_\varphi \mathcal{B}_0} \delta_* \mathbf{R} \cdot [\dot{\varphi} - \dot{\bar{\varphi}}] \, dA - \int_{\partial_\varphi \mathcal{B}_0} \mathbf{R} \cdot \delta_* \dot{\varphi} \\ & + \int_{\mathcal{B}_0} \delta_* \dot{C}_v : \mathbb{V}(\mathbf{C}_v) : \dot{C}_v \, dV + \int_{\mathcal{B}_0} \delta_* \bar{\Theta} \frac{R + D^{\text{tot}}}{\Theta} \, dV + \int_{\mathcal{B}_0} \frac{1}{\bar{\Theta}} \nabla(\delta_* \bar{\Theta}) \cdot \mathbf{Q} \, dV + \int_{\partial_\Theta \mathcal{B}_0} \lambda \delta_* \bar{\Theta} \, dA \\ & + \int_{\partial_Q \mathcal{B}_0} \frac{\delta_* \bar{\Theta}}{\Theta} \bar{Q} \, dA + \int_{\partial_\Theta \mathcal{B}_0} \delta_* \lambda [\bar{\Theta} - \bar{\Theta}] \, dA - \int_{\partial_\Theta \mathcal{B}_0} \delta_* h [\dot{\Theta} - \dot{\bar{\Theta}}] \, dA - \int_{\partial_\Theta \mathcal{B}_0} \delta_* \dot{\Theta} h \, dA \end{aligned}$$

Virtual internal power

$$\begin{aligned} \delta_* \dot{\Pi}^{\text{int}} := & \frac{1}{2} \int_{\mathcal{B}_0} \left\{ \left[2 \frac{\partial \Psi_M}{\partial \mathbf{C}} + \tilde{\mathbf{S}} - \mathbf{S} \right] : \delta_* \dot{\mathbf{C}} + \left[2 \frac{\partial \Psi_F}{\partial \mathbf{C}_F} + \tilde{S}_F - S_F \right] : \delta_* \dot{C}_F - \dot{\eta} \delta_* \bar{\Theta} \right\} \, dV \\ & - \frac{1}{2} \int_{\mathcal{B}_0} \delta_* \mathbf{S} : [\dot{\mathbf{C}} - \dot{\mathbf{C}}(\dot{\varphi})] \, dV + \int_{\mathcal{B}_0} \left\{ \nabla(\delta_* \dot{\varphi}) : \mathbf{F} [\mathbf{S} + S_F \mathbf{A}_0] + \delta_* \dot{C}_v : \frac{\partial \Psi}{\partial \mathbf{C}_v} \right\} \, dV \\ & - \frac{1}{2} \int_{\mathcal{B}_0} \delta_* \mathbf{S}_F : [\dot{C}_F - \dot{\mathbf{C}}(\dot{\varphi}) : \mathbf{A}_0] \, dV + \int_{\mathcal{B}_0} \left\{ \delta_* \dot{\Theta} \left[\frac{\partial \Psi}{\partial \Theta} + \eta \right] - \delta_* \dot{\eta} [\bar{\Theta} - \Theta] \right\} \, dV \end{aligned}$$

Euler-Lagrange equations

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Constitutive equations

$$\begin{aligned}\frac{\partial T}{\partial \mathbf{v}} &= \mathbf{p} & \forall t \geq t_0 & \quad \eta = -\frac{\partial \Psi}{\partial \Theta} \\ 2 \frac{\partial \Psi_M}{\partial \tilde{\mathbf{C}}} + \tilde{\mathbf{S}} &= \mathbf{S} & \forall t \geq t_0 & \quad \mathbf{S}_F = \left[2 \frac{\partial \Psi_F}{\partial \tilde{\mathbf{C}}_F} + \tilde{\mathbf{S}}_F \right] \mathbf{A}_0 \\ \dot{\tilde{\mathbf{C}}}(\dot{\varphi}) &= \dot{\tilde{\mathbf{C}}} \quad \text{with} \quad \tilde{\mathbf{C}}(t_0) = \mathbf{C}(\varphi_0) & -\frac{\partial \Psi_M}{\partial \mathbf{C}_v} &= \mathbb{V}(\mathbf{C}_v) \dot{\mathbf{C}}_v \\ \dot{\tilde{\mathbf{C}}}_F(\dot{\varphi}) : \mathbf{A}_0 &= \dot{\tilde{\mathbf{C}}}_F \quad \text{with} \quad \tilde{\mathbf{C}}_F(t_0) = \mathbf{C}_F(\varphi_0) : \mathbf{A}_0 & \tilde{\Theta} &= \Theta\end{aligned}$$

Neumann and Dirichlet boundary conditions

$$\begin{aligned}\mathbf{F}[\mathbf{S} + \mathbf{S}_F \mathbf{A}_0] \mathbf{N} &= \bar{\mathbf{T}} & \forall t \geq t_0 \quad \text{on} \quad \partial_T \mathcal{B}_0 \\ \mathbf{F}[\mathbf{S} + \mathbf{S}_F \mathbf{A}_0] \mathbf{N} &= \mathbf{R} & \dot{\varphi} = \dot{\bar{\varphi}} \quad \text{with} \quad \varphi(t_0) = \bar{\varphi}(t_0) \quad \text{on} \quad \partial_\varphi \mathcal{B}_0 \\ -\mathbf{Q} \cdot \mathbf{N} &= \bar{Q} & \forall t \geq t_0 \quad \text{on} \quad \partial_Q \mathcal{B}_0 \\ -\frac{\mathbf{Q} \cdot \mathbf{N}}{\Theta} &= \lambda & \tilde{\Theta} = \bar{\Theta} & \quad \forall t \geq t_0 \quad \text{on} \quad \partial_\Theta \mathcal{B}_0 \\ 0 &= h & \dot{\Theta} = \dot{\bar{\Theta}} \quad \text{with} \quad \Theta(t_0) = \bar{\Theta}(t_0) & \quad \text{on} \quad \partial_{\dot{\Theta}} \mathcal{B}_0\end{aligned}$$

Time evolution equations in first order form

(cf. Romero [2010])

$$\begin{aligned}\mathbf{v} &= \dot{\mathbf{u}} \quad \text{with} \quad \varphi(t_0) = \varphi_0 \\ \text{Div}[\mathbf{F}\mathbf{S} + \mathbf{F}_F \mathbf{S}_F] + \rho_0 \mathbf{B} &= \dot{\mathbf{p}} \quad \text{with} \quad \mathbf{p}(t_0) = \mathbf{p}_0 \equiv \frac{\partial T(\mathbf{v}_0)}{\partial \mathbf{v}} \\ -\frac{\text{Div}[\mathbf{Q}]}{\Theta} + \frac{R + D^{\text{int}}}{\Theta} &= \dot{\eta} \quad \text{with} \quad \eta(t_0) = \eta_0 \equiv -\frac{\partial \Psi(\varphi_0, \Theta_0)}{\partial \Theta}\end{aligned}$$

Discrete variational principle

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Discrete principle of virtual power

$$\sum_{n=0}^{N-1} \sum_{l,j,i=1}^{k_{mec}, k_{the}, k_{vis}} \delta_* \dot{\mathcal{H}}_h^n(\mathbf{z}_h^n(\xi_{l,j,i}), \mathbf{w}_h^n(\xi_{l,j,i}); \tilde{\mathbf{S}}_h^n(\xi_i), \tilde{\mathbf{S}}_{F_h}^n(\xi_i)) w_{l,j,i} h_n = 0 \quad \text{with} \quad \begin{aligned} \mathbf{z} &= (\dot{\varphi}, \dot{\mathbf{v}}, \dot{\mathbf{p}}, \dot{\mathbf{C}}_v, \dot{\mathbf{C}}, \dot{\mathbf{C}}_F, \dot{\Theta}, \dot{\eta}) \\ \mathbf{w} &= (\tilde{\Theta}, S, S_F, R, h, \lambda) \end{aligned}$$

$$\sum_{n=0}^{N-1} \delta_* \dot{\mathcal{H}}_d(\mathbf{q}, \mathbf{v}, \mathbf{p}, \mathbf{C}_v, \mathbf{C}, \mathbf{C}_F, \mathbf{o}, \mathbf{s}, \tilde{\mathbf{o}}, \mathbf{R}, \mathbf{h}, \boldsymbol{\lambda}, \tilde{\mathbf{S}}, \tilde{\mathbf{S}}_F; \tilde{\mathbf{S}}_h^n(\xi_i), \tilde{\mathbf{S}}_{F_h}^n(\xi_i)) h_n = 0 \quad \text{with} \quad \begin{aligned} \mathbf{q} &= (\varphi_2, \dots, \varphi_{k_{mec}+1}) \\ \tilde{\mathbf{o}} &= (\tilde{\Theta}_1, \dots, \tilde{\Theta}_{k_{the}}) \end{aligned}$$

Galerkin time approximation with Lagrange polynomials

$$\varphi_h^n(\alpha) := \sum_{j=1}^{k_{mec}+1} M_j(\alpha) \varphi_j^n \quad \delta_* \dot{\varphi}_h^n(\alpha) := \frac{1}{h_n} \sum_{i=1}^{k_{mec}} \tilde{M}_j(\alpha) \tilde{\varphi}_i^n \quad \delta_* \tilde{\Theta}_h^n(\alpha) := \sum_{i=1}^{k_{the}} \tilde{M}_i(\alpha) \tilde{\Theta}_i^n \quad \tilde{\Theta}_h^n(\alpha) := \sum_{i=1}^{k_{the}} \tilde{M}_i(\alpha) \tilde{\Theta}_i^n$$

Discrete Euler-Lagrange equations with space-time finite elements

Momentum equation: $[\tilde{\mathbf{B}} \otimes \mathbf{H}_q \otimes \mathbf{I}] [\rho_0 \mathbf{v} - \mathbf{p}] + \tilde{\mathbf{b}} \otimes [\mathbf{H}_q \otimes \mathbf{I}] [\rho_0 \mathbf{v}_1 - \mathbf{p}_1] = \mathbf{0}$

Velocity equation: $[\tilde{\mathbf{B}} \otimes \mathbf{H}_q \otimes \mathbf{I}] \mathbf{v} + \tilde{\mathbf{b}} \otimes [\mathbf{H}_q \otimes \mathbf{I}] \mathbf{v}_1 = \left[\frac{1}{h_n} \tilde{\mathbf{A}} \otimes \mathbf{H}_q \otimes \mathbf{I} \right] \mathbf{q} + \frac{1}{h_n} \tilde{\mathbf{a}} \otimes [\mathbf{H}_q \otimes \mathbf{I}] \mathbf{q}_1$

Positions on $\partial_\varphi \mathcal{B}_0$: $[\tilde{\mathbf{A}} \otimes \tilde{\mathbf{H}}_q \otimes \mathbf{I}] \tilde{\mathbf{q}} + \tilde{\mathbf{a}} \otimes [\tilde{\mathbf{H}}_q \otimes \mathbf{I}] \tilde{\mathbf{q}}_1 = \tilde{\mathbf{q}}$

momentum balance: $\left[\frac{1}{h_n} \tilde{\mathbf{A}} \otimes \mathbf{H}_q \otimes \mathbf{I} \right] \mathbf{p} + \frac{1}{h_n} \tilde{\mathbf{a}} \otimes [\mathbf{H}_q \otimes \mathbf{I}] \mathbf{p}_1 - \mathbf{F}^{\text{int}} - \mathbf{F}^{\text{ext}} - \tilde{\mathbf{F}}^{\text{ext}} = [\tilde{\mathbf{C}} \otimes \tilde{\mathbf{H}}_q \otimes \mathbf{I}] \mathbf{R}$

Temperature | Entropy equation: $[\tilde{\mathbf{C}} \otimes \mathbf{H}_o] \tilde{\mathbf{o}} = [\tilde{\mathbf{B}} \otimes \mathbf{H}_o] \mathbf{o} + \tilde{\mathbf{b}} \otimes \mathbf{H}_o \mathbf{o}_1 \quad \Phi + [\tilde{\mathbf{B}} \otimes \mathbf{H}_o] \mathbf{s} + \tilde{\mathbf{b}} \otimes \mathbf{H}_o \mathbf{s}_1 = [\tilde{\mathbf{C}} \otimes \tilde{\mathbf{H}}_o] \tilde{\mathbf{h}}$

Temperatures on $\partial_\Theta \mathcal{B}_0 | \partial_\Theta \mathcal{B}_0$: $[\tilde{\mathbf{A}} \otimes \tilde{\mathbf{H}}_o] \tilde{\mathbf{o}} + \tilde{\mathbf{a}} \otimes [\tilde{\mathbf{H}}_o] \tilde{\mathbf{o}}_1 = \tilde{\mathbf{o}} \quad \tilde{\mathbf{o}} = \mathbf{e}_k \otimes \tilde{\mathbf{o}}$

Entropy balance: $\left[\frac{1}{h_n} \tilde{\mathbf{A}} \otimes \mathbf{H}_o \right] \mathbf{s} + \frac{1}{h_n} \tilde{\mathbf{a}} \otimes \mathbf{H}_o \mathbf{s}_1 - \mathbf{S}^{\text{con}} - \mathbf{S}^{\text{cdu}} - \mathbf{S}^{\text{int}} - \tilde{\mathbf{S}}^{\text{ext}} = [\tilde{\mathbf{C}} \otimes \tilde{\mathbf{H}}_o] \boldsymbol{\lambda}$

Local discrete Euler-Lagrange equations

Stress equations at the Gauss points in space and time

$$S(\xi_i, \chi_I) = 2 \frac{\partial \Psi_M(\xi_i, \chi_I)}{\partial \tilde{C}} + \tilde{S}_h^n(\xi_i, \chi_I) \quad S_F(\xi_i, \chi_I) = 2 \frac{\partial \Psi_F(\xi_i, \chi_I)}{\partial \tilde{C}_F} + \tilde{S}_{Fh}^n(\xi_i, \chi_I) \quad (\xi_i = 1, \dots, k_{\text{mec}})$$

Viscous time evolution equations at the Gauss points in space

$$\Upsilon(\mathbf{C}_v(\chi_I)) = \frac{1}{h_n} \mathbf{V}(\mathbf{C}_v(\chi_I)) \rightarrow \text{local level Newton-Raphson method} \quad \leadsto \mathbf{C}_v(\chi_I) \in \mathbb{R}^{6 k_{\text{vis}}}$$

Discrete weak assumed strain equations on the element

$$\sum_{i=1}^{k_{\text{mec}}} \delta_* S_h^{n,e}(\xi_i, \chi_I) : \left[\frac{d \tilde{C}_h^{n,e}(\xi_i, \chi_I)}{d\alpha} - \overset{\circ}{C}(\overset{\circ}{\varphi}_h^{n,e}(\xi_i, \chi_I)) \right] w_i = 0 \quad (i = 1, \dots, k_{\text{mec}})$$

Discrete assumed strain equations at the Gauss points in space

$$\frac{d \tilde{C}_h^n(\xi_l, \chi_I)}{d\alpha} = \overset{\circ}{C}(\overset{\circ}{\varphi}_h^n(\xi_l, \chi_I)) \quad l = 1, \dots, k_{\text{mec}} \quad \frac{d \tilde{C}_h^n(\xi_l, \chi_I)}{d\alpha} = \sum_{j=1}^{k_{\text{mec}}+1} \overset{\circ}{M}_j(\xi_l) C_j^n(\chi_I) \equiv \sum_{i=1}^{k_{\text{mec}}} \tilde{M}_i(\xi_l) \tilde{C}_i^n(\chi_I)$$

Assumed strains at the time nodes $C_l^n(\chi_I)$, $l = 2, \dots, k_{\text{mec}}$

$$C_l^n(\chi_I) := \sum_{i=1}^{k_{\text{mec}}} m_{li} \overset{\circ}{C}(\overset{\circ}{\varphi}_h^n(\xi_i, \chi_I)) + C_1^n(\chi_I) \quad \text{with} \quad m = \begin{bmatrix} \overset{\circ}{M}_2(\xi_1) & \dots & \overset{\circ}{M}_{k+1}(\xi_1) \\ \vdots & \dots & \vdots \\ \overset{\circ}{M}_2(\xi_k) & \dots & \overset{\circ}{M}_{k+1}(\xi_k) \end{bmatrix}^{-1}$$

Discrete mechanical energy balance

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Discrete kinetic energy balance

(cf. G. & Betsch [2011])

$$\begin{aligned}
 \frac{T_{n+1} - T_n}{h_n} &= \frac{1}{2 h_n} \{ \mathbf{v}_{k_{\text{mec}}+1}^T [\mathbf{M} \otimes \mathbf{I}] \mathbf{v}_{k_{\text{mec}}+1} - \mathbf{v}_1^T [\mathbf{M} \otimes \mathbf{I}] \mathbf{v}_1 \} \\
 &= \frac{1}{2 h_n} \begin{bmatrix} \mathbf{v}_1 \\ \mathbf{v} \end{bmatrix}^T [2 \mathbf{J}^{\text{sym}} \otimes \mathbf{M} \otimes \mathbf{I}] \begin{bmatrix} \mathbf{v}_1 \\ \mathbf{v} \end{bmatrix} \quad \text{with } 2 \mathbf{J}^{\text{sym}} := \text{diag}(\overbrace{-1, 0, \dots, 0}^{k_{\text{mec}}}, 1) \\
 &= \begin{bmatrix} \mathbf{p}_1 \\ \mathbf{p} \end{bmatrix}^T \begin{bmatrix} \frac{1}{h_n} \mathbf{J}^T \otimes \mathbf{H}_q \otimes \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{v}_1 \\ \mathbf{v} \end{bmatrix} \quad \text{with momentum equation and } a \mathbf{A} a = a \mathbf{A}^T a \\
 &= \begin{bmatrix} \mathbf{p}_1 \\ \mathbf{p} \end{bmatrix}^T \begin{bmatrix} \frac{1}{(h_n)^2} [\tilde{\mathbf{a}} | \tilde{\mathbf{A}}]^T \tilde{\mathbf{C}}^{-T} [\tilde{\mathbf{a}} | \tilde{\mathbf{A}}] \otimes \mathbf{H}_q \otimes \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{q}_1 \\ \mathbf{q} \end{bmatrix} \quad \text{with velocity equation} \\
 &= \begin{bmatrix} \mathbf{q}_1 \\ \mathbf{q} \end{bmatrix}^T \begin{bmatrix} \frac{1}{(h_n)^2} \tilde{\mathbf{T}}_1^T [\tilde{\mathbf{a}} | \tilde{\mathbf{A}}] \otimes \mathbf{H}_q \otimes \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{p}_1 \\ \mathbf{p} \end{bmatrix} \quad \text{with } \tilde{\mathbf{T}}_1 := \tilde{\mathbf{C}}^{-1} [\tilde{\mathbf{a}} | \tilde{\mathbf{A}}] \text{ and } a \mathbf{A} b = b \mathbf{A}^T a \\
 \frac{T_{n+1} - T_n}{h_n} &= \frac{1}{h_n} \begin{bmatrix} \mathbf{q}_1 \\ \mathbf{q} \end{bmatrix}^T \left[\tilde{\mathbf{T}}_1^T \otimes \mathbf{I}_q \otimes \mathbf{I} \right] \left\{ \mathbf{F}^{\text{int}} + \mathbf{F}^{\text{ext}} + \tilde{\mathbf{F}}^{\text{ext}} \right\} \quad \text{with momentum balance} \\
 &+ \frac{1}{h_n} \begin{bmatrix} \mathbf{q}_1 \\ \mathbf{q} \end{bmatrix}^T \left[\tilde{\mathbf{T}}_1^T \otimes \mathbf{I}_q \otimes \mathbf{I} \right] \cancel{[\tilde{\mathbf{C}} \otimes \tilde{\mathbf{H}}_q \otimes \mathbf{I}] \mathbf{R}}^0 \stackrel{(\perp)}{\rightarrow} \begin{bmatrix} \mathbf{q}_1 \\ \mathbf{q} \end{bmatrix}^T \left[\tilde{\mathbf{T}}_1^T \otimes \mathbf{I}_q \otimes \mathbf{I} \right] \equiv \dot{\mathbf{q}}^T
 \end{aligned}$$

Discrete potential energy balance with dead loads $\mathbf{F}^{\text{ext}}$

$$\begin{aligned}
 \sum_{I=1}^{N_q} [\Psi_{n+1}(\chi_I) - \Psi_n(\chi_I)] W_I &= - \dot{\mathbf{q}}^T [\mathbf{F}^{\text{int}} + \mathbf{F}^{\text{ext}}] - [\Pi_{n+1}^{\text{ext}} - \Pi_n^{\text{ext}}] \\
 &+ \sum_{i=1}^{k_{\text{vis}}} \sum_{I=1}^{N_q} \left[\frac{\partial \Psi_M}{\partial \mathbf{C}_v} : \dot{\mathbf{C}}_v \right] (\xi_i, \chi_I) W_I w_i + \sum_{j=1}^{k_{\text{the}}} \sum_{I=1}^{N_q} \left[\frac{\partial \Psi}{\partial \Theta} \dot{\Theta} \right] (\xi_j, \chi_I) W_I w_j \\
 \Pi_{n+1}^{\text{pot}} - \Pi_n^{\text{pot}} &- \sum_{i,j,l} \sum_I \left[\frac{\partial \Psi_M}{\partial \tilde{\mathbf{C}}} : \dot{\tilde{\mathbf{C}}} + \frac{\partial \Psi_F}{\partial \tilde{\mathbf{C}}_F} \dot{\tilde{\mathbf{C}}}_F + \frac{\partial \Psi_M}{\partial \mathbf{C}_v} : \dot{\mathbf{C}}_v + \frac{\partial \Psi}{\partial \Theta} \dot{\Theta} \right] (\xi_{i,j,l}, \chi_I) W_I w_{i,j,l} \\
 &= \sum_{l=1}^{k_{\text{mec}}} \sum_{I=1}^{N_q} \frac{1}{2} \left[\tilde{\mathbf{S}} : \dot{\tilde{\mathbf{C}}} + \tilde{\mathbf{S}}_F : \dot{\tilde{\mathbf{C}}}_F \right] (\xi_l, \chi_I) W_I w_l \quad \text{with stress equations}
 \end{aligned}$$

Discrete superimposed fiber stress ($k_{\text{mec}} = k_{\text{the}} = k_{\text{vis}} = 1$)

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Discrete claim for the fiber stress at the Gauss points in space

$$\left[\frac{\partial \Psi_F(\tilde{C}_F, \Theta)_{n+\frac{1}{2}}}{\partial \tilde{C}_F} + \frac{1}{2} \tilde{S}_{F_{n+\frac{1}{2}}} \right] \underbrace{\mathbf{A}_0 : [\mathbf{C}_{n+1} - \mathbf{C}_n]}_{\mathbf{C}_{F_{n+1}} - \mathbf{C}_{F_n}} + \frac{\partial \Psi_F(\tilde{C}_F, \Theta)_{n+\frac{1}{2}}}{\partial \Theta} [\Theta_{n+1} - \Theta_n] = \Psi_F(\tilde{C}_F, \Theta)_{n+1} - \Psi_F(\tilde{C}_F, \Theta)_n$$

Variational problem

(cf. Gauss's principle in Ramm [2011])

$$\mathcal{L}(\mu, \tilde{S}_{F_{n+\frac{1}{2}}}) := \frac{1}{2} (\tilde{S}_{F_{n+\frac{1}{2}}})^2 + \mu \mathcal{G}(\tilde{S}_{F_{n+\frac{1}{2}}}) \quad \delta_* \mathcal{L}(\mu, \tilde{S}_{F_{n+\frac{1}{2}}}) = 0$$

Discrete claim as constraint

(cf. Hesch & Betsch [2011], G. & Betsch [2011])

$$\mathcal{G}(\tilde{S}_{F_{n+\frac{1}{2}}}) := \Psi_F(\tilde{C}_F, \Theta)_{n+1} - \Psi_F(\tilde{C}_F, \Theta)_n - \left[\frac{\partial \Psi_F(\tilde{C}_F, \Theta)_{n+\frac{1}{2}}}{\partial \tilde{C}_F} + \frac{1}{2} \tilde{S}_{F_{n+\frac{1}{2}}} \right] [\mathbf{C}_{F_{n+1}} - \mathbf{C}_{F_n}] - \frac{\partial \Psi_F(\tilde{C}_F, \Theta)_{n+\frac{1}{2}}}{\partial \Theta} [\Theta_{n+1} - \Theta_n] = 0$$

Discrete Euler-Lagrange equations

$$\frac{\partial \mathcal{L}}{\partial \tilde{S}_{F_{n+\frac{1}{2}}}} \equiv \tilde{S}_{F_{n+\frac{1}{2}}} - \frac{\mu}{2} [\mathbf{C}_{F_{n+1}} - \mathbf{C}_{F_n}] = 0 \quad \frac{\partial \mathcal{L}}{\partial \mu} \equiv \mathcal{G}(\tilde{S}_{F_{n+\frac{1}{2}}}) = 0$$

Discrete superimposed fiber stress

(cf. Gonzalez [2000], Hesch & Betsch [2011])

$$\tilde{S}_{F_{n+\frac{1}{2}}} = 2 \frac{\mathcal{G}(O)}{[\mathbf{C}_{F_{n+1}} - \mathbf{C}_{F_n}] [\mathbf{C}_{F_{n+1}} - \mathbf{C}_{F_n}]} [\mathbf{C}_{F_{n+1}} - \mathbf{C}_{F_n}]$$

Discrete superimposed stress tensor $(k_{mec} = k_{the} = k_{vis} = 1)$

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Discrete claim for the matrix stress tensor

(one equation for 6 unknowns)

$$\left[\frac{\partial \Psi_M(\tilde{\mathbf{C}}, \mathbf{C}_v, \Theta)_{n+\frac{1}{2}}}{\partial \tilde{\mathbf{C}}} + \frac{1}{2} \tilde{\mathbf{S}}_{n+\frac{1}{2}} \right] : [\mathbf{C}_{n+1} - \mathbf{C}_n] + \frac{\partial \Psi_M(\tilde{\mathbf{C}}, \mathbf{C}_v, \Theta)_{n+\frac{1}{2}}}{\partial \mathbf{C}_v} + \frac{\partial \Psi_M(\tilde{\mathbf{C}}, \mathbf{C}_v, \Theta)_{n+\frac{1}{2}}}{\partial \Theta} \\ = \Psi_M(\tilde{\mathbf{C}}, \mathbf{C}_v, \Theta)_{n+1} - \Psi_M(\tilde{\mathbf{C}}, \mathbf{C}_v, \Theta)_n$$

Constrained variational problem with the Mandel stress tensor

$$\mathcal{L}(\mu, \tilde{\mathbf{S}}_{n+\frac{1}{2}}) := \frac{1}{2} \tilde{\mathbf{C}}_{n+\frac{1}{2}} \tilde{\mathbf{S}}_{n+\frac{1}{2}} : \tilde{\mathbf{S}}_{n+\frac{1}{2}} \tilde{\mathbf{C}}_{n+\frac{1}{2}} + \mu \mathcal{G}(\tilde{\mathbf{S}}_{n+\frac{1}{2}}) \quad \delta_* \mathcal{L}(\mu, \tilde{\mathbf{S}}_{n+\frac{1}{2}}) = 0$$

Discrete claim as constraint

(cf. Hesch & Betsch [2011], G. & Betsch [2011])

$$\mathcal{G}(\tilde{\mathbf{S}}_{n+\frac{1}{2}}) := \Psi_M(\tilde{\mathbf{C}}, \mathbf{C}_v, \Theta)_{n+1} - \Psi_M(\tilde{\mathbf{C}}, \mathbf{C}_v, \Theta)_n - \left[\frac{\partial \Psi_M(\tilde{\mathbf{C}}, \mathbf{C}_v, \Theta)_{n+\frac{1}{2}}}{\partial \tilde{\mathbf{C}}} + \frac{1}{2} \tilde{\mathbf{S}}_{n+\frac{1}{2}} \right] : [\mathbf{C}_{n+1} - \mathbf{C}_n] \\ - \frac{\partial \Psi_M(\tilde{\mathbf{C}}, \mathbf{C}_v, \Theta)_{n+\frac{1}{2}}}{\partial \mathbf{C}_v} - \frac{\partial \Psi_M(\tilde{\mathbf{C}}, \mathbf{C}_v, \Theta)_{n+\frac{1}{2}}}{\partial \Theta}$$

Discrete Euler-Lagrange equations

$$\frac{\partial \mathcal{L}}{\partial \tilde{\mathbf{S}}_{n+\frac{1}{2}}} \equiv \tilde{\mathbf{C}}_{n+\frac{1}{2}} \tilde{\mathbf{S}}_{n+\frac{1}{2}} \tilde{\mathbf{C}}_{n+\frac{1}{2}} - \frac{\mu}{2} [\mathbf{C}_{n+1} - \mathbf{C}_n] = \mathbf{O} \quad \frac{\partial \mathcal{L}}{\partial \mu} \equiv \mathcal{G}(\tilde{\mathbf{S}}_{n+\frac{1}{2}}) = 0$$

Discrete superimposed stress tensor

(cf. Armero & Zambrana-Rojas [2007])

$$\tilde{\mathbf{S}}_{n+\frac{1}{2}} = 2 \frac{\mathcal{G}(\mathbf{O})}{\tilde{\mathbf{C}}_{n+\frac{1}{2}}^{-1} [\mathbf{C}_{n+1} - \mathbf{C}_n] : [\mathbf{C}_{n+1} - \mathbf{C}_n] \tilde{\mathbf{C}}_{n+\frac{1}{2}}^{-1}} \tilde{\mathbf{C}}_{n+\frac{1}{2}}^{-1} [\mathbf{C}_{n+1} - \mathbf{C}_n] \tilde{\mathbf{C}}_{n+\frac{1}{2}}^{-1}$$

Higher-order variational vs. Galerkin schemes

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Galerkin scheme ($k_{\text{mec}} = 2$)

$$\mathbf{C}_n \equiv \mathbf{C}_1^n := (\mathbf{F}_1^n)^T \mathbf{F}_1^n$$

$$\mathbf{C}_2^n := (\mathbf{F}_2^n)^T \mathbf{F}_2^n$$

$$\mathbf{C}_{n+1} \equiv \mathbf{C}_3^n := (\mathbf{F}_3^n)^T \mathbf{F}_3^n$$

Variational scheme for $k_{\text{mec}} = 2$

$$\mathbf{C}_n \equiv \mathbf{C}_1^n := (\mathbf{F}_1^n)^T \mathbf{F}_1^n$$

$$\mathbf{C}_2^n := \frac{1}{3} \left[\frac{\mathbf{F}_1^n + \mathbf{F}_3^n}{2} - \mathbf{F}_2^n \right]^T \left[\frac{\mathbf{F}_1^n + \mathbf{F}_3^n}{2} - \mathbf{F}_2^n \right] + (\mathbf{F}_2^n)^T \mathbf{F}_2^n$$

$$\mathbf{C}_{n+1} \equiv \mathbf{C}_3^n := (\mathbf{F}_3^n)^T \mathbf{F}_3^n$$

Superimposed stress tensor of Galerkin schemes

(cf. Mohr, Menzel, Steinmann [2008])

$$\tilde{\mathbf{S}}_h^n(\xi_i) := 2 \frac{\mathcal{G}(\mathcal{O})}{\sum_{l=1}^{k_{\text{mec}}} \tilde{\mathcal{C}}_h^n(\xi_l) : \overset{\circ}{\mathcal{C}}(\overset{\circ}{\varphi}_h^n)(\xi_l) w_l} \overset{\circ}{\tilde{\mathcal{C}}}_h^n(\xi_i)$$

(energy consistent, **but not** variationally consistent approximation)

with

$$\tilde{\mathcal{C}}_h^n(\alpha) = \sum_{j=1}^{k_{\text{mec}}+1} M_{j+1}(\alpha) [\mathbf{F}_j^n]^T \mathbf{F}_j^n \quad (i = 1, \dots, k_{\text{mec}})$$

Superimposed stress tensor of variational schemes

(cf. G. & Dietzsch [2017])

$$\tilde{\mathbf{S}}_h^n(\xi_i) := 2 \frac{\mathcal{G}(\mathcal{O})}{\sum_{l=1}^{k_{\text{mec}}} [\tilde{\mathcal{C}}_h^n(\xi_l)]^{-1} \overset{\circ}{\tilde{\mathcal{C}}}_h^n(\xi_l) : \overset{\circ}{\tilde{\mathcal{C}}}_h^n(\xi_l) [\tilde{\mathcal{C}}_h^n(\xi_l)]^{-1} w_l} [\tilde{\mathcal{C}}_h^n(\xi_i)]^{-1} \overset{\circ}{\tilde{\mathcal{C}}}_h^n(\xi_i) [\tilde{\mathcal{C}}_h^n(\xi_i)]^{-1}$$

with

$$\tilde{\mathcal{C}}_h^n(\alpha) = \sum_{j=1}^{k_{\text{mec}}+1} M_{j+1}(\alpha) \mathbf{C}_j^n \quad (i = 1, \dots, k_{\text{mec}})$$

Discrete balances of thermal and total energy

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Discrete thermal energy balance

$$\begin{aligned}
 \frac{\Pi_{n+1}^{\text{the}} - \Pi_n^{\text{the}}}{h_n} &= \frac{1}{h_n} \left\{ \mathbf{o}_{k_{\text{the}}+1}^T \mathbf{H}_o \mathbf{s}_{k_{\text{the}}+1} - \mathbf{o}_1^T \mathbf{H}_o \mathbf{s}_1 \right\} & \text{with } \Pi_\alpha^{\text{the}} &:= \sum_{I=1}^{N_q} \Theta(\chi_I, \alpha) \eta(\chi_I, \alpha) W_I \\
 &= \begin{bmatrix} \mathbf{o}_1 \\ \mathbf{o} \end{bmatrix}^T \left[\frac{2}{h_n} \mathbf{J}^{\text{sym}} \otimes \mathbf{H}_o \right] \begin{bmatrix} \mathbf{s}_1 \\ \mathbf{s} \end{bmatrix} & \text{with } 2\mathbf{J}^{\text{sym}} &:= \text{diag} \left(\overbrace{-1, 0, \dots, 0}^{k_{\text{the}}}, 1 \right) \\
 &= \begin{bmatrix} \mathbf{o}_1 \\ \mathbf{o} \end{bmatrix}^T \left[\frac{1}{h_n} (\mathbf{J} + \mathbf{J}^T) \otimes \mathbf{H}_o \right] \begin{bmatrix} \mathbf{s}_1 \\ \mathbf{s} \end{bmatrix} & \text{with } \mathbf{J}^T &\equiv [\tilde{\mathbf{a}} | \tilde{\mathbf{A}}]^T \overbrace{\tilde{\mathbf{C}}^{-T}}^{\tilde{\mathbf{T}}_2} [\tilde{\mathbf{b}} | \tilde{\mathbf{B}}] \equiv \tilde{\mathbf{T}}_1^T [\tilde{\mathbf{b}} | \tilde{\mathbf{B}}] \\
 &= \underbrace{\begin{bmatrix} \mathbf{o}_1 \\ \mathbf{o} \end{bmatrix}^T}_{\tilde{\Theta}^T} \underbrace{\left[\tilde{\mathbf{T}}_2^T \otimes \mathbf{I}_o \right]}_{\tilde{\Theta}^T} \underbrace{\left[\frac{1}{h_n} [[\tilde{\mathbf{a}} | \tilde{\mathbf{A}}] \otimes \mathbf{H}_o] \right]}_{\text{entropy balance}} \underbrace{\begin{bmatrix} \mathbf{s}_1 \\ \mathbf{s} \end{bmatrix}}_{\text{entropy equation}} + \frac{1}{h_n} \underbrace{\begin{bmatrix} \mathbf{o}_1 \\ \mathbf{o} \end{bmatrix}^T}_{\tilde{\Theta}^T} \underbrace{\left[\tilde{\mathbf{T}}_1^T \otimes \mathbf{I}_o \right]}_{\tilde{\Theta}^T} \underbrace{[[\tilde{\mathbf{b}} | \tilde{\mathbf{B}}] \otimes \mathbf{H}_o]}_{\text{entropy equation}} \underbrace{\begin{bmatrix} \mathbf{s}_1 \\ \mathbf{s} \end{bmatrix}}_{\text{entropy equation}} \\
 \frac{\Pi_{n+1}^{\text{the}} - \Pi_n^{\text{the}}}{h_n} &= \tilde{\Theta}^T \left[\cancel{\mathbf{s}^{\text{con}}} + \mathbf{s}^{\text{edu}} \right] + \tilde{\Theta}^T \left\{ \mathbf{s}^{\text{int}} + \bar{\mathbf{s}}^{\text{ext}} + [\tilde{\mathbf{C}} \otimes \bar{\mathbf{H}}_o] \lambda \right\} - \frac{1}{h_n} \tilde{\Theta}^T \left\{ \Phi - [\tilde{\mathbf{C}} \otimes \bar{\mathbf{H}}_o] \bar{\mathbf{h}} \right\}
 \end{aligned}$$

Discrete total energy balance

$$\begin{aligned}
 \frac{\mathcal{H}_{n+1} - \mathcal{H}_n}{h_n} &= \frac{T_{n+1} - T_n}{h_n} + \frac{\Pi_{n+1}^{\text{pot}} - \Pi_n^{\text{pot}}}{h_n} + \frac{\Pi_{n+1}^{\text{ext}} - \Pi_n^{\text{ext}}}{h_n} + \frac{\Pi_{n+1}^{\text{the}} - \Pi_n^{\text{the}}}{h_n} \\
 &= \frac{1}{h_n} \mathring{\mathbf{q}}^T \left\{ \cancel{\mathbf{F}^{\text{int}}} + \mathbf{F}^{\text{ext}} + \bar{\mathbf{F}}^{\text{ext}} \right\} \\
 &\quad - \frac{1}{h_n} \mathring{\mathbf{q}}^T \left\{ \cancel{\mathbf{F}^{\text{int}}} + \mathbf{F}^{\text{ext}} \right\} + \sum_{I=1}^{N_q} \left\{ \sum_{i=1}^{k_{\text{vis}}} \left[\frac{\partial \Psi_M}{\partial \mathbf{C}_v} : \mathring{\mathbf{C}}_v \right] (\xi_i, \chi_I) \frac{w_i}{h_n} + \sum_{j=1}^{k_{\text{the}}} \left[\frac{\partial \Psi}{\partial \Theta} \right] (\xi_j, \chi_I) \frac{w_j}{h_n} \right\} W_I \\
 &\quad - \frac{1}{h_n} \tilde{\Theta}^T \left\{ \cancel{\mathbf{s}} - [\tilde{\mathbf{C}} \otimes \mathbf{H}_o] \bar{\mathbf{h}} \right\} + \tilde{\Theta}^T \left\{ \cancel{\mathbf{s}^{\text{int}}} + \bar{\mathbf{s}}^{\text{ext}} + [\tilde{\mathbf{C}} \otimes \bar{\mathbf{H}}_o] \lambda \right\} \\
 \frac{\mathcal{H}_{n+1} - \mathcal{H}_n}{h_n} &= \frac{1}{h_n} \mathring{\mathbf{q}}^T \bar{\mathbf{F}}^{\text{ext}} + \tilde{\Theta}^T \left\{ \bar{\mathbf{s}}^{\text{ext}} + [\tilde{\mathbf{C}} \otimes \bar{\mathbf{H}}_o] \lambda \right\} + \frac{1}{h_n} \tilde{\Theta}^T [\tilde{\mathbf{C}} \otimes \mathbf{H}_o] \bar{\mathbf{h}}
 \end{aligned}$$

Discrete balances of total momenta

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Discrete balance of total angular momentum

(cf. G. & Betsch [2011])

$$\begin{aligned}
 \frac{\mathcal{J}_{n+1} - \mathcal{J}_n}{h_n} &= \frac{1}{h_n} \left\{ \mathbf{q}_{k_{mec}+1}^T \left[\mathbf{M} \otimes \mathbf{W}_{\xi_0}^T \right] \mathbf{v}_{k_{mec}+1} - \mathbf{q}_1^T \left[\mathbf{M} \otimes \mathbf{W}_{\xi_0}^T \right] \mathbf{v}_1 \right\} \quad \text{with } \mathbf{W}_{\xi_0} := \text{spin}[\xi_0] \\
 &= \begin{bmatrix} \mathbf{q}_1 \\ \mathbf{q} \end{bmatrix}^T \left[\frac{2}{h_n} \mathbf{J}^{\text{sym}} \otimes \mathbf{M} \otimes \mathbf{W}_{\xi_0}^T \right] \begin{bmatrix} \mathbf{v}_1 \\ \mathbf{v} \end{bmatrix} \quad \text{with } 2\mathbf{J}^{\text{sym}} := \text{diag}(\overbrace{-1, 0, \dots, 0}^{k_{the}}, 1) \\
 &= \begin{bmatrix} \mathbf{q}_1 \\ \mathbf{q} \end{bmatrix}^T \left[\frac{1}{h_n} (\mathbf{J} + \mathbf{J}^T) \otimes \mathbf{H}_q \otimes \mathbf{W}_{\xi_0}^T \right] \begin{bmatrix} \mathbf{p}_1 \\ \mathbf{p} \end{bmatrix} \quad \text{with momentum equation} \\
 &= \begin{bmatrix} \mathbf{q}_1 \\ \mathbf{q} \end{bmatrix}^T \left[\tilde{\mathbf{T}}_2^T \otimes \mathbf{I}_q \otimes \mathbf{W}_{\xi_0}^T \right] \left\{ \frac{1}{h_n} [[\tilde{\mathbf{a}}|\tilde{\mathbf{A}}] \otimes \mathbf{H}_q \otimes \mathbf{I}] \begin{bmatrix} \mathbf{p}_1 \\ \mathbf{p} \end{bmatrix} \right\} \quad \text{momentum balance} \\
 &+ \frac{1}{h_n} \begin{bmatrix} \mathbf{q}_1 \\ \mathbf{q} \end{bmatrix}^T \left[\tilde{\mathbf{T}}_1^T \otimes \rho_0 \mathbf{I}_q \otimes \mathbf{W}_{\xi_0}^T \right] \left\{ [[\tilde{\mathbf{b}}|\tilde{\mathbf{B}}] \otimes \mathbf{H}_q \otimes \mathbf{I}] \begin{bmatrix} \mathbf{v}_1 \\ \mathbf{v} \end{bmatrix} \right\} \quad \text{velocity equation} \\
 \frac{\mathcal{J}_{n+1} - \mathcal{J}_n}{h_n} &= \begin{bmatrix} \mathbf{q}_1 \\ \mathbf{q} \end{bmatrix}^T \left[\tilde{\mathbf{T}}_2^T \otimes \mathbf{I}_q \otimes \mathbf{W}_{\xi_0}^T \right] \left\{ \cancel{\mathbf{F}^{\text{int}}} + \mathbf{F}^{\text{ext}} + \bar{\mathbf{F}}^{\text{ext}} + [\tilde{\mathbf{C}} \otimes \bar{\mathbf{H}}_q \otimes \mathbf{I}] \mathbf{R} \right\} \quad \text{with } \mathbf{S} = \mathbf{S}^T \\
 &+ \frac{1}{(h_n)^2} \begin{bmatrix} \mathbf{q}_1 \\ \mathbf{q} \end{bmatrix}^T \left[[\tilde{\mathbf{a}}|\tilde{\mathbf{A}}]^T \tilde{\mathbf{C}}^{-T} [\tilde{\mathbf{a}}|\tilde{\mathbf{A}}] \otimes \mathbf{M} \otimes \mathbf{W}_{\xi_0}^T \right] \begin{bmatrix} \mathbf{q}_1 \\ \mathbf{q} \end{bmatrix} \quad \text{with } \mathbf{M} = \mathbf{M}^T
 \end{aligned}$$

Discrete balance of total linear momentum

(cf. G. & Betsch [2011])

$$\begin{aligned}
 \frac{\mathcal{P}_{n+1} - \mathcal{P}_n}{h_n} &= \frac{1}{h_n} \mathbf{c}^T \left\{ [\mathbf{H}_q \otimes \mathbf{I}] \mathbf{p}_{k_{mec}+1} - [\mathbf{H}_q \otimes \mathbf{I}] \mathbf{p}_1 \right\} \quad \text{with } \mathbf{c}^T := [\xi_0^T, \dots, \xi_0^T] \in \mathbb{R}^{1 \times n_{\text{dof}}} \\
 &= [\mathbf{e}_{k_{mec}} \otimes \mathbf{c}]^T \left\{ \frac{1}{h_n} [[\tilde{\mathbf{a}}|\tilde{\mathbf{A}}] \otimes \mathbf{H}_q \otimes \mathbf{I}] \begin{bmatrix} \mathbf{p}_1 \\ \mathbf{p} \end{bmatrix} \right\} \quad \text{momentum balance} \\
 &= [\mathbf{e} \otimes \mathbf{c}]^T \left\{ \cancel{\mathbf{F}^{\text{int}}} + \mathbf{F}^{\text{ext}} + \bar{\mathbf{F}}^{\text{ext}} + [\tilde{\mathbf{C}} \otimes \bar{\mathbf{H}}_q \otimes \mathbf{I}] \mathbf{R} \right\} \quad \text{with } \sum_{I=1}^{N_q} \nabla N_I = 0 \\
 \frac{\mathcal{P}_{n+1} - \mathcal{P}_n}{h_n} &= [\mathbf{e} \otimes \mathbf{c}]^T \left\{ \mathbf{F}^{\text{ext}} + \bar{\mathbf{F}}^{\text{ext}} + [\tilde{\mathbf{C}} \otimes \bar{\mathbf{H}}_q \otimes \mathbf{I}] \mathbf{R} \right\} \quad \mathbf{e}_{k_{mec}}^T := [1, \dots, 1] \in \mathbb{R}^{1 \times k_{mec}}
 \end{aligned}$$

Discrete balance of total entropy

Discrete balance of total entropy or thermal momentum

$$\begin{aligned}\frac{S_{n+1} - S_n}{h_n} &= \frac{1}{h_n} \mathbf{e}_\Theta^T \{ [\mathbf{H}_q] \mathbf{s}_{k_{\text{the}}+1} - [\mathbf{H}_q] \mathbf{s}_1 \} && \text{with } \mathbf{e}_\Theta^T := [1, \dots, 1] \in \mathbb{R}^{1 \times n_{\text{node}}} \\ &= [\mathbf{e}_{k_{\text{the}}} \otimes \mathbf{e}_\Theta]^T \underbrace{\frac{1}{h_n} [[\tilde{\mathbf{a}}[\tilde{\mathbf{A}}] \otimes \mathbf{H}_q] \begin{bmatrix} \mathbf{s}_1 \\ \mathbf{s} \end{bmatrix} }_{\text{momentum balance}} && \text{with } \mathbf{e}_{k_{\text{the}}}^T := [1, \dots, 1] \in \mathbb{R}^{1 \times k_{\text{the}}} \\ \frac{S_{n+1} - S_n}{h_n} &= [\mathbf{e}_{k_{\text{the}}} \otimes \mathbf{e}_\Theta]^T \left\{ \mathbf{s}^{\text{con}} + \mathbf{s}^{\text{cdu}} + \mathbf{s}^{\text{int}} + \bar{\mathbf{s}}^{\text{ext}} + [\tilde{\mathbf{C}} \otimes \bar{\mathbf{H}}_o] \boldsymbol{\lambda} \right\} && \text{with } \sum_{I=1}^{N_q} \nabla N_I = 0\end{aligned}$$

In the case without **transient Dirichlet** and **Neumann** boundary conditions, we obtain at $\partial_\Theta \mathcal{B}_0$

$$[\mathbf{e}_{k_{\text{the}}} \otimes \bar{\mathbf{e}}_\Theta]^T \left\{ \left[\frac{1}{h_n} \tilde{\mathbf{A}} \otimes \bar{\mathbf{H}}_o \right] \mathbf{s} + \frac{1}{h_n} \mathbf{a} \otimes \mathbf{H}_o \mathbf{s}_1 - \bar{\mathbf{s}}^{\text{con}} - \bar{\mathbf{s}}^{\text{cdu}} - \bar{\mathbf{s}}^{\text{int}} - \bar{\mathbf{s}}^{\text{ext}} \right\} = [\mathbf{e}_{k_{\text{the}}} \otimes \bar{\mathbf{e}}_\Theta]^T [\tilde{\mathbf{C}} \otimes \bar{\mathbf{H}}_o] \boldsymbol{\lambda} \leq 0$$

Discrete balance of Lyapunov function

$$\begin{aligned}\frac{\mathcal{F}_{n+1} - \mathcal{F}_n}{h_n} &= \frac{\mathcal{H}_{n+1} - \mathcal{H}_n}{h_n} - \Theta_\infty \frac{S_{n+1} - S_n}{h_n} && \text{with } \Theta_\infty^T := \Theta_\infty [\mathbf{e}_{k_{\text{the}}} \otimes \mathbf{e}_\Theta]^T \\ &= \frac{1}{h_n} \overset{\circ}{\mathbf{q}}^T \left\{ \bar{\mathbf{F}}^{\text{ext}} + [\tilde{\mathbf{C}} \otimes \bar{\mathbf{H}}_q \otimes \mathbf{I}] \mathbf{R} \right\} + [\tilde{\Theta} - \Theta_\infty]^T \left\{ \bar{\mathbf{s}}^{\text{ext}} + [\tilde{\mathbf{C}} \otimes \bar{\mathbf{H}}_o] \boldsymbol{\lambda} \right\} \\ &- \Theta_\infty^T \left\{ \mathbf{s}^{\text{cdu}} + \mathbf{s}^{\text{int}} \right\} + \frac{1}{h_n} \overset{\circ}{\Theta}^T [\tilde{\mathbf{C}} \otimes \mathbf{H}_o] \bar{\mathbf{h}}\end{aligned}$$

In the case without **transient Dirichlet** and **Neumann** boundary conditions, we arrive at

$$\begin{aligned}\frac{\mathcal{F}_{n+1} - \mathcal{F}_n}{h_n} &= \frac{1}{h_n} \overset{\circ}{\mathbf{q}}^T \left\{ \bar{\mathbf{F}}^{\text{ext}} + [\tilde{\mathbf{C}} \otimes \bar{\mathbf{H}}_q \otimes \mathbf{I}] \mathbf{R} \right\} + [\tilde{\Theta} - \Theta_\infty]^T \bar{\mathbf{s}}^{\text{ext}} \\ &- \Theta_\infty^T \left\{ \mathbf{s}^{\text{cdu}} + \mathbf{s}^{\text{int}} \right\} + \frac{1}{h_n} \overset{\circ}{\Theta}^T [\tilde{\mathbf{C}} \otimes \mathbf{H}_o] \bar{\mathbf{h}} \\ \frac{\mathcal{F}_{n+1} - \mathcal{F}_n}{h_n} &= - \Theta_\infty^T \left\{ \mathbf{s}^{\text{cdu}} + \mathbf{s}^{\text{int}} \right\} \leq 0\end{aligned}$$

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Characteristics $\Theta_{\infty} = 298.15 \text{ K}$

Geometry

Edge length $l_{\text{edge}} = 1$

Mesh

Element: 10-node

Element number: $n_{\text{el}} = 20$

Node number: $n_{\text{no}} = 59$

Boundary conditions

Red face: x -dof fixed

Green face: y -dof fixed

Blue face: z -dof fixed

$\Theta^A = \Theta_{\infty}$

Yellow face: $\Theta^A = \Theta_{\infty}$

Initial conditions

Initial velocity: $v_0^A = -10 \mathbf{e}_z$

Initial angular velocity: $\omega_0^A = \mathbf{0}$

Initial temperature: $\Theta_0^A = 308.15$

Dirichlet loads

Displacement profile: no

Temperature profile: no

Neumann loads

Traction load: no

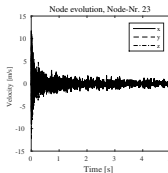
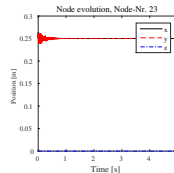
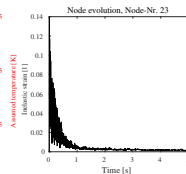
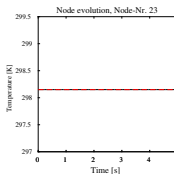
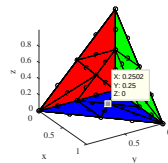
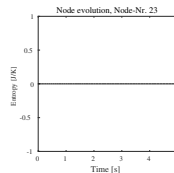
Pressure load: no

Heat flux load: no

Volume loads

Standard gravity $g = 9.81$

Time evolutions of node 23 (bottom)



Dynamic Taylor impact test with a tetrahedron

('Decreasing'-Test of balance laws; $k_{\text{mec}} = 2, k_{\text{the}} = 2, k_{\text{vis}} = 1$)

Characteristics $\Theta_{\infty} = 298.15 \text{ K}$

Geometry

Edge length $l_{\text{edge}} = 1$

Mesh

Element: 10-node

Element number: $n_{\text{el}} = 20$

Node number: $n_{\text{no}} = 59$

Boundary conditions

Red face: x -dof fixed

Green face: y -dof fixed

Blue face: z -dof fixed

$\Theta^A = \Theta_{\infty}$

Yellow face: $\Theta^A = \Theta_{\infty}$

Initial conditions

Initial velocity: $v_0^A = -10 e_z$

Initial angular velocity: $\omega_0^A = 0$

Initial temperature: $\Theta_0^A = 308.15$

Dirichlet loads

Displacement profile: no

Temperature profile: no

Neumann loads

Traction load: no

Pressure load: no

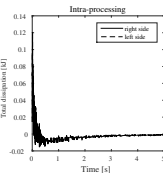
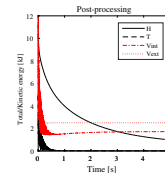
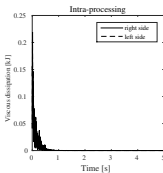
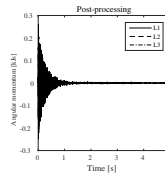
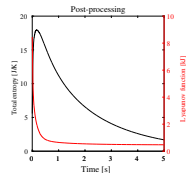
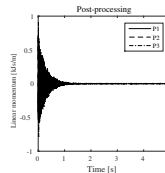
Heat flux load: no

Volume loads

Standard gravity $g = 9.81$

Balance properties

$\text{tol} = 10^{-2} \text{ J} / \text{tolevo} = 10^{-10} \text{ J}$



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Dynamic Taylor impact test with a tetrahedron (**'Decreasing'**-Test of balance laws; $k_{\text{mec}} = 2, k_{\text{the}} = 2, k_{\text{vis}} = 1$)

Characteristics $\Theta_{\infty} = 298.15 \text{ K}$

Geometry

Edge length $l_{\text{edge}} = 1$

Mesh

Element: 10-node

Element number: $n_{\text{el}} = 20$

Node number: $n_{\text{no}} = 59$

Boundary conditions

Red face: x -dof fixed

Green face: y -dof fixed

Blue face: z -dof fixed

$\Theta^A = \Theta_{\infty}$

Yellow face: $\Theta^A = \Theta_{\infty}$

Initial conditions

Initial velocity: $v_0^A = -10 e_z$

Initial angular velocity: $\omega_0^A = 0$

Initial temperature: $\Theta_0^A = 308.15$

Dirichlet loads

Displacement profile: no

Temperature profile: no

Neumann loads

Traction load: no

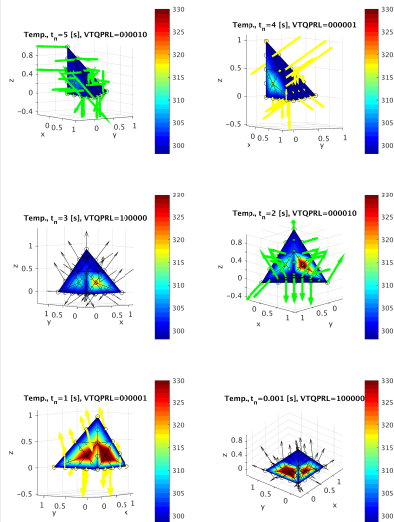
Pressure load: no

Heat flux load: no

Volume loads

Standard gravity $g = 9.81$

Snapshots of the motion with reactions



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Dynamic Taylor impact test with a tetrahedron (**'Decreasing'**-Test of balance laws; $k_{\text{mec}} = 2, k_{\text{the}} = 2, k_{\text{vis}} = 1$)

Characteristics $\Theta_{\infty} = 298.15 \text{ K}$

Geometry

Edge length $l_{\text{edge}} = 1$

Mesh

Element: 10-node

Element number: $n_{\text{el}} = 20$

Node number: $n_{\text{no}} = 59$

Boundary conditions

Red face: x -dof fixed

Green face: y -dof fixed

Blue face: z -dof fixed

$\Theta^A = \Theta_{\infty}$

Yellow face: $\Theta^A = \Theta_{\infty}$

Initial conditions

Initial velocity: $v_0^A = -10 e_z$

Initial angular velocity: $\omega_0^A = 0$

Initial temperature: $\Theta_0^A = 308.15$

Dirichlet loads

Displacement profile: no

Temperature profile: no

Neumann loads

Traction load: no

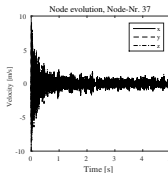
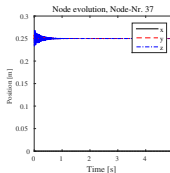
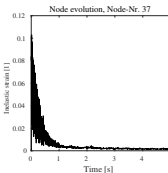
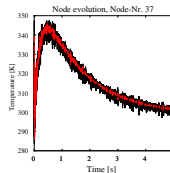
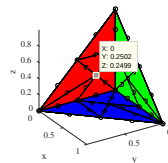
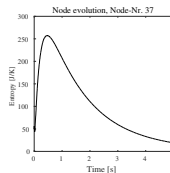
Pressure load: no

Heat flux load: no

Volume loads

Standard gravity $g = 9.81$

Time evolutions of node 37 (right)



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Dynamic Taylor impact test with a tetrahedron (**'Decreasing'**-Test of balance laws; $k_{\text{mec}} = 2, k_{\text{the}} = 2, k_{\text{vis}} = 1$)

Characteristics $\Theta_{\infty} = 298.15 \text{ K}$

Geometry

Edge length $l_{\text{edge}} = 1$

Mesh

Element: 10-node

Element number: $n_{\text{el}} = 20$

Node number: $n_{\text{no}} = 59$

Boundary conditions

Red face: x -dof fixed

Green face: y -dof fixed

Blue face: z -dof fixed

$\Theta^A = \Theta_{\infty}$

Yellow face: $\Theta^A = \Theta_{\infty}$

Initial conditions

Initial velocity: $v_0^A = -10 e_z$

Initial angular velocity: $\omega_0^A = 0$

Initial temperature: $\Theta_0^A = 308.15$

Dirichlet loads

Displacement profile: no

Temperature profile: no

Neumann loads

Traction load: no

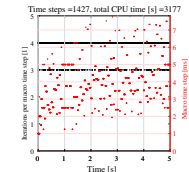
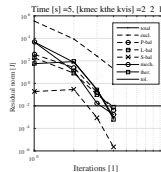
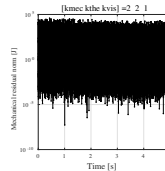
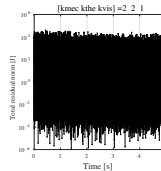
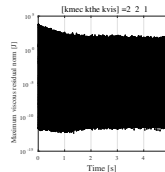
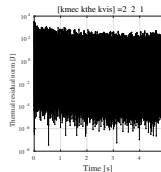
Pressure load: no

Heat flux load: no

Volume loads

Standard gravity $g = 9.81$

Time steps and CPU time $h_n^{\min} = 10^{-6} \text{ s}$



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('Decreasing'-Test of balance laws; $k_{\text{mec}} = 1, k_{\text{the}} = 1, k_{\text{vis}} = 1$)

Characteristics $\Theta_{\infty} = 298.15 \text{ K}$

Geometry

Edge length $l_{\text{edge}} = 1$

Mesh

Element: 10-node

Element number: $n_{\text{el}} = 20$

Node number: $n_{\text{no}} = 59$

Boundary conditions

Red face: x -dof fixed

Green face: y -dof fixed

Blue face: z -dof fixed

$\Theta^A = \Theta_{\infty}$

Yellow face: $\Theta^A = \Theta_{\infty}$

Initial conditions

Initial velocity: $v_0^A = -10 e_z$

Initial angular velocity: $\omega_0^A = 0$

Initial temperature: $\Theta_0^A = 308.15$

Dirichlet loads

Displacement profile: no

Temperature profile: no

Neumann loads

Traction load: no

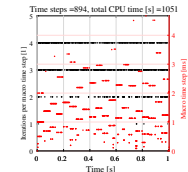
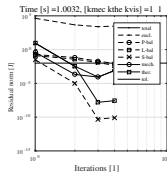
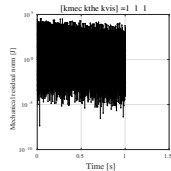
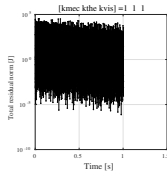
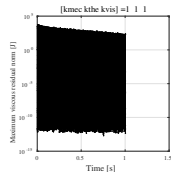
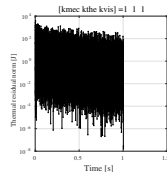
Pressure load: no

Heat flux load: no

Volume loads

Standard gravity $g = 9.81$

Time steps and CPU time $h_n^{\min} = 10^{-6} \text{ s}$



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Dynamic Taylor impact test with a tetrahedron (**'Decreasing'**-Test of balance laws; $k_{\text{mec}} = 2, k_{\text{the}} = 2, k_{\text{vis}} = 1$)

Characteristics $\Theta_{\infty} = 298.15 \text{ K}$

Geometry

Edge length $l_{\text{edge}} = 1$

Mesh

Element: 10-node

Element number: $n_{\text{el}} = 20$

Node number: $n_{\text{no}} = 59$

Boundary conditions

Red face: x -dof fixed

Green face: y -dof fixed

Blue face: z -dof fixed

$\Theta^A = \Theta_{\infty}$

Yellow face: $\Theta^A = \Theta_{\infty}$

Initial conditions

Initial velocity: $v_0^A = -10 e_z$

Initial angular velocity: $\omega_0^A = 0$

Initial temperature: $\Theta_0^A = 308.15$

Dirichlet loads

Displacement profile: no

Temperature profile: no

Neumann loads

Traction load: no

Pressure load: no

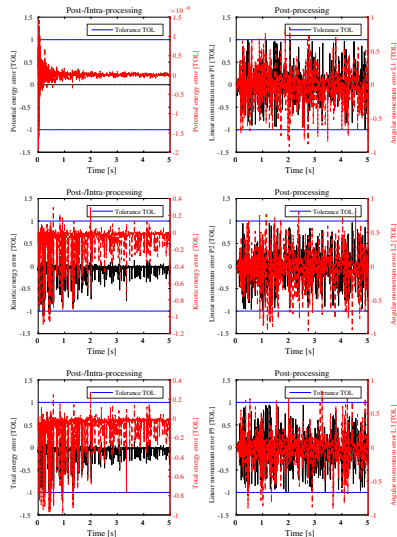
Heat flux load: no

Volume loads

Standard gravity $g = 9.81$

Mechanical balance errors

$\text{tol} = 10^{-2} \text{ J}$



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Characteristics $\Theta_{\infty} = 298.15 \text{ K}$

Geometry

Edge length $l_{\text{edge}} = 1$

Mesh

Element: 10-node

Element number: $n_{\text{el}} = 20$

Node number: $n_{\text{no}} = 59$

Boundary conditions

Red face: x -dof fixed

Green face: y -dof fixed

Blue face: z -dof fixed

$\Theta^A = \Theta_{\infty}$

Yellow face: $\Theta^A = \Theta_{\infty}$

Initial conditions

Initial velocity: $v_0^A = -10 e_z$

Initial angular velocity: $\omega_0^A = 0$

Initial temperature: $\Theta_0^A = 308.15$

Dirichlet loads

Displacement profile: no

Temperature profile: no

Neumann loads

Traction load: no

Pressure load: no

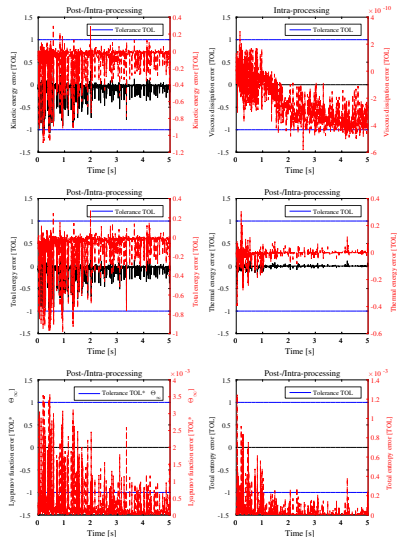
Heat flux load: no

Volume loads

Standard gravity $g = 9.81$

Thermal balance errors

$\text{tol} = 10^{-2} \text{ J}$



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Pressure and temperature load on a tetrahedron

(Mechanical Neumann/Thermal Dirichlet load; $k_{\text{mec}} = 2$, $k_{\text{the}} = 2$, $k_{\text{vis}} = 1$)

Characteristics $\Theta_{\infty} = 298.15 \text{ K}$

Geometry

Edge length $l_{\text{edge}} = 1$

Mesh

Element: 10-node

Element number: $n_{\text{el}} = 65$

Node number: $n_{\text{no}} = 158$

Boundary conditions

Red face: x -dof fixed

Green face: y -dof fixed

Blue face: z -dof fixed

$\Theta^A = \Theta_{\infty}$

Yellow face: $T_{\text{load}} = 0.5$

$\omega_{\text{load}} = 10\pi$

Initial conditions

Initial velocity: $\mathbf{v}_0^A = \mathbf{0}$

Initial angular velocity: $\boldsymbol{\omega}_0^A = \mathbf{0}$

Initial temperature: $\Theta_0^A = 308.15$

Dirichlet loads

Displacement profile: no

Temperature profile: $\hat{\Theta} = 10$

Neumann loads

Traction load: no

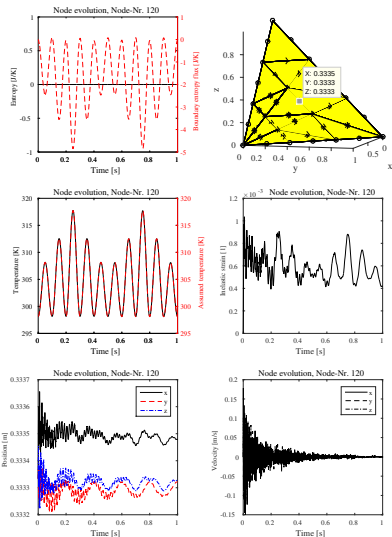
Pressure load: $\hat{p} = 4 \cdot 10^4$

Heat flux load: no

Volume loads

Standard gravity $g = 9.81$

Time evolutions of node 120 (front)



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Pressure and temperature load on a tetrahedron

(Mechanical Neumann/Thermal Dirichlet load; $k_{\text{mec}} = 2$, $k_{\text{the}} = 2$, $k_{\text{vis}} = 1$)

Characteristics $\Theta_{\infty} = 298.15 \text{ K}$

Geometry

Edge length $l_{\text{edge}} = 1$

Mesh

Element: 10-node

Element number: $n_{\text{el}} = 65$

Node number: $n_{\text{no}} = 158$

Boundary conditions

Red face: x -dof fixed

Green face: y -dof fixed

Blue face: z -dof fixed

$\Theta^A = \Theta_{\infty}$

Yellow face: $T_{\text{load}} = 0.5$

$\omega_{\text{load}} = 10\pi$

Initial conditions

Initial velocity: $\mathbf{v}_0^A = \mathbf{0}$

Initial angular velocity: $\boldsymbol{\omega}_0^A = \mathbf{0}$

Initial temperature: $\Theta_0^A = 308.15$

Dirichlet loads

Displacement profile: no

Temperature profile: $\hat{\Theta} = 10$

Neumann loads

Traction load: no

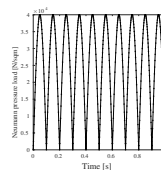
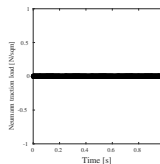
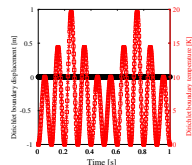
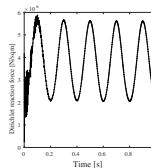
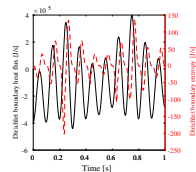
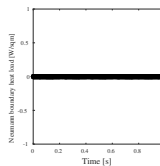
Pressure load: $\hat{p} = 4 \cdot 10^4$

Heat flux load: no

Volume loads

Standard gravity $g = 9.81$

Time evolutions of loads and reactions



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Total momenta balances

Total entropy balance

Numerical studies

Summary

Pressure and temperature load on a tetrahedron

(Mechanical Neumann/Thermal Dirichlet load; $k_{\text{mec}} = 2$, $k_{\text{the}} = 2$, $k_{\text{vis}} = 1$)

Characteristics $\Theta_{\infty} = 298.15 \text{ K}$

Geometry

Edge length $l_{\text{edge}} = 1$

Mesh

Element: 10-node

Element number: $n_{\text{el}} = 65$

Node number: $n_{\text{no}} = 158$

Boundary conditions

Red face: x -dof fixed

Green face: y -dof fixed

Blue face: z -dof fixed

$\Theta^A = \Theta_{\infty}$

Yellow face: $T_{\text{load}} = 0.5$

$\omega_{\text{load}} = 10\pi$

Initial conditions

Initial velocity: $\mathbf{v}_0^A = \mathbf{0}$

Initial angular velocity: $\boldsymbol{\omega}_0^A = \mathbf{0}$

Initial temperature: $\Theta_0^A = 308.15$

Dirichlet loads

Displacement profile: no

Temperature profile: $\hat{\Theta} = 10$

Neumann loads

Traction load: no

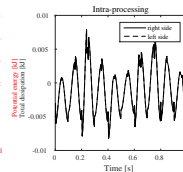
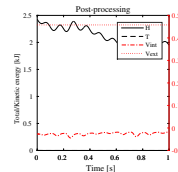
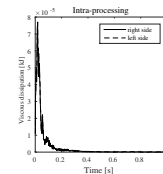
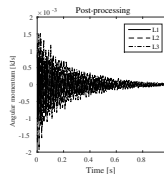
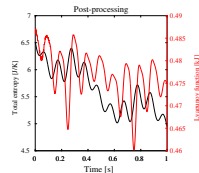
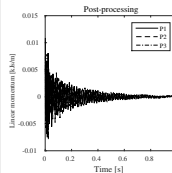
Pressure load: $\hat{p} = 4 \cdot 10^4$

Heat flux load: no

Volume loads

Standard gravity $g = 9.81$

Balance properties



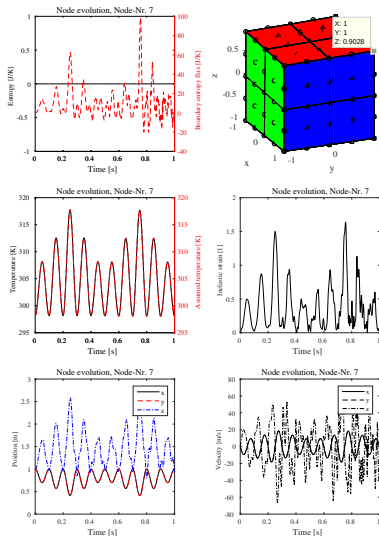
Compression test with heating on a cube

(Mechanical Dirichlet/Thermal Dirichlet load; $k_{\text{mec}} = 1$, $k_{\text{the}} = 2$, $k_{\text{vis}} = 2$)

Characteristics $\Theta_{\infty} = 298.15 \text{ K}$

Geometry	
Edge length	$l_{\text{edge}} = 2$
Mesh	
Element:	27-node
Element number:	$n_{\text{el}} = 8$
Node number:	$n_{\text{no}} = 125$
Boundary conditions	
Green yz-face:	x -dof fixed
Green xz-face:	y -dof fixed
Yellow xy-face:	z -dof fixed
	$\Theta^A = 10 f(t)$
Red xy-face:	$\Theta^A = 10 f(t)$
Blue yz-face:	$\Theta^A = \Theta_{\infty}$
	$u_x^A = -0.3 f(t)$
Blue xz-face:	$\Theta^A = \Theta_{\infty}$
	$u_y^A = -0.3 f(t)$
Initial conditions	
Initial velocities:	$\mathbf{v}_0^A = \mathbf{0} = \boldsymbol{\omega}_0^A$
Initial temperature:	$\Theta_0^A = 308.15$
Dirichlet loads	
Displacements with $f(t)$:	$T_{\text{load}} = 0.5$
Temperatures with $f(t)$:	$\omega_{\text{load}} = 10\pi$
Neumann loads	
Traction load:	no
Pressure load:	no
Heat flux load:	no
Volume loads	
Standard gravity	$g = 9.81$

Time evolutions of node 7 (corner)



Compression test with heating on a cube

(Mechanical Dirichlet/Thermal Dirichlet load; $k_{\text{mec}} = 1$, $k_{\text{the}} = 2$, $k_{\text{vis}} = 2$)

Characteristics $\Theta_{\infty} = 298.15 \text{ K}$

Geometry

Edge length $l_{\text{edge}} = 2$

Mesh

Element: 27-node

Element number: $n_{\text{el}} = 8$

Node number: $n_{\text{no}} = 125$

Boundary conditions

Green yz-face: x -dof fixed

Green xz-face: y -dof fixed

Yellow xy-face: z -dof fixed

$\Theta^A = 10 f(t)$

Red xy-face: $\Theta^A = 10 f(t)$

Blue yz-face: $\Theta^A = \Theta_{\infty}$

$u_x^A = -0.3 f(t)$

Blue xz-face: $\Theta^A = \Theta_{\infty}$

$u_y^A = -0.3 f(t)$

Initial conditions

Initial velocities: $v_0^A = \mathbf{0} = \omega_0^A$

Initial temperature: $\Theta_0^A = 308.15$

Dirichlet loads

Displacements with $f(t)$: $T_{\text{load}} = 0.5$

Temperatures with $f(t)$: $\omega_{\text{load}} = 10\pi$

Neumann loads

Traction load: no

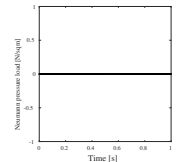
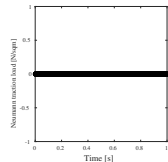
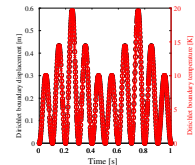
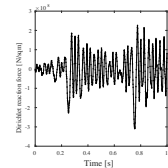
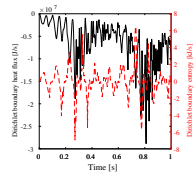
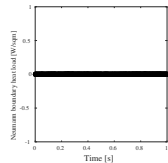
Pressure load: no

Heat flux load: no

Volume loads

Standard gravity $g = 9.81$

Time evolutions of loads and reactions



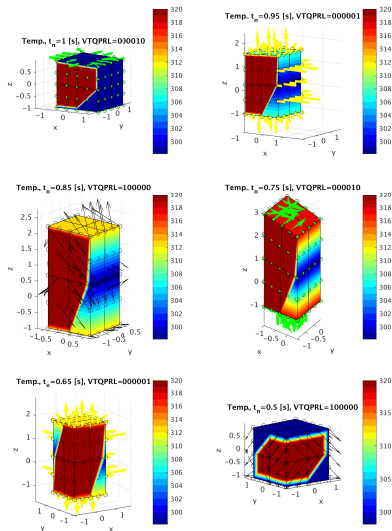
Compression test with heating on a cube

(Mechanical Dirichlet/Thermal Dirichlet load; $k_{\text{mec}} = 1$, $k_{\text{the}} = 2$, $k_{\text{vis}} = 2$)

Characteristics $\Theta_{\infty} = 298.15 \text{ K}$

Geometry	
Edge length	$l_{\text{edge}} = 2$
Mesh	
Element:	27-node
Element number:	$n_{\text{el}} = 8$
Node number:	$n_{\text{no}} = 125$
Boundary conditions	
Green yz-face:	x -dof fixed
Green xz-face:	y -dof fixed
Yellow xy-face:	z -dof fixed
	$\Theta^A = 10 f(t)$
Red xy-face:	$\Theta^A = 10 f(t)$
Blue yz-face	$\Theta^A = \Theta_{\infty}$
	$u_x^A = -0.3 f(t)$
Blue xz-face	$\Theta^A = \Theta_{\infty}$
	$u_y^A = -0.3 f(t)$
Initial conditions	
Initial velocities:	$\mathbf{v}_0^A = \mathbf{0} = \boldsymbol{\omega}_0^A$
Initial temperature:	$\Theta_0^A = 308.15$
Dirichlet loads	
Displacements with $f(t)$:	$T_{\text{load}} = 0.5$
Temperatures with $f(t)$:	$\omega_{\text{load}} = 10\pi$
Neumann loads	
Traction load:	no
Pressure load:	no
Heat flux load:	no
Volume loads	
Standard gravity	$g = 9.81$

Snapshots of the motion with reactions



Compression test with heating on a cube

(Mechanical Dirichlet/Thermal Dirichlet load; $k_{\text{mec}} = 1$, $k_{\text{the}} = 2$, $k_{\text{vis}} = 2$)

Characteristics $\Theta_{\infty} = 298.15 \text{ K}$

Geometry

Edge length $l_{\text{edge}} = 2$

Mesh

Element: 27-node

Element number: $n_{\text{el}} = 8$

Node number: $n_{\text{no}} = 125$

Boundary conditions

Green yz-face: x -dof fixed

Green xz-face: y -dof fixed

Yellow xy-face: z -dof fixed

$\Theta^A = 10 f(t)$

Red xy-face: $\Theta^A = 10 f(t)$

Blue yz-face: $\Theta^A = \Theta_{\infty}$

$u_x^A = -0.3 f(t)$

Blue xz-face: $\Theta^A = \Theta_{\infty}$

$u_y^A = -0.3 f(t)$

Initial conditions

Initial velocities: $v_0^A = \mathbf{0} = \omega_0^A$

Initial temperature: $\Theta_0^A = 308.15$

Dirichlet loads

Displacements with $f(t)$: $T_{\text{load}} = 0.5$

Temperatures with $f(t)$: $\omega_{\text{load}} = 10\pi$

Neumann loads

Traction load: no

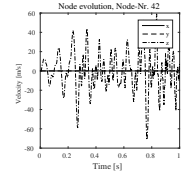
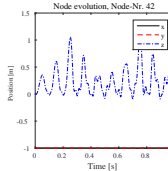
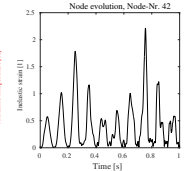
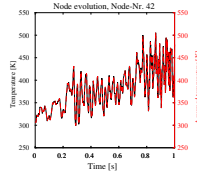
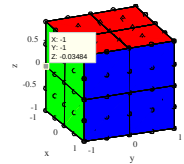
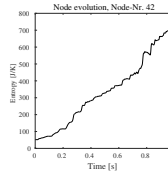
Pressure load: no

Heat flux load: no

Volume loads

Standard gravity $g = 9.81$

Time evolutions of node 42 (corner)



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Total momenta balances

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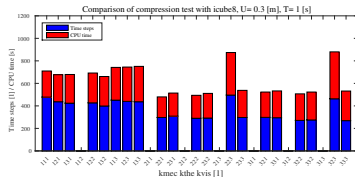
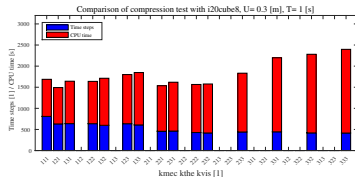
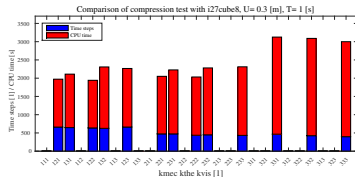
Compression test with heating on a cube

(Mechanical Dirichlet/Thermal Dirichlet load; $n_{el} = 8$)

Characteristics $\Theta_{\infty} = 298.15 \text{ K}$

Geometry	
Edge length	$l_{edge} = 2$
Mesh	
Element:	8/20/27-node
Element number:	$n_{el} = 8$
Node number:	$n_{no} = 27/81/125$
Boundary conditions	
Green yz-face:	x -dof fixed
Green xz-face:	y -dof fixed
Yellow xy-face:	z -dof fixed
	$\Theta^A = 10 f(t)$
Red xy-face:	$\Theta^A = 10 f(t)$
Blue yz-face	$\Theta^A = \Theta_{\infty}$
	$u_x^A = -0.3 f(t)$
Blue xz-face	$\Theta^A = \Theta_{\infty}$
	$u_y^A = -0.3 f(t)$
Initial conditions	
Initial velocities:	$\mathbf{v}_0^A = \mathbf{0} = \boldsymbol{\omega}_0^A$
Initial temperature:	$\Theta_0^A = 308.15$
Dirichlet loads	
Displacements $[f(t)]$:	$T_{load} = 0.5$
Temperatures $[f(t)]$:	$\omega_{load} = 10\pi$
Neumann loads	
Traction load:	no
Pressure load:	no
Heat flux load:	no
Volume loads	
Standard gravity	$g = 9.81$

Time steps and CPU time $h_n^{\min} = 10^{-6} \text{ s}$



Compression test with heating on a cube

(Mechanical Dirichlet/Thermal Dirichlet load; $n_{el} = 64$)

Characteristics $\Theta_{\infty} = 298.15 \text{ K}$

Geometry

Edge length $l_{edge} = 2$

Mesh

Element: 8/20/27-node

Element number: $n_{el} = 64$

Node number: $n_{no} = 125/425/729$

Boundary conditions

Green yz-face: x -dof fixed

Green xz-face: y -dof fixed

Yellow xy-face: z -dof fixed

$\Theta^A = 10 f(t)$

Red xy-face: $\Theta^A = 10 f(t)$

Blue yz-face: $\Theta^A = \Theta_{\infty}$

$u_x^A = -0.3 f(t)$

Blue xz-face: $\Theta^A = \Theta_{\infty}$

$u_y^A = -0.3 f(t)$

Initial conditions

Initial velocities: $v_0^A = 0 = \omega_0^A$

Initial temperature: $\Theta_0^A = 308.15$

Dirichlet loads

Displacements $[f(t)]$: $T_{load} = 0.5$

Temperatures $[f(t)]$: $\omega_{load} = 10\pi$

Neumann loads

Traction load: no

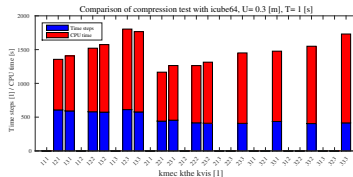
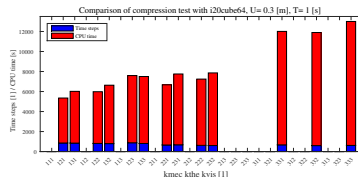
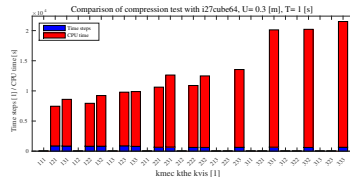
Pressure load: no

Heat flux load: no

Volume loads

Standard gravity $g = 9.81$

Time steps and CPU time $h_n^{\min} = 10^{-6} \text{ s}$



Compression with cooling on a 'Cook-like' cube

(Mechanical Neumann/Thermal Neumann load; $k_{\text{mec}} = 1, k_{\text{the}} = 2, k_{\text{vis}} = 1$)

Characteristics $\Theta_{\infty} = 298.15 \text{ K}$

Geometry

Edge lengths	$l_{\text{edge}_1} = 1.5$
	$l_{\text{edge}_2} = 2$
	$l_{\text{edge}_3} = 2.5$

Mesh

Element:	10-node
Element number:	$n_{\text{el}} = 46$
Node number:	$n_{\text{no}} = 121$

Boundary conditions

Green yz-face:	x -dof fixed
Green xz-face:	y -dof fixed
Yellow xy-face:	z -dof fixed
Red faces:	$Q^A = -2000 f(t)$
Blue face	$\Theta^A = \Theta_{\infty}$
	$T_z^A = -400000 f(t)$

Initial conditions

Initial velocities:	$\mathbf{v}_0^A = \mathbf{0} = \boldsymbol{\omega}_0^A$
Initial temperature:	$\Theta_0^A = 308.15$

Dirichlet loads

Displacement profile:	no
Temperature profile:	no

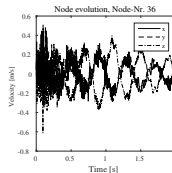
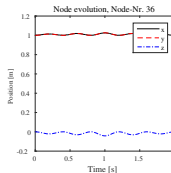
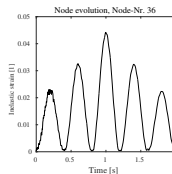
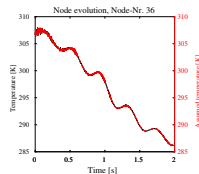
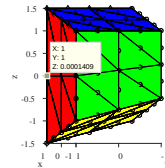
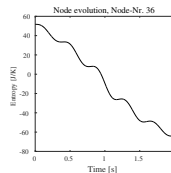
Neumann loads

Heat flux load $[f(t)]$:	$T_{\text{load}} = 2$
Traction load $[f(t)]$:	$\omega_{\text{load}} = 2.5\pi$
Pressure load:	no

Volume loads

Standard gravity	$g = 9.81$
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Time evolutions of node 36 (long edge)



Compression with cooling on a 'Cook-like' cube

(Mechanical Neumann/Thermal Neumann load; $k_{\text{mec}} = 1$, $k_{\text{the}} = 2$, $k_{\text{vis}} = 1$)

Characteristics $\Theta_{\infty} = 298.15 \text{ K}$

Geometry

Edge lengths	$l_{\text{edge}_1} = 1.5$
	$l_{\text{edge}_2} = 2$
	$l_{\text{edge}_3} = 2.5$

Mesh

Element:	10-node
Element number:	$n_{\text{el}} = 46$
Node number:	$n_{\text{no}} = 121$

Boundary conditions

Green yz-face:	x -dof fixed
Green xz-face:	y -dof fixed
Yellow xy-face:	z -dof fixed
Red faces:	$Q^A = -2000 f(t)$
Blue face	$\Theta^A = \Theta_{\infty}$
	$T_{,z}^A = -400000 f(t)$

Initial conditions

Initial velocities:	$v_0^A = \mathbf{0} = \omega_0^A$
Initial temperature:	$\Theta_0^A = 308.15$

Dirichlet loads

Displacement profile:	no
Temperature profile:	no

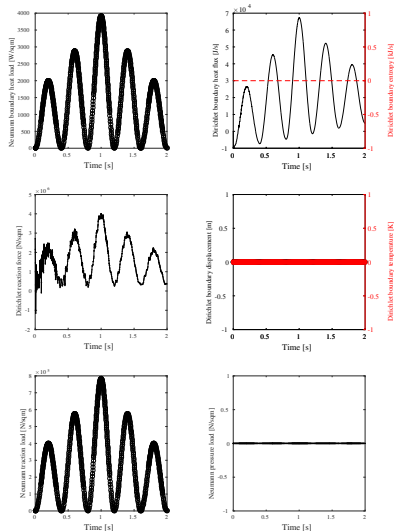
Neumann loads

Heat flux load $[f(t)]$:	$T_{\text{load}} = 2$
Traction load $[f(t)]$:	$\omega_{\text{load}} = 2.5\pi$
Pressure load:	no

Volume loads

Standard gravity	$g = 9.81$
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Time evolutions of loads and reactions



Compression with cooling on a 'Cook-like' cube

(Mechanical Neumann/Thermal Neumann load; $k_{\text{mec}} = 1, k_{\text{the}} = 2, k_{\text{vis}} = 1$)

Characteristics $\Theta_{\infty} = 298.15 \text{ K}$

Geometry

Edge lengths	$l_{\text{edge}_1} = 1.5$
	$l_{\text{edge}_2} = 2$
	$l_{\text{edge}_3} = 2.5$

Mesh

Element:	10-node
Element number:	$n_{\text{el}} = 46$
Node number:	$n_{\text{no}} = 121$

Boundary conditions

Green yz-face:	x -dof fixed
Green xz-face:	y -dof fixed
Yellow xy-face:	z -dof fixed
Red faces:	$Q^A = -2000 f(t)$
Blue face	$\Theta^A = \Theta_{\infty}$
	$T_{\varepsilon}^A = -400000 f(t)$

Initial conditions

Initial velocities:	$\mathbf{v}_0^A = \mathbf{0} = \boldsymbol{\omega}_0^A$
Initial temperature:	$\Theta_0^A = 308.15$

Dirichlet loads

Displacement profile:	no
Temperature profile:	no

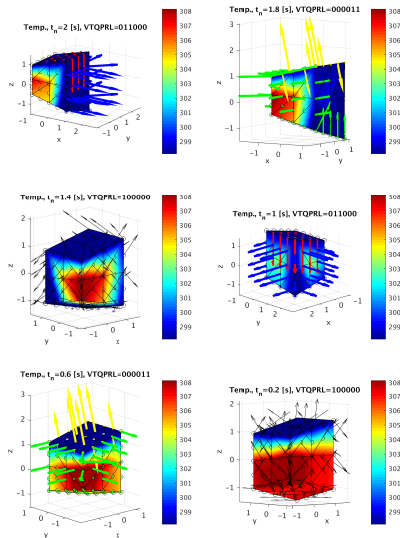
Neumann loads

Heat flux load $[f(t)]$:	$T_{\text{load}} = 2$
Traction load $[f(t)]$:	$\omega_{\text{load}} = 2.5\pi$
Pressure load:	no

Volume loads

Standard gravity	$g = 9.81$
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Snapshots of the motion with reactions



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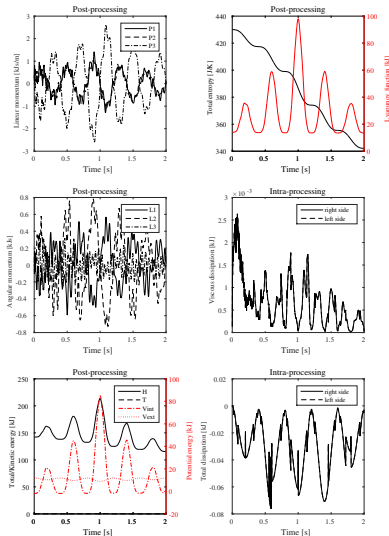
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Balance properties



Summary and Outlook

Dynamic
thermo-mechanical
coupling in
fiber-reinforced
bodies simulated
by higher-
order variational
energy-momentum
schemes

Michael Groß and
Julian Dietzsch

Introduction

Variational setting

Continuum model

Variational principle

Euler-Lagrange equations

Discrete setting

Global E-L equations

Local E-L equations

Mechanical energy balance

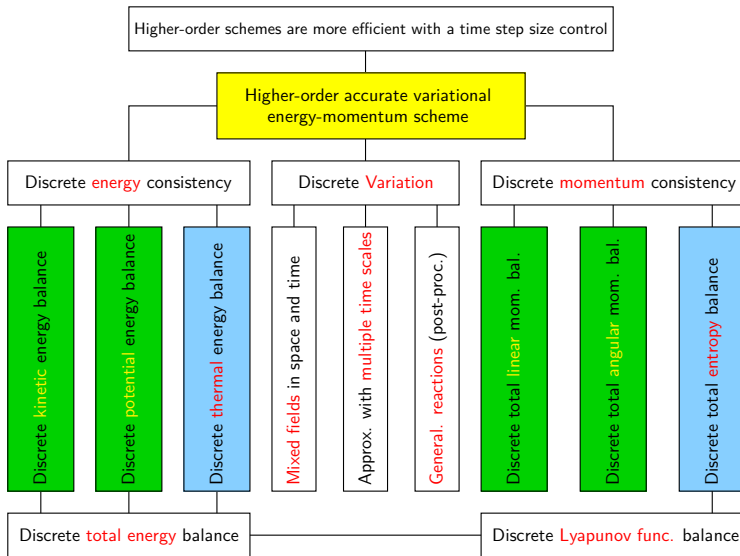
Total energy balance

Total momenta balances

Total entropy balance

Numerical studies

Summary



Outlook: Mixed finite element stress fields