



A mixed assumed strain FE formulation for variational-based energy-momentum time integrations in thermodynamics of fiber-reinforced continua

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June 14, 2018

ECCM-ECFD 2018 – MS 53A

Time integration methods for single and multi-physical problems I

Acknowledgments: This research is provided by **DFG** under the grant GR 3297/4-1

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D2V1F1 and D1V0F0

D1V0F0 and D1F0 and D1

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Motivation, goals and strategy

A **mixed** assumed strain FE formulation for **variational-based** energy-momentum time integrations in thermodynamics of **fiber-reinforced** continua

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Motivation: New simulation methods for **fiber-reinforced materials**

- 1 **Energy-momentum schemes** and **locking-free FE methods** are well-known algorithms
- 2 Usually developed separately; without a 'smart algorithmic interface' between both
- 3 **Idea:** appropriate discrete **variational principles** can serve as such a 'smart interface'

Goal 1: **Locking-free** FE methods within **energy-momentum** schemes

Locking in volume elements

Simo, Taylor, Pister [1985]
Weiss, Govindjee et al. [1996]
Schröder et al. [2011, 2016]
Bonet, Gil et al. [2015] ...

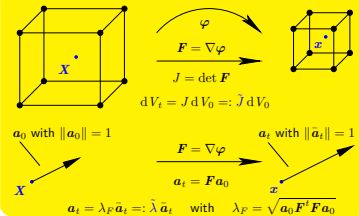
Energy-momentum schemes

Simo, Tarnow [1992]
Betsch, Steinmann [2000]
Noels, Stainier et al. [2004]
Romero [2010] ...

Locking-free energy-momentum schemes

Kuhl, Ramm [2000] Miehe, Schröder [2001] ...
Sansour et al. [2002] Armero [2008] Betsch et al. [2018]

Goal 2: **volumetric locking** in matrix & **line locking** in fibers



Strategy: Hu-Washizu functionals in the principle of **virtual power**

- 1 We design **mixed variational** principles which **avoid static** E.-L. equations
- 2 We derive **energy-momentum** schemes as **discrete Euler-Lagrange** equations



Hu-Washizu method and virtual power principle

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Principle of virtual work / Hamilton's principle (Simo, Taylor, Pister [1985])

1 Internal energy functional

$$\Pi_{\text{STP}}(\varphi, \tilde{J}, p) := \int_{\mathcal{B}_0} \Psi^{\text{iso}}(\varphi) \, dV + \int_{\mathcal{B}_0} \Psi^{\text{vol}}(\tilde{J}) \, dV - \int_{\mathcal{B}_0} p [\tilde{J} - \det(\nabla \varphi)] \, dV$$

2 Euler-Lagrange equations for $\tilde{J}$ and φ

$$\tilde{J} = \det(\nabla \varphi) \quad \rho_0 \ddot{\varphi} = \text{Div} \left[2 \nabla \varphi \frac{\partial \Psi^{\text{iso}}}{\partial C} + p \text{cof}(\nabla \varphi) \right] \quad \text{with} \quad C = F^t F$$

Energy-momentum time integration (cf. Betsch & Steinmann [2002], Armero [2008])

1 Preservation of balance law of total energy $H := T(\dot{\varphi}) + \Psi^{\text{iso}}(\varphi) + \Psi^{\text{vol}}(\tilde{J})$

$$\mathcal{H}_{t_{n+1}} - \mathcal{H}_{t_n} = \int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} \left[\frac{\partial H}{\partial \dot{\varphi}} \cdot \ddot{\varphi} + \frac{\partial H}{\partial \varphi} \cdot \dot{\varphi} + \frac{\partial H}{\partial \tilde{J}} \dot{\tilde{J}} \right] \, dV \, dt$$

2 Time evolution of volume dilatation $\tilde{J}$

$$\int_{t_n}^{t_{n+1}} \int_{\mathcal{B}_0} \delta p \, \dot{G} \, dt = 0 \quad \text{with} \quad G(\varphi, \tilde{J}) := \tilde{J} - \det(\nabla \varphi)$$

Virtual power principle (cf. Schröder & Kuhl [2015])

$$\int_{t_n}^{t_{n+1}} \delta_* \dot{\mathcal{H}}(\dot{\varphi}, \dot{\tilde{J}}, p) \, dt = 0 \quad \text{with} \quad \mathcal{H} := \frac{1}{2} \int_{\mathcal{B}_0} \rho_0 \dot{\varphi} \cdot \dot{\varphi} \, dV + \Pi_{\text{STP}}(\varphi, \tilde{J}, p)$$

Continuum model of a fiber-reinforced body I

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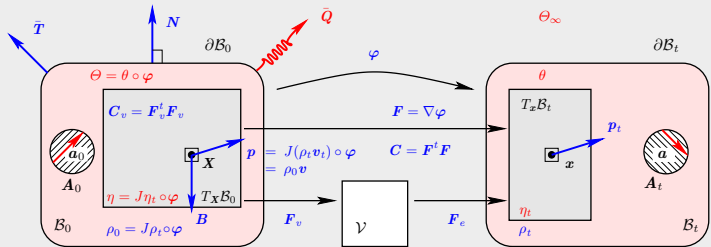
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Transversely isotropic material in motion

(cf. Schröder, Neff & Balzani [2005])



Deformation of fibers and matrix

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

1 Deformation of the fibers

$$\mathbf{F}_F := \mathbf{a}_t \otimes \mathbf{a}_0 = \mathbf{F} \mathbf{A}_0 \quad \mathbf{a}_t = \mathbf{F} \mathbf{a}_0 \quad \mathbf{A}_0 := \mathbf{a}_0 \otimes \mathbf{a}_0$$

2 Fiber and volume dilatation

$$\mathbf{C}_F := \mathbf{F}_F^t \mathbf{F}_F := \mathbf{C}_F \mathbf{A}_0 \quad \mathbf{C}_F := \mathbf{C} : \mathbf{A}_0 \quad \mathbf{C}_V := [\det(\mathbf{C})]^{\frac{1}{n_{\text{dim}}}}$$

3 Isotropic viscoelastic matrix

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

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Thermo-viscoelastic free energy

(cf. Reese [2001])

1 Hyperelastic strain energy

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

2 Thermoelastic free energy

$$\begin{aligned} \Psi^{\text{the}}(\Theta, C_V, C_F) = & \hat{\Psi}^{\text{cap}}(\Theta) - 2\sqrt{C_V^{2-n_{\text{dim}}}} \beta_M [\Theta - \Theta_\infty] \text{D}\hat{\Psi}_M^{\text{vol}}(C_V) \\ & - 2\sqrt{C_F^{2-1}} \beta_F [\Theta - \Theta_\infty] \text{D}\hat{\Psi}_F^{\text{ela}}(C_F) \end{aligned}$$

3 Viscoelastic free energy

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

Non-equilibrium and total stress

(cf. Reese [2001])

1 Viscous evolution equation and non-equilibrium stress tensor

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

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

2 Total second Piola-Kirchhoff stress tensor

$$\mathbf{S} := \mathbf{S}_M^{\text{iso}} + \mathbf{S}_M^{\text{vis}} + \mathbf{S}_V^{\text{vol}} + \mathbf{S}_F^{\text{ela}} \mathbf{A}_0 \quad \mathbf{A}^{\text{vol}} := \frac{1}{n_{\text{dim}}} \det(\mathbf{C})^{\frac{1}{n_{\text{dim}}}} \mathbf{C}^{-1}$$



Basis of the principle of virtual power I

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Total energy **balance law** in functional form

$$\dot{\mathcal{H}}(\dot{\varphi}, \dot{\mathbf{v}}, \dot{\mathbf{p}}, \dot{\mathbf{C}}_v, \dot{\tilde{\mathbf{C}}}, \dot{\mathbf{C}}_V, \dot{\mathbf{C}}_F, \dot{\eta}, \dot{\Theta}, \dot{\tilde{\Theta}}, \mathbf{S}, S_V, S_F, \mathbf{R}, h, \lambda; \tilde{\mathbf{S}}, \tilde{S}_V, \tilde{S}_F) = 0 \quad \text{with} \quad \dot{\mathcal{H}} = \dot{\mathcal{T}} + \dot{H}^{\text{int}} + \dot{H}^{\text{ext}}$$

Kinetic energy in Hu-Washizu form

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

Kinetic **power** functional

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

External **power** functional

$$D^{\text{tot}} := D^{\text{int}} + D^{\text{edu}} \quad D^{\text{edu}} = -\nabla(\ln \Theta) \cdot \mathbf{Q}$$

$$\begin{aligned} \dot{H}^{\text{ext}} := & - \int_{\mathcal{B}_0} \rho_0 \mathbf{B} \cdot \dot{\varphi} \, dV & - \int_{\partial_T \mathcal{B}_0} \bar{\mathbf{T}} \cdot \dot{\varphi} \, dA & + \int_{\partial_Q \mathcal{B}_0} \frac{\tilde{\Theta}}{\bar{\Theta}} \bar{Q} \, dA \\ & - \int_{\mathcal{B}_0} \frac{1}{\bar{\Theta}} \nabla \tilde{\Theta} \cdot \boldsymbol{\kappa}_0 \nabla \Theta \, dV & + \int_{\mathcal{B}_0} \frac{\tilde{\Theta}}{\bar{\Theta}} D^{\text{tot}} \, dV & + \int_{\mathcal{B}_0} \frac{1}{2} \dot{\mathbf{C}}_v : \mathbb{V}(\mathbf{C}_v) : \dot{\mathbf{C}}_v \, dV \\ & + \int_{\partial_\Theta \mathcal{B}_0} \lambda [\tilde{\Theta} - \Theta_\infty] \, dA & - \int_{\partial_\Theta \mathcal{B}_0} h [\dot{\Theta} - \dot{\tilde{\Theta}}] \, dA & - \int_{\partial_\varphi \mathcal{B}_0} \mathbf{R} \cdot [\dot{\varphi} - \dot{\varphi}] \, dA \\ & + \int_{\mathcal{B}_0} \frac{1}{2} \tilde{\mathbf{S}} : \dot{\mathbf{C}} \, dV & + \int_{\mathcal{B}_0} \frac{1}{2} \tilde{S}_V \dot{\mathbf{C}}_V \, dV & + \int_{\mathcal{B}_0} \frac{1}{2} \tilde{S}_F \dot{\mathbf{C}}_F \, dV \end{aligned}$$



Basis of the principle of virtual power II

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Fourier's law of transversely isotropic heat conduction

Al-Kinani [2014]

$$\mathbf{q} := -\boldsymbol{\kappa} \mathbf{F}^{-T} \nabla \Theta \quad \boldsymbol{\kappa} := k \mathbf{I} + \frac{k_F - k}{\|\mathbf{a}\|^2} \mathbf{a} \otimes \mathbf{a} \quad \boldsymbol{\kappa}_0 := k_0 \mathbf{C}^{-1} + \frac{k_{F_0} - k_0}{C_F} \mathbf{A}_0$$

Internal energy

$$\begin{aligned} \Pi^{\text{int}} := & \int_{\mathcal{B}_0} \left[\hat{\Psi}_M(\mathbf{C}_v, \tilde{\mathbf{C}}, \tilde{\mathbf{C}}_V, \Theta; \mathbf{A}_0) + \hat{\Psi}_F(\tilde{\mathbf{C}}_F, \Theta) \right] dV \\ & - \frac{1}{2} \int_{\mathcal{B}_0} \mathbf{S} : [\tilde{\mathbf{C}} - (\nabla \boldsymbol{\varphi})^t \nabla \boldsymbol{\varphi}] dV \quad - \frac{1}{2} \int_{\mathcal{B}_0} S_F : [\tilde{\mathbf{C}}_F - \tilde{\mathbf{C}} : \mathbf{A}_0] dV \\ & - \frac{1}{2} \int_{\mathcal{B}_0} S_V : [\tilde{\mathbf{C}}_V - \det(\tilde{\mathbf{C}})^{\frac{1}{n_{\text{dim}}}}] dV - \int_{\mathcal{B}_0} \eta [\tilde{\Theta} - \Theta] dV \end{aligned}$$

Internal power functional

$$\mathbf{C} := (\nabla \boldsymbol{\varphi})^t \nabla \boldsymbol{\varphi}$$

$$\begin{aligned} \dot{\Pi}^{\text{int}} := & \frac{1}{2} \int_{\mathcal{B}_0} \left\{ \left[2 \frac{\partial \hat{\Psi}_M}{\partial \mathbf{C}} + S_V \mathbf{A}^{\text{vol}} + S_F \mathbf{A}_0 - \mathbf{S} \right] : \dot{\tilde{\mathbf{C}}} + \left[2 \frac{\partial \hat{\Psi}_M}{\partial \tilde{\mathbf{C}}_V} - S_V \right] : \dot{\tilde{\mathbf{C}}}_V \right\} dV \\ & + \frac{1}{2} \int_{\mathcal{B}_0} \left[2 \frac{\partial \hat{\Psi}_F}{\partial \tilde{\mathbf{C}}_F} - S_F \right] : \dot{\tilde{\mathbf{C}}}_F dV - \frac{1}{2} \int_{\mathcal{B}_0} \dot{\mathbf{S}} : [\tilde{\mathbf{C}} - \mathbf{C}] dV + \frac{1}{2} \int_{\mathcal{B}_0} \mathbf{S} : \dot{\mathbf{C}} dV \\ & - \frac{1}{2} \int_{\mathcal{B}_0} \dot{S}_V : [\tilde{\mathbf{C}}_V - \det(\tilde{\mathbf{C}})^{\frac{1}{n_{\text{dim}}}}] dV - \frac{1}{2} \int_{\mathcal{B}_0} \dot{S}_F : [\tilde{\mathbf{C}}_F - \tilde{\mathbf{C}} : \mathbf{A}_0] dV \\ & + \int_{\mathcal{B}_0} \dot{\eta} [\tilde{\Theta} - \Theta] dV + \int_{\mathcal{B}_0} \dot{\Theta} \left[\eta + \frac{\partial \Psi}{\partial \Theta} \right] dV + \int_{\mathcal{B}_0} \eta \dot{\Theta} dV + \int_{\mathcal{B}_0} \frac{\partial \hat{\Psi}_M}{\partial \mathbf{C}_v} : \dot{\mathbf{C}}_v dV \end{aligned}$$



Principle of virtual power

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

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Principle of virtual power

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

Virtual kinetic power

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

Virtual external power

$$\begin{aligned} \delta_* \dot{I}^{\text{ext}} := & - \int_{\mathcal{B}_0} \rho_0 \mathbf{B} \cdot \delta_* \dot{\varphi} \, dV - \int_{\partial_T \mathcal{B}_0} \bar{\mathbf{T}} \cdot \delta_* \dot{\varphi} \, dA - \int_{\partial_\varphi \mathcal{B}_0} \delta_* \mathbf{R} \cdot [\dot{\varphi} - \dot{\varphi}] \, dA - \int_{\partial_\varphi \mathcal{B}_0} \mathbf{R} \cdot \delta_* \dot{\varphi} \\ & + \int_{\mathcal{B}_0} \delta_* \dot{\mathbf{C}}_v : \mathbb{V}(\mathbf{C}_v) : \dot{\mathbf{C}}_v \, dV + \int_{\mathcal{B}_0} \delta_* \tilde{\Theta} \frac{D^{\text{tot}}}{\Theta} \, dV - \int_{\mathcal{B}_0} \frac{1}{\Theta} \nabla(\delta_* \tilde{\Theta}) \cdot \boldsymbol{\kappa}_0 \nabla \Theta \, dV + \int_{\partial_\Theta \mathcal{B}_0} \lambda \delta_* \tilde{\Theta} \, dA \\ & + \int_{\partial_Q \mathcal{B}_0} \frac{\delta_* \tilde{\Theta}}{\Theta} \bar{Q} \, dA + \int_{\partial_\Theta \mathcal{B}_0} \delta_* \lambda [\tilde{\Theta} - \Theta_\infty] \, dA - \int_{\partial_\Theta \mathcal{B}_0} \delta_* h [\dot{\Theta} - \dot{\tilde{\Theta}}] \, dA - \int_{\partial_\Theta \mathcal{B}_0} \delta_* \dot{\Theta} h \, dA \\ & + \int_{\mathcal{B}_0} \frac{1}{2} \tilde{\mathbf{S}} : \delta_* \dot{\mathbf{C}} \, dV + \int_{\mathcal{B}_0} \frac{1}{2} \tilde{\mathbf{S}}_V \delta_* \dot{\mathbf{C}}_V \, dV + \int_{\mathcal{B}_0} \frac{1}{2} \tilde{\mathbf{S}}_F \delta_* \dot{\mathbf{C}}_F \, dV \end{aligned}$$

Virtual internal power

$$\mathbf{F} := \nabla \varphi \quad \mathbf{C} := (\nabla \varphi)^t \nabla \varphi$$

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

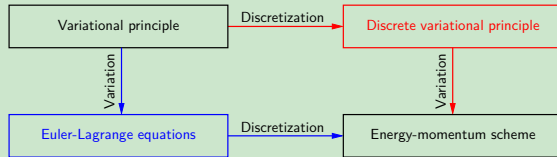


Design of the energy-momentum schemes

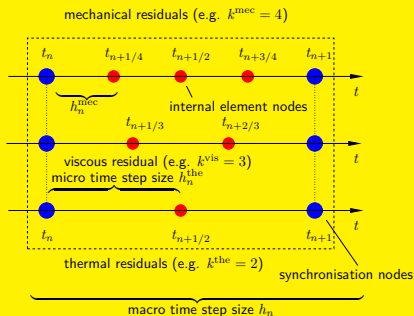
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Schematic process of the energy-momentum scheme design (cf. Yavari [2008])



Different time scales in the time integration (cf. Kassiotis et al. [2009])



k	$M_I(\alpha)$	α_I	$\tilde{M}_I(\alpha)$	$\tilde{\alpha}_I$
1	$1 - \alpha$	0	1	1
2	$(2\alpha - 1)(\alpha - 1)$ $-4\alpha(\alpha - 1)$ $(2\alpha - 1)\alpha$	0 $\frac{1}{2}$ 1	$1 - \alpha$ α	0 1
3	$-\frac{2}{3}(\alpha - \frac{1}{2})(\alpha - \frac{1}{3})(\alpha - 1)$ $-\frac{4}{3}(\alpha - \frac{1}{2})(\alpha - 1)\alpha$ $-\frac{2}{3}(\alpha - \frac{1}{3})(\alpha - 1)\alpha$ $\frac{2}{3}(\alpha - \frac{1}{2})(\alpha - \frac{2}{3})\alpha$	0 $\frac{1}{3}$ $\frac{2}{3}$ 1	$(2\alpha - 1)(\alpha - 1)$ $-4\alpha(\alpha - 1)$ $(2\alpha - 1)\alpha$	0 $\frac{1}{3}$ $\frac{2}{3}$ 1
4	$\frac{1}{24}(\alpha - \frac{1}{4})(\alpha - \frac{1}{2})(\alpha - \frac{3}{4})(\alpha - 1)$ $-\frac{1}{24}(\alpha - \frac{1}{4})(\alpha - \frac{1}{2})(\alpha - 1)\alpha$ $-\frac{1}{24}(\alpha - \frac{1}{2})(\alpha - \frac{3}{4})(\alpha - 1)\alpha$ $-\frac{1}{24}(\alpha - \frac{1}{4})(\alpha - \frac{3}{4})(\alpha - 1)\alpha$ $\frac{1}{24}(\alpha - \frac{1}{4})(\alpha - \frac{1}{2})(\alpha - \frac{3}{4})\alpha$	0 $\frac{1}{4}$ $\frac{1}{2}$ $\frac{3}{4}$ 1	$-\frac{2}{3}(\alpha - \frac{1}{2})(\alpha - \frac{1}{3})(\alpha - 1)$ $-\frac{4}{3}(\alpha - \frac{1}{2})(\alpha - 1)\alpha$ $-\frac{2}{3}(\alpha - \frac{1}{3})(\alpha - 1)\alpha$ $\frac{2}{3}(\alpha - \frac{1}{2})(\alpha - \frac{2}{3})\alpha$	0 $\frac{1}{4}$ $\frac{1}{2}$ $\frac{3}{4}$ 1

$$\phi^n(\alpha) := \sum_{I=1}^{k^{\text{mec}}+1} M_I^{\text{mec}}(\alpha) \phi_I$$

$$\alpha(t) := \frac{t - t_n}{h_n} \in [0, 1]$$



Features of the energy-momentum schemes

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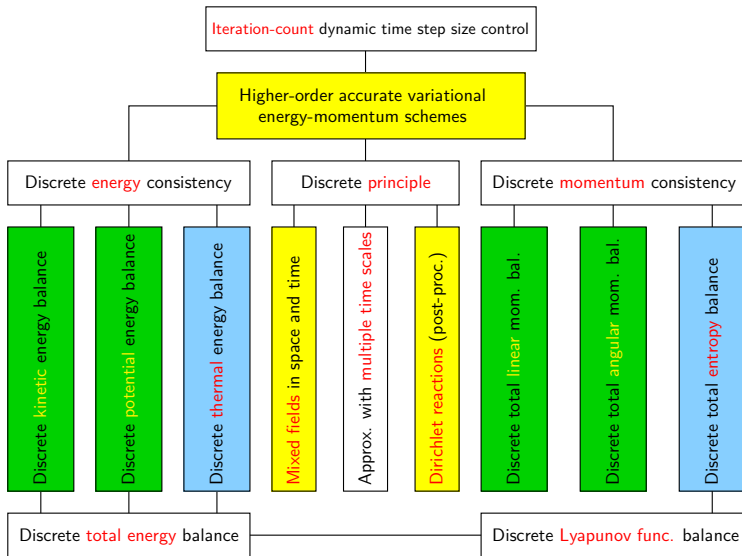
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Summary



$$\mathcal{H} := \mathcal{T} + \Pi^{\text{pot}} + \Pi^{\text{the}}$$

$$\Pi^{\text{the}} := \int_{\mathcal{B}_0} \Theta \eta \, dV$$

$$\mathcal{F} := \mathcal{H} - \Theta_\infty \mathcal{S}$$



Fiber-reinforced spherical shell with a slit

(Boundary and initial conditions; $k_{\text{mec}} = 1, k_{\text{the}} = 2, k_{\text{vis}} = 1$)

A mixed assumed strain FE formulation for variational-based energy-momentum time integrations in thermodynamics of fiber-reinforced continua

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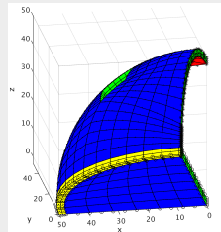
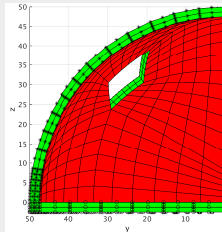
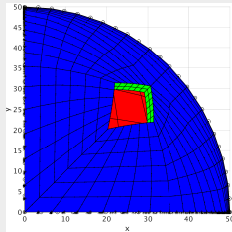
Balance laws over time

D2V1F1 and D1V0F0

D1V0F0 and D1F0 and D1

Summary

Boundary Status Monitor



Temperature profile (yellow patches) $f_L(t) := \sin(\omega_{\text{load}} t)$

$$f(t) = \begin{cases} (1.0 f_L(t))^2 & \forall T_{\text{load}}(0.0 + c_{\text{load}}) < t \leq T_{\text{load}}(0.2 + c_{\text{load}}) \\ (1.2 f_L(t))^2 & \forall T_{\text{load}}(0.2 + c_{\text{load}}) < t \leq T_{\text{load}}(0.4 + c_{\text{load}}) \\ (1.4 f_L(t))^2 & \forall T_{\text{load}}(0.4 + c_{\text{load}}) < t \leq T_{\text{load}}(0.6 + c_{\text{load}}) \\ (1.2 f_L(t))^2 & \forall T_{\text{load}}(0.6 + c_{\text{load}}) < t \leq T_{\text{load}}(0.8 + c_{\text{load}}) \\ (1.0 f_L(t))^2 & \forall T_{\text{load}}(0.8 + c_{\text{load}}) < t \leq T_{\text{load}}(1.0 + c_{\text{load}}) \end{cases}$$

Dirichlet and Neumann boundary conditions

$$\theta_t^A = \theta_\infty \text{ (blue patches)} \quad \varphi_t^A = X^A \text{ (circular markers)}$$

Thermal insulation $\bar{Q} := 0$ (red and green patches)

Transient pressure (follower load in star markers)

$$f_p(t) := \hat{p} |\sin(\omega_{\text{load},p} t)|$$

Initial conditions (Ambient temp. $\theta_\infty = 298.15$)

$$\varphi_0^A = X^A$$

$$\mathbf{v}_0^A = \mathbf{0}$$

$$\theta_0^A = \theta_\infty + 10$$



Fiber-reinforced spherical shell with a slit

(Parameters and fiber directions; $k_{mec} = 1, k_{the} = 2, k_{vis} = 1$)

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Simulation parameters

$$\Theta_{\infty} = 298.15$$

Initial conditions

Initial velocity: $v_0^A = 0$
Initial temperature: $\Theta_0^A = \Theta_{\infty} + 10 = 308.15$

Boundary conditions

Green patches in xz-plane: y -dof fixed
Green patches in yz-plane: x -dof fixed
Yellow patches in xy-plane (with circular markers): z -dof fixed
Yellow patches: $\Theta^A = \hat{\Theta} f(t)$
Blue patches: $\Theta^A = \Theta_{\infty}$
Green and red patches: $\bar{Q} = 0$ (thermal insulation)

Dirichlet loads

Temperature profile: $f(t)$ with $\hat{\Theta} = 10$
(yellow patches) $T_{load} = 2.0, \omega_{load} = 10\pi$

Neumann loads

Pressure load: $f_p(t)$ with $\hat{p} = 1 \cdot 10^5$
(green patches with star marker) $T_{load,p} = 2.0, \omega_{load,p} = 10\pi$

Volume loads

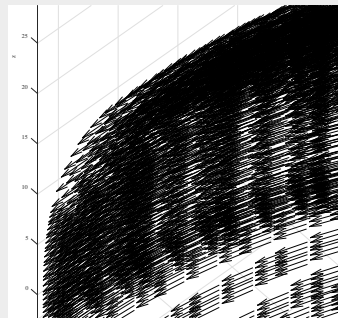
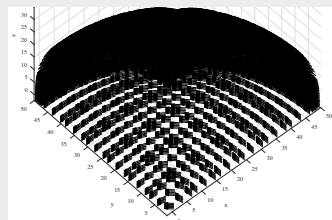
Standard gravity $g = 9.81$ with $e_g = -e_z$

Material parameters

$$\begin{aligned} \rho_0 &= 1.120 \cdot 10^3 & \kappa^{vol} &= 1.000 \cdot 10^7 & \mu_{01} &= 0.250 \cdot 10^4 \\ \mu_{10} &= 0.250 \cdot 10^7 & \mu_{20} &= 0.021 \cdot 10^7 & Y_1 &= 0.1631 \cdot 10^7 \\ Y_2 &= 0.6 & \kappa_{ani} &= 0.250 \cdot 10^7 & g_0 &= 0.300 \cdot 10^7 \\ g_c &= 4 & \beta_M &= 20 \cdot 10^{-6} & c_{M0} &= 1539.50\% \\ c_{M1} &= 0.00375 & k &= 0.2595 & \beta_F &= 206 \cdot 10^{-6} \\ c_{F0} &= 1539.50\% & c_{F1} &= 0.00375 & k_F &= 200 \text{ k} \\ V_{dev} &= 10^3 & V_{vol} &= 5 \cdot 10^3 & \kappa_v^{vol} &= 1.000 \cdot 10^6 \\ \mu_{01}^v &= 0.250 \cdot 10^3 & \mu_{10}^v &= 0.250 \cdot 10^6 & \mu_{20}^v &= 0.021 \cdot 10^6 \\ Y_1^v &= 0.1631 \cdot 10^6 & Y_2^v &= 0.6 \end{aligned}$$

Fiber directions

$$a_0 := e_z \times X / \|X\|$$





Fiber-reinforced spherical shell with a slit

(Free energy functions and loads; $k_{\text{mec}} = 1$, $k_{\text{the}} = 2$, $k_{\text{vis}} = 1$)

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Free energy

$$(C^{\text{iso}} := [I_3^C]^{-\frac{1}{3}} C, \Theta_\infty = 298.15)$$

Elastic free energy functions

$$\begin{aligned} \psi_M^{\text{ela}} &:= \mu_{10} [I_1(C^{\text{iso}}) - I_1(I)] \\ &\quad + \mu_{20} [I_1(C^{\text{iso}}) - I_1(I)]^2 \\ &\quad + \mu_{01} [I_2(C^{\text{iso}}) - I_2(I)] \\ &\quad + \frac{Y_1}{Y_2} \{1 - \exp[-Y_2 (I_1(C^{\text{iso}}) - I_1(I))]\} \\ &\quad + \frac{\kappa_{\text{uni}}}{3} \left[(I_4(C^{\text{iso}}))^{3/2} + 3 (I_4(C^{\text{iso}}))^{-1/2} - 4 \right] \end{aligned}$$

$$\begin{aligned} \psi_M^{\text{vol}} &:= \frac{\kappa^{\text{vol}}}{50} \left[(\tilde{C}_V)^{5n_{\text{dim}}/2} + (\tilde{C}_V)^{-5n_{\text{dim}}/2} - 2 \right] \\ \psi_F^{\text{ela}} &:= \frac{g_0}{(2g_c)} \left[\exp[g_c(\tilde{C}_F - 1)^2] - 1 \right] \end{aligned}$$

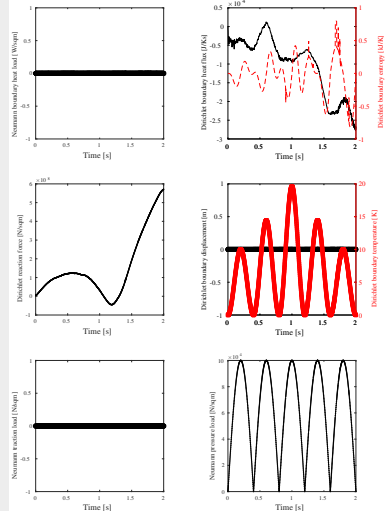
Thermoelastic free energy function

$$\begin{aligned} \psi^{\text{cap}} &:= c_0 (1 - \Theta_\infty c_1) \left[\Theta - \Theta_\infty - \Theta \ln \left(\frac{\Theta}{\Theta_\infty} \right) \right] \\ &\quad - \frac{1}{2} c_0 c_1 (\Theta - \Theta_\infty)^2 \\ \hat{\psi}_M^{\text{the}} &:= \hat{\psi}_M^{\text{cap}} - 2 \sqrt{C_V^2 - n_{\text{dim}}} \beta_M (\Theta - \Theta_\infty) D \hat{\psi}_M^{\text{vol}}(C_V) \\ \hat{\psi}_F^{\text{the}} &:= \hat{\psi}_F^{\text{cap}} - 2 \sqrt{C_F} \beta_F (\Theta - \Theta_\infty) D \hat{\psi}_F^{\text{ela}}(C_F) \end{aligned}$$

Viscoelastic free energy function

$$\begin{aligned} \psi_M^{\text{vis}} &:= \mu_{10}^v [I_1(A^{\text{iso}}) - I_1(I)] \\ &\quad + \mu_{20}^v [I_1(A^{\text{iso}}) - I_1(I)]^2 \\ &\quad + \mu_{01}^v [I_2(A^{\text{iso}}) - I_2(I)] \\ &\quad + \frac{Y_1^v}{Y_2^v} \{1 - \exp[-Y_2^v (I_1(A^{\text{iso}}) - I_1(I))]\} \\ &\quad + \frac{\kappa_{\text{vis}}}{50} \left[(I_3(A))^{5/2} + (I_3(A))^{-5/2} - 2 \right] \end{aligned}$$

Time evolutions of loads/reactions



Fiber-reinforced spherical shell with a slit

(Current configurations I; $k_{mec} = 1, k_{the} = 2, k_{vis} = 1$)

A mixed assumed strain FE formulation for variational-based energy-momentum time integrations in thermodynamics of fiber-reinforced continua

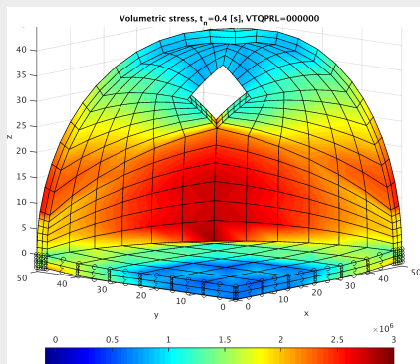
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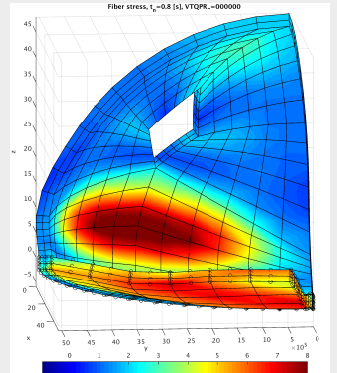
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Volumetric stress S_V at $t_n = 0.4$



Fiber stress S_F at $t_n = 0.8$



1 Volumetric stress

(fiber stress analogous)

$$\mathbf{S}_V^{n,e} = [\mathbf{I}_{k_{mec}} \otimes \tilde{\mathbf{H}}^{-1}] \int_{\Omega_{\square}} \tilde{\mathbf{m}}^{mec} \left[2\Psi_V^{n,e}(\zeta) + \tilde{\mathbf{S}}_V^{n,e}(\zeta) \right] \otimes \tilde{\mathbf{N}}(\zeta) dV_{\square}$$

2 Volumetric strain

(fiber strain analogous)

$$\mathbf{C}_V^{n,e} = [\mathbf{I}_{k_{mec}} \otimes \tilde{\mathbf{H}}^{-1}] \int_{\Omega_{\square}} [\tilde{\mathbf{m}}^{mec} \mathbf{c}_V^{n,e}(\zeta)] \otimes \tilde{\mathbf{N}}(\zeta) dV_{\square} + [\mathbf{e}_{k_{mec}} \otimes \mathbf{C}_{V_1}^e]$$



Fiber-reinforced spherical shell with a slit

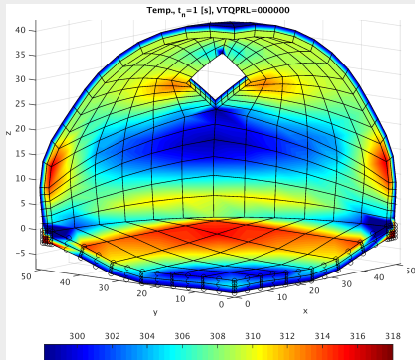
(Current configurations II; $k_{\text{mec}} = 1, k_{\text{the}} = 2, k_{\text{vis}} = 1$)

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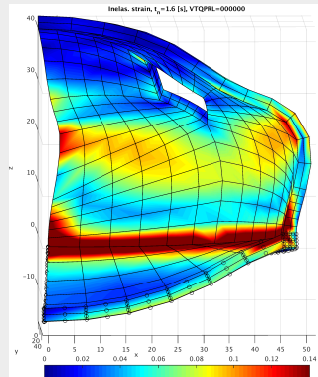
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Temperature Θ at $t_n = 1.0$



Viscous strain E_v at $t_n = 1.6$



- 1 Entropy equation (determines the temperature in the entropy balance)

$$\mathbf{R}^{\text{ent}} := \Psi(\mathbf{x}, \mathbf{o}) + [\tilde{\mathbf{B}}_o \otimes \mathbf{H}] \mathbf{s} + \tilde{\mathbf{b}}_o \otimes \mathbf{H} \mathbf{s}_1 = [\tilde{\mathbf{C}}_o \otimes \bar{\mathbf{H}}] \mathbf{h}$$

- 2 Viscous time evolution equation (determines the viscous strain)

$$\sum_{l=1}^{k^{\text{vis}}} \frac{\circ}{\delta_* \mathbf{C}_v^{n,e}}(\xi_l^{\text{vis}}, \chi_B) : \mathbf{Y}^{n,e}(\xi_l^{\text{vis}}, \chi_B) \mathbf{w}_l^{\text{vis}} = \sum_{i=1}^{k^{\text{the}}} \frac{\circ}{\delta_* \mathbf{C}_v^{n,e}}(\xi_i^{\text{the}}, \chi_B) : \mathbf{V}(\mathbf{C}_v^{n,e}(\xi_i^{\text{the}}, \chi_B)) : \frac{\circ}{\mathbf{C}_v^{n,e}}(\xi_i^{\text{the}}, \chi_B) \frac{\mathbf{w}_i^{\text{the}}}{h_n}$$



Fiber-reinforced spherical shell with a slit

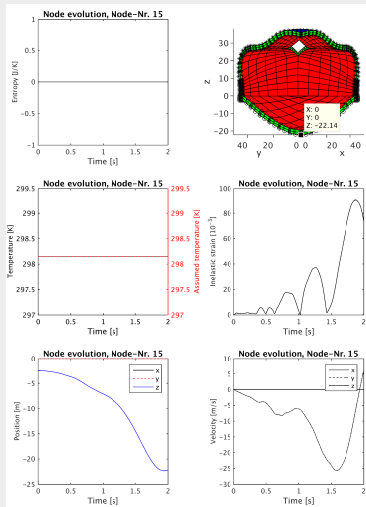
(Solutions over time; $k_{\text{mec}} = 1$, $k_{\text{the}} = 2$, $k_{\text{vis}} = 1$)

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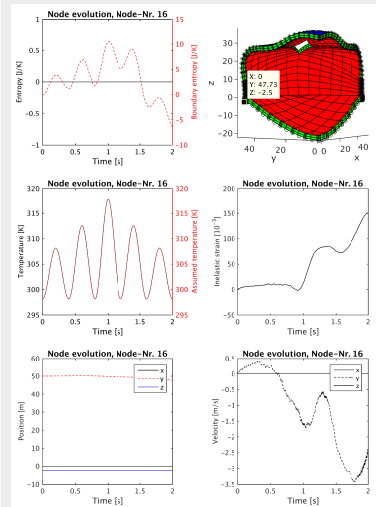
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Tip node on boundaries $\partial_{\Theta}\mathcal{B}_0$, $\partial_{\varphi}\mathcal{B}_0$



Kink node on boundaries $\partial_{\Theta}\mathcal{B}_0$, $\partial_{\varphi}\mathcal{B}_0$



1 Large deflection/velocity increase during the buckling



Fiber-reinforced spherical shell with a slit

(Error in balance laws over time; $k_{mec} = 1, k_{the} = 2, k_{vis} = 1$)

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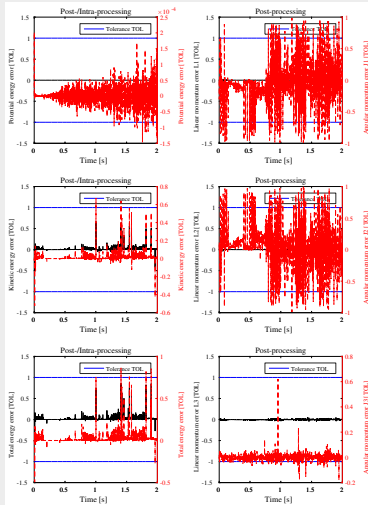
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D2V1F1 and D1V0F0

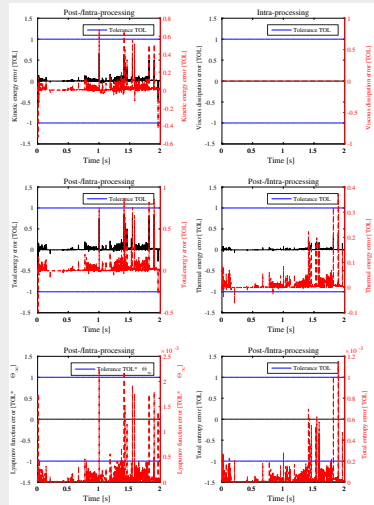
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Mechanical balance laws



Thermal balance laws

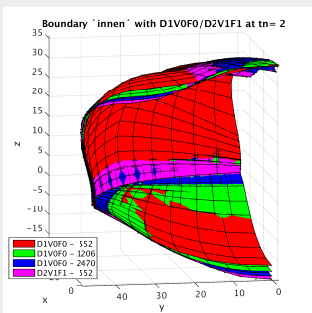
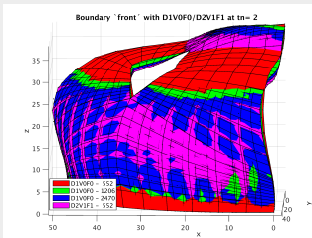


① Exact algorithmic preservation $\leadsto$ balance errors $<$ TOL

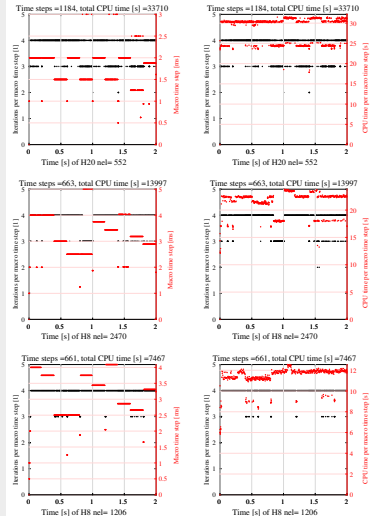


Fiber-reinforced spherical shell with a slit (D2V1F1 and D1V0F0; $k_{\text{mec}} = 1, k_{\text{the}} = 2, k_{\text{vis}} = 1$)

Sections of the shell at $t_n = 2$



Iterations per time step



H8 = D1V0F0

H20 = D2V1F1

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Fiber-reinforced spherical shell with a slit

(D1V0F0 and D1F0 and D1; $k_{\text{mec}} = 1, k_{\text{the}} = 2, k_{\text{vis}} = 1$)

A **mixed** assumed strain FE formulation for **variational-based** energy-momentum time integrations in thermodynamics of **fiber-reinforced** continua

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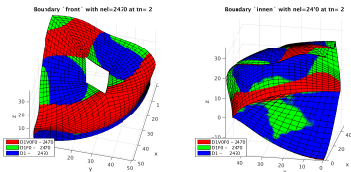
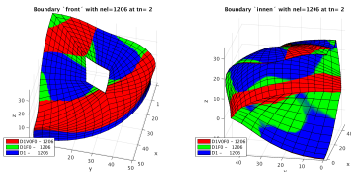
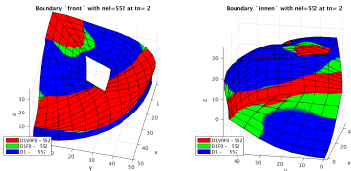
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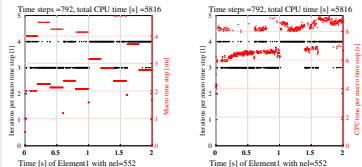
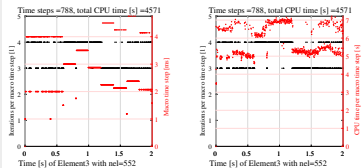
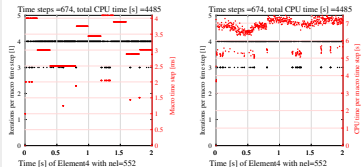
D1V0F0 and D1F0 and D1

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Sections of the shell at $t_n = 2$



Iterations per time step: $n_{\text{el}} = 552$



Element1= D1

Element3= D1F0

Element4= D1V0F0



Fiber-reinforced spherical shell with a slit

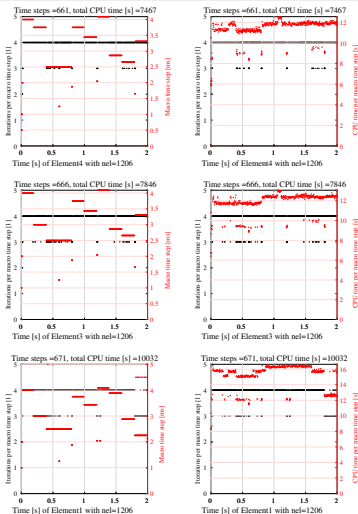
(D1V0F0 and D1F0 and D1; $k_{\text{mec}} = 1, k_{\text{the}} = 2, k_{\text{vis}} = 1$)

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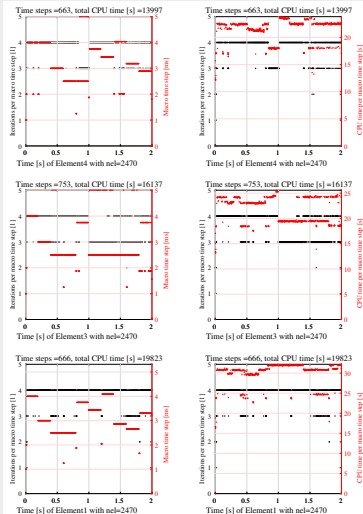
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Iterations per time step: $n_{\text{el}} = 1206$



Iterations per time step: $n_{\text{el}} = 2470$



Element1= D1

Element3= D1F0

Element4= D1V0F0

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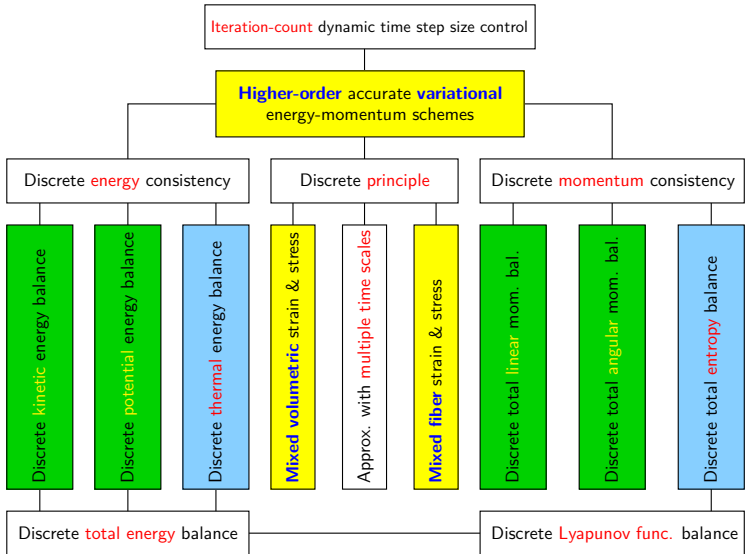
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D1V0F0 and D1F0 and D1

Summary



RESULT: This mixed formulation avoids locking and is more efficient due to larger time steps