



Locking-free
higher-order
energy-momentum
schemes for
thermo-viscoelastic
fiber-reinforced
materials derived
by the principle of
virtual power

Michael Groß,
Julian Dietzsch &
Chris Rübiger

Locking-free higher-order energy-momentum schemes for thermo-viscoelastic fiber-reinforced materials derived by the principle of virtual power

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including Solution Approaches by Extensions of Standard Numerical Methods

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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 **Problem:** usually developed separately without a 'smart 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]
Simo, Armero, Taylor [1993]
Kasper, Taylor [2000, 2004]
Schröder et al. [2011, 2016]

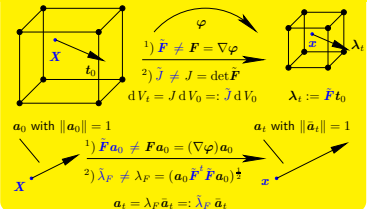
Energy-momentum schemes

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 $\tilde{J}$

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

Principle of virtual power

(cf. Schröder & Kuhl [2015])

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

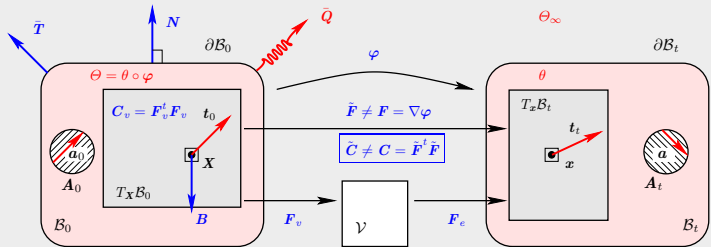
Continuum model of a fiber-reinforced body (I)

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Continuum model

Transversely isotropic material in non-isothermal motions



Deformation of fibers and matrix

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

- ### 1 Deformation of the fibers

$$F_F := a_t \otimes a_0 = \tilde{F} A_0 \quad A_0 := a_0 \otimes a_0 \quad C_F := F_F^t F_F := C_F A_0$$

- ## 2 Fiber and volume dilatation

$$\tilde{C}_F \neq C_F := \tilde{\mathbf{C}} : \mathbf{A}_0 \qquad \tilde{C}_V \neq C_V := [\det(\tilde{\mathbf{C}})]^{\frac{1}{n_{\text{dim}}}}$$

- ### 3 Isotropic viscoelastic matrix

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

Continuum model of a fiber-reinforced body (II)

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Thermo-viscoelastic free energy

1 Hyperelastic strain energy

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

2 Thermoelastic free energy

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

3 Viscoelastic free energy

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

Non-equilibrium and total stress

(cf. Reese [2001])

1 Viscous evolution equation and non-equilibrium stress tensor

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

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

2 Total second Piola-Kirchhoff stress tensor

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



Basis of the principle of virtual power (I)

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Total energy **balance law** in functional form with independent fields

$$\underbrace{\dot{\mathcal{H}}(\dot{\varphi}, \dot{v}, \dot{p}, \dot{C}_w, \dot{\Theta}, \dot{\eta}, \dot{F}, \dot{C}, \dot{C}_V, \dot{C}_F)}_{\text{temporally continuous}}; \underbrace{\tilde{\Theta}, P, S, S_V, S_F, R, h, \lambda}_{\text{temporally discontinuous parameters}}; \underbrace{\tilde{S}, \tilde{S}_V, \tilde{S}_F}_{\text{temporally discontinuous parameters}}) = 0 \quad \text{with} \quad \dot{\mathcal{H}} = \dot{T} + \dot{I}^{\text{int}} + \dot{I}^{\text{ext}}$$

External **power functional**

$$D^{\text{cd}} = -\nabla(\ln \Theta) \cdot Q$$

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

Kinetic energy in Hu-Washizu form

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

Kinetic **power functional** (with independent time rate fields)

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

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Fourier's law of transversely isotropic heat conduction

Al-Kinani [2014]

$$\mathbf{q} := -\kappa \mathbf{F}^{-T} \nabla \Theta \quad \kappa := k \mathbf{I} + \frac{k_F - k}{\|\mathbf{a}\|^2} \mathbf{a} \otimes \mathbf{a} \quad \kappa_0 := k_0 \mathbf{C}^{-1} + \frac{k_{F_0} - k_0}{C_F} \mathbf{A}_0 \quad \mathbf{Q} := -\kappa_0 \nabla \Theta$$

Internal energy

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

Internal power functional

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



Principle of virtual power

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

Principle of virtual power

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

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

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

Virtual internal power

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

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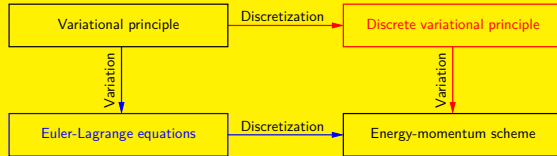
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Design of the mixed time discretization

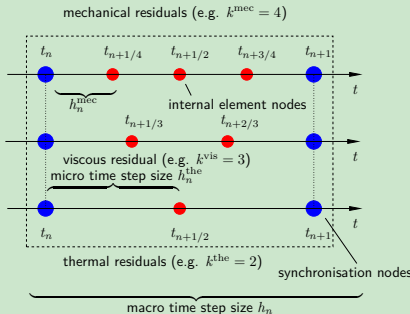
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Schematic process of the energy-momentum scheme design (cf. Yavari [2008])



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
	α	1		
2	$(2\alpha - 1)(\alpha - 1)$	0	$1 - \alpha$	0
	$-4\alpha(\alpha - 1)$	$\frac{1}{2}$	$-4\alpha(\alpha - 1)$	$\frac{1}{2}$
	$(2\alpha - 1)\alpha$	1	α	1
3	$-\frac{2}{3}(\alpha - \frac{1}{2})(\alpha - \frac{1}{3})(\alpha - 1)$	0	$(2\alpha - 1)(\alpha - 1)$	0
	$-\frac{4}{3}(\alpha - \frac{1}{2})(\alpha - 1)\alpha$	$\frac{1}{3}$	$-4\alpha(\alpha - 1)$	$\frac{1}{3}$
	$-\frac{4}{3}(\alpha - \frac{1}{2})(\alpha - 1)\alpha$	$\frac{2}{3}$	$(2\alpha - 1)\alpha$	$\frac{2}{3}$
	$\frac{2}{3}(\alpha - \frac{1}{2})(\alpha - \frac{2}{3})\alpha$	1		1
4	$-\frac{2}{3}(\alpha - \frac{1}{2})(\alpha - \frac{1}{3})(\alpha - \frac{1}{4})(\alpha - 1)$	0	$-\frac{2}{3}(\alpha - \frac{1}{2})(\alpha - \frac{1}{3})(\alpha - 1)$	0
	$-\frac{4}{3}(\alpha - \frac{1}{2})(\alpha - \frac{1}{3})(\alpha - 1)\alpha$	$\frac{1}{4}$	$-\frac{4}{3}(\alpha - \frac{1}{2})(\alpha - 1)\alpha$	$\frac{1}{4}$
	$64(\alpha - \frac{1}{2})(\alpha - \frac{1}{3})(\alpha - 1)\alpha$	$\frac{1}{3}$	$-\frac{4}{3}(\alpha - \frac{1}{2})(\alpha - 1)\alpha$	$\frac{1}{3}$
	$-\frac{4}{3}(\alpha - \frac{1}{2})(\alpha - \frac{1}{4})(\alpha - 1)\alpha$	$\frac{2}{3}$	$\frac{2}{3}(\alpha - \frac{1}{2})(\alpha - \frac{2}{3})\alpha$	$\frac{2}{3}$
	$\frac{2}{3}(\alpha - \frac{1}{2})(\alpha - \frac{1}{3})(\alpha - \frac{1}{4})\alpha$	1		1

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

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



Design of the mixed space discretization

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Analytical static condensation of mixed fields

- 1 First Piola-Kirchhoff stress tensor $\mathbf{P}$ is condensed out $\leadsto$ only a new 'B-matrix'
- 2 $\tilde{\mathbf{F}}$, $\tilde{\mathbf{C}}_F$, $\tilde{\mathbf{C}}_V$ are temporally continuous fields $\leadsto$ initial value is taken into account

Space approximation of mixed fields

$\deg[X] = \text{degree of spatial shape functions of } X$

- 1 $\underbrace{\deg[\dot{\varphi}, \dot{v}, \dot{p}, \dot{\theta}, \dot{\eta}, \dot{\theta}]}_{\text{spatially continuous}} \geq \underbrace{\deg[\dot{\tilde{\mathbf{F}}}, \mathbf{P}]}_{\text{spatially discontinuous}} \geq \deg[\dot{\mathbf{C}}_V, \dot{\mathbf{C}}_F, S_V, S_F]$ (motivated by Q1P0, Q2P1 etc.)
- 2 Evaluation of $\tilde{\mathbf{C}}$, $\mathbf{C}_v$ and $\mathbf{S}$ at spatial quadrature points

Strategy for choosing shape functions of mixed fields

(cf. Mahnen et al. [2008])

- 1 Choose $\deg[\dot{\varphi}, \dot{v}, \dot{p}, \dot{\theta}, \dot{\eta}, \dot{\theta}]$ and they kind of shape functions (hexahedral or tetrahedral)
- 2 Determine independent spatial shape functions N_A , $\tilde{N}_B^{\text{def}}$, $\tilde{N}_C^{\text{str}}$, which fulfill the condition

$$\deg[\dot{\varphi}, \dot{v}, \dot{p}, \dot{\theta}, \dot{\eta}] = \deg[\dot{\tilde{\mathbf{F}}}, \mathbf{P}] + 1 = \deg[\dot{\mathbf{C}}_V, \dot{\mathbf{C}}_F, S_V, S_F] + 2$$
- 3 Extend the shape functions $\tilde{N}_B^{\text{def}}$, $\tilde{N}_C^{\text{str}}$ by area bubbles in order to include each monomial and fulfill the completeness conditions

$$\sum_{B=1}^{\tilde{n}_{\text{def}}} \tilde{N}_B^{\text{def}} = 1$$

$$\sum_{C=1}^{\tilde{n}_{\text{str}}} \tilde{N}_C^{\text{str}} = 1$$

Example: Mesh of 8-node hexahedral elements

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Motivation: time discretization

(cf. Betsch & Steinmann [2002])

- 1 **Example:** Trial functions for the deformation φ of degree $k = 2$, given by

$$M_1(\alpha) = (2\alpha - 1)(\alpha - 1) \quad M_2(\alpha) = -4\alpha(\alpha - 1) \quad M_3(\alpha) = \alpha(2\alpha - 1)$$

demands for the variation $\delta\varphi$ test functions of degree $k - 1 = 1$ of the form

$$\tilde{M}_1(\alpha) = 1 - \alpha \quad \tilde{M}_2(\alpha) = \alpha$$

- 2 **Proof:** The time functions $M'_1(\alpha) = 4\alpha - 3$, $M'_2(\alpha) = 4 - 8\alpha$ and $M'_3(\alpha) = 4\alpha - 1$ are not independent, which means

$$\sum_{i=1}^{k+1} a_i M'_i(\alpha) = 0 \quad \text{leads to } a_i = \lambda_1 \in \mathbb{R} \text{ with } p = 1 \text{ parameter}$$

Therefore, only $k - p = 2$ functions $\tilde{M}_j$ are independent, and (i) gives the identity

$$\sum_{i=1}^{k+1} M'_i(\alpha) z_i = \sum_{j=1}^k \tilde{M}_j z_j \quad \text{and (ii) includes the required monomials } 1, \alpha$$

Application: space discretization with 8-node hexahedrons

(cf. Armero [2008])

- 1 The 8 shape functions N_A have 4 independent derivatives, which leads to

$$\tilde{N}_1^{\text{def}} = 1 - \xi - \eta - \zeta \quad \tilde{N}_2^{\text{def}} = \xi \quad \tilde{N}_3^{\text{def}} = \eta \quad \tilde{N}_4^{\text{def}} = \zeta$$

- 2 The 4 shape functions $\tilde{N}_B^{\text{def}}$ have 1 independent derivative $\tilde{N}^{\text{str}} = 1$.

- 3 Since the derivatives of N_A include the monomials $\xi\eta$, $\xi\zeta$ and $\eta\zeta$, we define

$$\tilde{N}_1^{\text{def}} := \tilde{N}_1^{\text{def}} - \xi\eta - \xi\zeta - \eta\zeta \quad \tilde{N}_2^{\text{def}} := \tilde{N}_2^{\text{def}} + \eta\zeta \quad \tilde{N}_3^{\text{def}} := \tilde{N}_3^{\text{def}} + \xi\zeta \quad \tilde{N}_4^{\text{def}} := \tilde{N}_4^{\text{def}} + \xi\eta$$



Fiber-reinforced air beam with two cells

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

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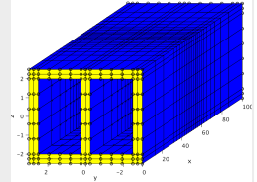
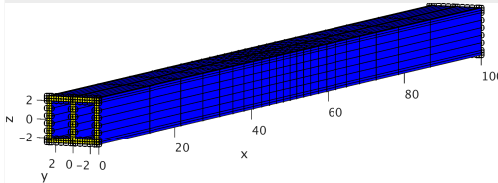
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Boundary Status Monitor

(cf. Nguyen et al. [2015])



Dirichlet and Neumann boundary conditions

$$\varphi_t^A = \mathbf{X}^A \text{ (circular markers)}$$

$$\Theta_t^A = \Theta_\infty \text{ (blue patches)}$$

(clamped at both ends)

No thermal insulation $\bar{Q} := 0$

Transient pressure

(follower load in star markers)

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

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

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

Initial conditions

(Ambient temp. $\Theta_\infty = 298.15$)

$$\varphi_0^A = \mathbf{X}^A$$

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

$$\Theta_0^A = \Theta_\infty + 10$$



Fiber-reinforced air beam with two cells

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

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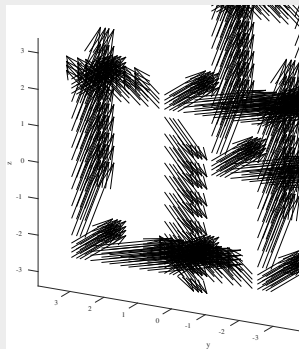
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Simulation parameters

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

Initial conditions	
Initial velocity:	$v_0^A = 0$
Initial temperature:	$\Theta_0^A = \Theta_{\infty} + 10 = 308.15$
Boundary conditions	
Yellow patches in yz-plane (with circular markers):	x-dof, y-dof and z-dof fixed
Yellow patches:	$\Theta^A = \hat{\Theta} f(t)$
Blue patches:	$\Theta^A = \Theta_{\infty}$
Dirichlet loads	
Temperature profile: (yellow patches)	$f(t)$ with $\hat{\Theta} = 10$ $T_{load} = 2.0$ $\omega_{load} = 10\pi$
Neumann loads	
Pressure load: (blue patches with star markers)	$f_p(t)$ with $\hat{p} = 1 \cdot 10^5$ $T_{load,p} = 2.0$ $\omega_{load,p} = 10\pi$
Volume loads	
Standard gravity	$g = 9.81$ with $e_g = -e_z$

Material Status Monitor



Material parameters

$$\begin{aligned}
 \rho_0 &= 1.120 \cdot 10^3 & \kappa^{\text{vol}} &= 1.000 \cdot 10^7 & \mu_{01} &= 0.250 \cdot 10^4 \\
 \mu_{10} &= 0.250 \cdot 10^7 & \mu_{20} &= 0.021 \cdot 10^7 & Y_1 &= 0.1631 \cdot 10^7 \\
 Y_2 &= 0.6 & \kappa_{\text{ani}} &= 0.250 \cdot 10^7 & g_0 &= 0.300 \cdot 10^7 \\
 g_c &= 4 & \beta_M &= 20 \cdot 10^{-6} & c_{M_0} &= 1539 \cdot 50\% \\
 c_{M_1} &= 0.00375 & k &= 0.2595 & \beta_F &= 206 \cdot 10^{-6} \\
 c_{F_0} &= 1539 \cdot 50\% & c_{F_1} &= 0.00375 & k_F &= 200 \text{ k} \\
 V_{\text{dev}} &= 10^3 & V_{\text{vol}} &= 5 \cdot 10^3 & \kappa_v^{\text{vol}} &= 1.000 \cdot 10^6 \\
 \mu_{01}^v &= 0.250 \cdot 10^3 & \mu_{10}^v &= 0.250 \cdot 10^6 & \mu_{20}^v &= 0.021 \cdot 10^6 \\
 Y_1^v &= 0.1631 \cdot 10^6 & Y_2^v &= 0.6 & &
 \end{aligned}$$

Fiber directions

$$\begin{aligned}
 \text{Side walls} &: \mathbf{a}_0 = \sin \phi \mathbf{e}_x + \cos \phi \mathbf{e}_z, \phi = \frac{\pi}{4} \\
 \text{Middle wall} &: \mathbf{a}_0 = \sin \phi \mathbf{e}_x + \cos \phi \mathbf{e}_z, \phi = \frac{3\pi}{4} \\
 \text{Bottom left/ top right} &: \mathbf{a}_0 = \sin \phi \mathbf{e}_x + \cos \phi \mathbf{e}_y, \phi = \frac{3\pi}{4} \\
 \text{Bottom right/ top left} &: \mathbf{a}_0 = \sin \phi \mathbf{e}_x + \cos \phi \mathbf{e}_y, \phi = \frac{\pi}{4} \\
 \text{Chamber corners} &: \mathbf{a}_0 = \sin \phi \mathbf{e}_x + \cos \phi \mathbf{e}_y, \phi = \frac{\pi}{2}
 \end{aligned}$$



Fiber-reinforced air beam with two cells

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

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Free energy

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

Elastic free energy functions

$$\begin{aligned}\psi_M^{\text{ela}} &:= \mu_{10} [I_1(C^{\text{iso}}) - I_1(I)] \\ &\quad + \mu_{20} [I_1(C^{\text{iso}}) - I_1(I)]^2 \\ &\quad + \mu_{01} [I_2(C^{\text{iso}}) - I_2(I)] \\ &\quad + \frac{Y_1}{Y_2} \{1 - \exp[-Y_2 (I_1(C^{\text{iso}}) - I_1(I))]\} \\ &\quad + \frac{\kappa^{\text{ani}}}{3} [(I_4(C^{\text{iso}}))^{3/2} + 3 (I_4(C^{\text{iso}}))^{-1/2} - 4] \\ \psi_M^{\text{vol}} &:= \frac{\kappa^{\text{vol}}}{50} [(\tilde{C}_V)^{5n_{\text{dim}}/2} + (\tilde{C}_V)^{-5n_{\text{dim}}/2} - 2] \\ \psi_F^{\text{ela}} &:= \frac{g_0}{(2g_c)} [\exp[g_c(\tilde{C}_F - 1)^2] - 1]\end{aligned}$$

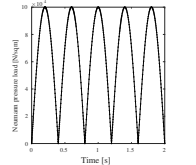
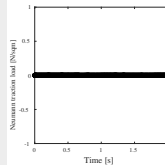
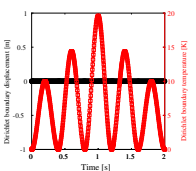
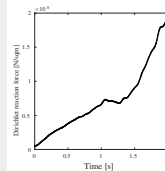
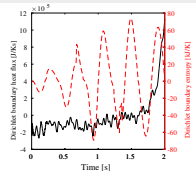
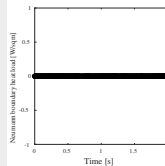
Thermoelastic free energy function

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

Viscoelastic free energy function

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

Time evolutions of loads/reactions





Fiber-reinforced air beam with two cells

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

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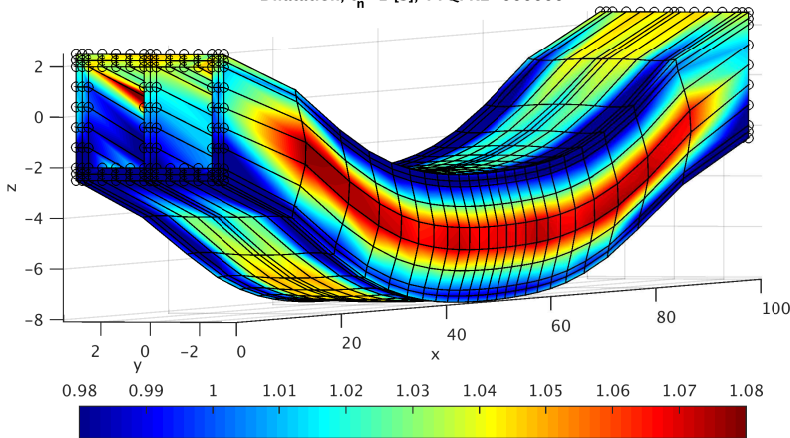
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Motion Status Monitor: Volume dilatation $\det(\tilde{\mathbf{F}})$ at $t_n = 1.0$

Dilatation, $t_n = 1$ [s], VTQPRL=000000





Fiber-reinforced air beam with two cells

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

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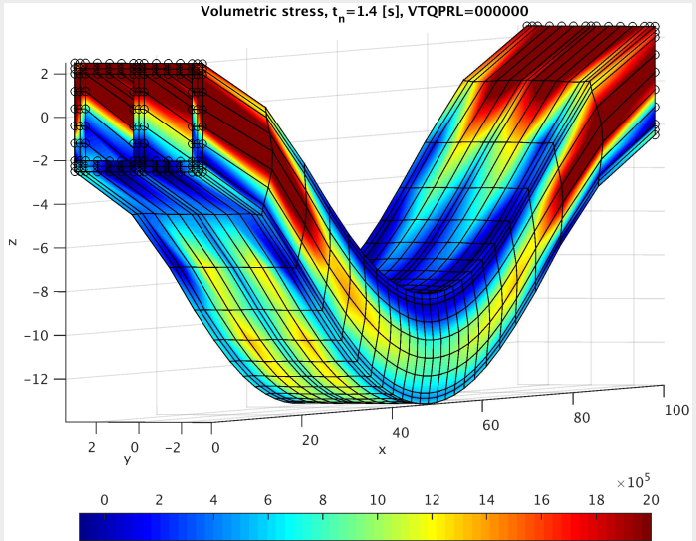
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Motion Status Monitor: Volumetric stress S_V at $t_n = 1.4$





Fiber-reinforced air beam with two cells

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

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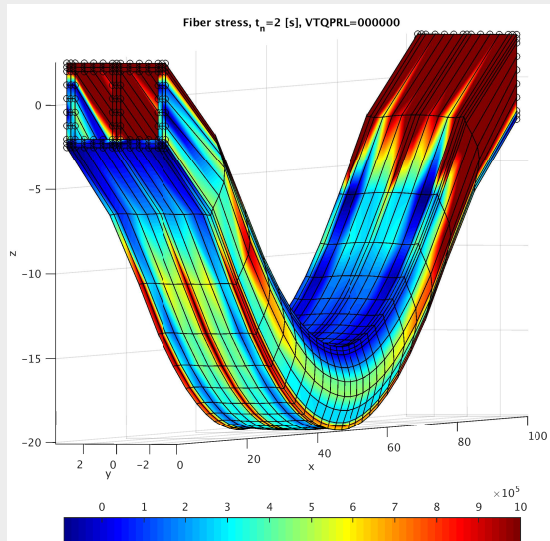
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Motion Status Monitor: Fiber stress S_F at $t_n = 2.0$





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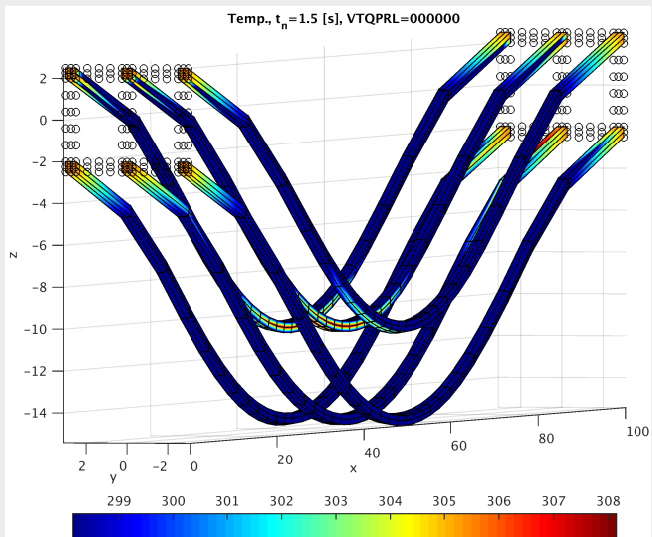
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Motion Status Monitor: Temperature Θ at $t_n = 1.5$ INSIDE the cell corners





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

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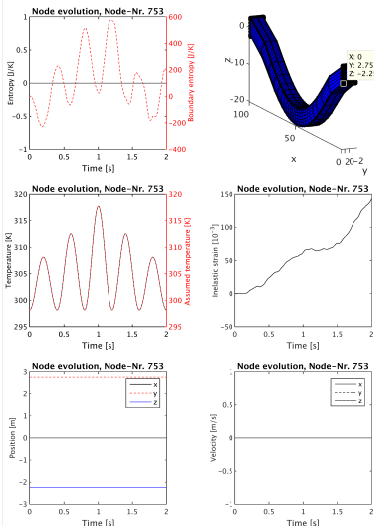
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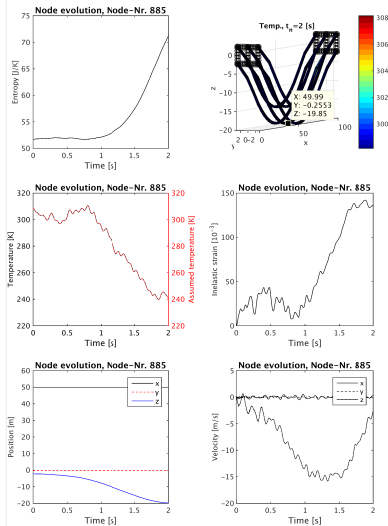
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Fixed node on the boundaries $\partial_{\dot{\mathcal{B}}_0}$, $\partial_{\varphi}\mathcal{B}_0$



Free node of the middle corner at the center

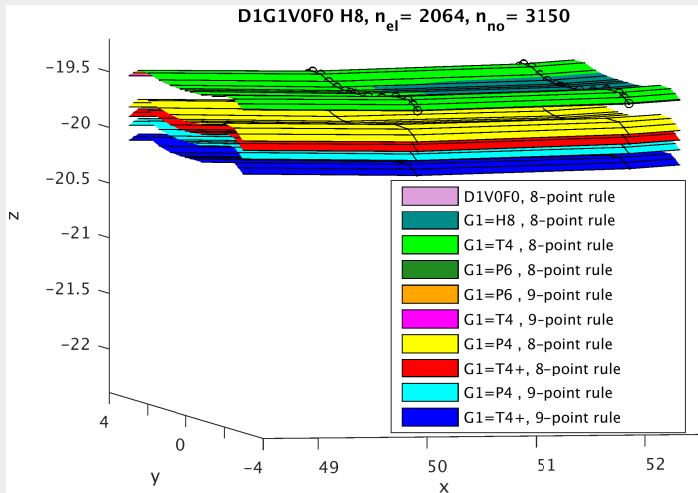




Fiber-reinforced air beam with two cells

(Comparison of $\tilde{N}_B$ (I); $k_{\text{mec}} = 1, k_{\text{the}} = 2, k_{\text{vis}} = 1$)

Current configurations at $t_n = 2.0$: Zoom on bottom surfaces of the beams



Hourglass functions

(cf. Simo, Armero, Taylor [1993])

$$\mathcal{H}_1(\xi, \eta, \zeta) := \xi \eta$$

$$\mathcal{H}_2(\xi, \eta, \zeta) := \xi \zeta$$

$$\mathcal{H}_3(\xi, \eta, \zeta) := \eta \zeta$$

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Shape functions of $T4+-\tilde{F}$ -element

$$\tilde{N}_1 = 1 - \xi - \eta - \zeta - \xi\zeta - \eta\zeta - \xi\eta$$

$$\tilde{N}_2 = \xi + \eta\zeta$$

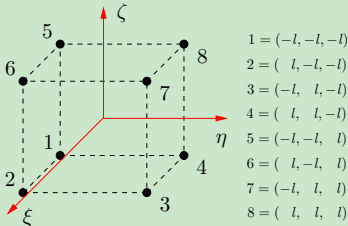
$$\tilde{N}_3 = \eta + \xi\zeta$$

$$\tilde{N}_4 = \zeta + \xi\eta$$

8-point product Gauss rule

(Felippa [2001], Wriggers [2001])

$$l = \sqrt{1/3}, \quad w = 1/(3l^2)$$



Shape functions of $P4-\tilde{F}$ -element

$$\tilde{N}_1 = \frac{1}{2} [1 - \xi - \eta + \xi\zeta + \eta\zeta]$$

$$\tilde{N}_2 = \frac{1}{2} [\xi - \xi\zeta]$$

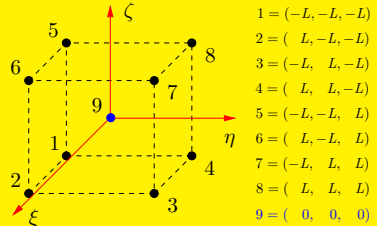
$$\tilde{N}_3 = \frac{1}{2} [\eta - \eta\zeta]$$

$$\tilde{N}_4 = \frac{1}{2} [1 + \zeta]$$

9-point non-product Gauss rule

(Simo, Armero, Taylor [1993], Felippa [2001])

$$L = \sqrt{3/5} > l, \quad W = 1/(3L^2) < w, \quad W_9 = 8 - 8W$$





Fiber-reinforced air beam with two cells

(Computational costs; $k_{\text{mec}} = 1$, $k_{\text{the}} = 2$, $k_{\text{vis}} = 1$)

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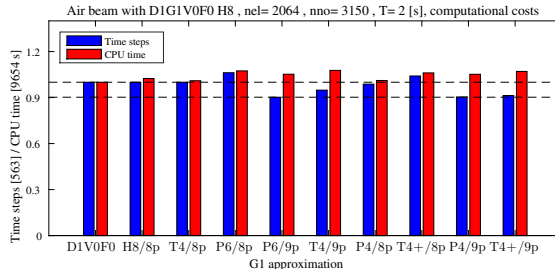
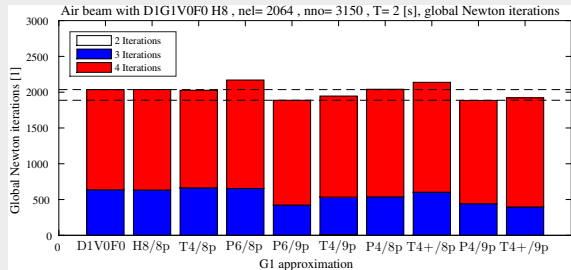
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Number of time steps / Total cpu time / Number of global iterations



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1 Motivation:

- ▶ Energy-momentum schemes for fiber-reinforced materials
- ▶ related with locking-free meshes for thin-walled structures

2 Goals:

- ▶ Independent space-time approximations
- ▶ of the stretch vector $\lambda_t(\tilde{\mathbf{F}})$, and
- ▶ of the volume as well as fiber dilatation $(\tilde{C}_V, \tilde{C}_F)$

3 Strategy:

- ▶ Discretization of a mixed principle of virtual power
- ▶ Design of independent shape functions for spatial derivatives
- ▶ Introduction of appropriate quadrature rules in space

4 Important results:

- ▶ Reduction of locking in meshes of thin-walled structures
- ▶ Increase of maximum time step size due to less artificial stiffness

5 Outlook:

- ▶ Generalization to higher-order hexahedral/tetrahedral meshes



Fiber-reinforced air beam with two cells

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

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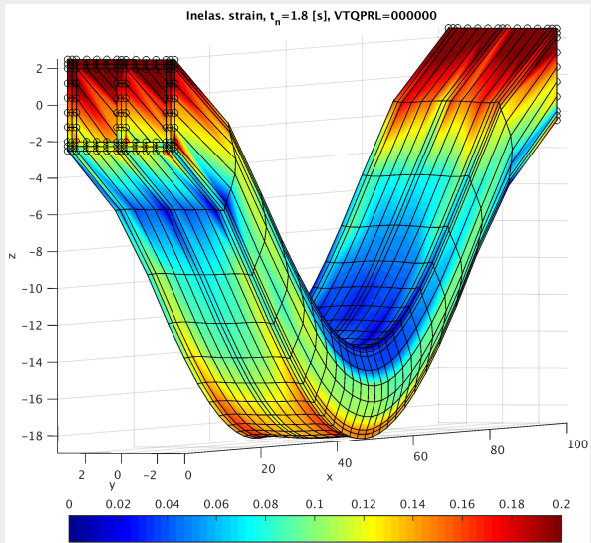
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Motion Status Monitor: Inelastic strain $\|C_i\|$ at $t_n = 1.8$





Fiber-reinforced air beam with two cells

(Mechanical/thermal balance laws; $k_{\text{mec}} = 1, k_{\text{the}} = 2, k_{\text{vis}} = 1$)

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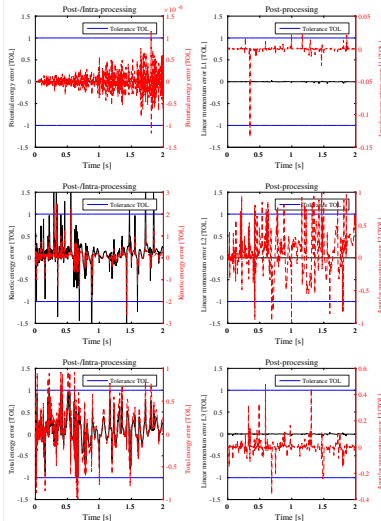
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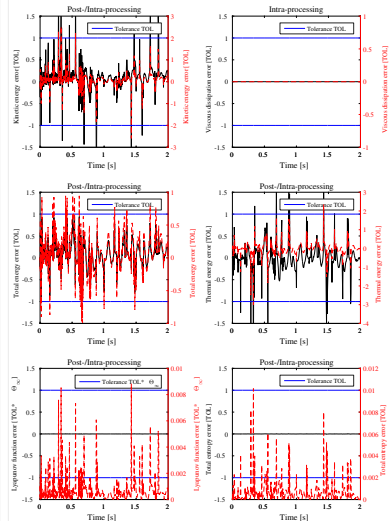
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M-Balance Status Monitor



T-Balance Status Monitor



Fiber-reinforced air beam with two cells

(Comparison of $\tilde{N}_B$ (III); $k_{\text{mec}} = 1$, $k_{\text{the}} = 2$, $k_{\text{vis}} = 1$)

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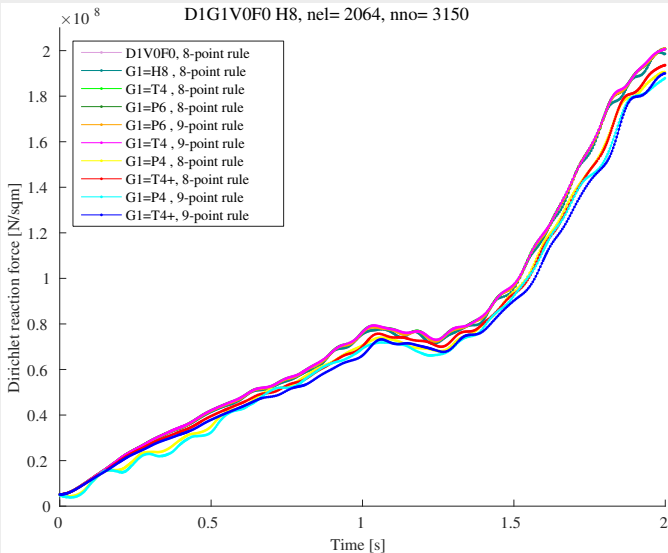
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Time evolutions of reaction force in the clamping

(cf. Kasper & Taylor [2004])





Fiber-reinforced air beam with two cells

(Comparison of $\tilde{N}_B$ (IV); $k_{\text{mec}} = 1$, $k_{\text{the}} = 2$, $k_{\text{vis}} = 1$)

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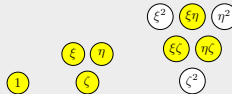
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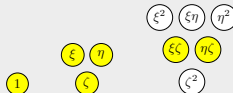
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Monomials of the H8-derivative (Layers 0,1,2 of Pascal's pyramid)

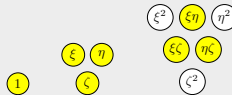


Monomials of the P4 element (Layers 0,1,2 of Pascal's pyramid)



► Missing monomial: $\xi\eta$

Monomials of the T4+ element (Layers 0,1,2 of Pascal's pyramid)





Fiber-reinforced air beam with two cells (H20)

(Comparison of $\tilde{N}_B$ (I); $k_{\text{mec}} = 1$, $k_{\text{the}} = 2$, $k_{\text{vis}} = 1$)

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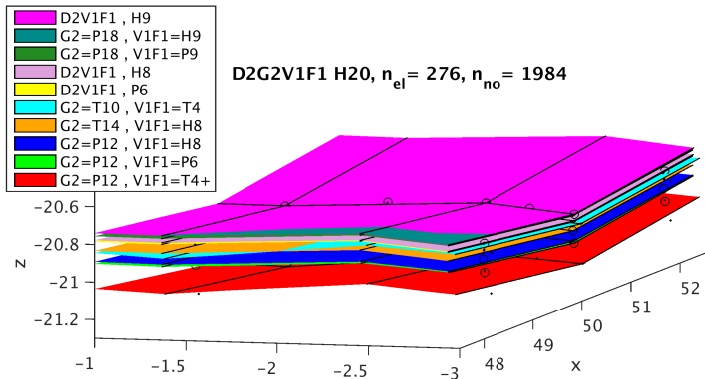
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Current configurations at $t_n = 2.0$: Zoom on bottom surfaces of the beams





Fiber-reinforced air beam with two cells (H20)

(Comparison of $\tilde{N}_B$ (II); $k_{\text{mec}} = 1, k_{\text{the}} = 2, k_{\text{vis}} = 1$)

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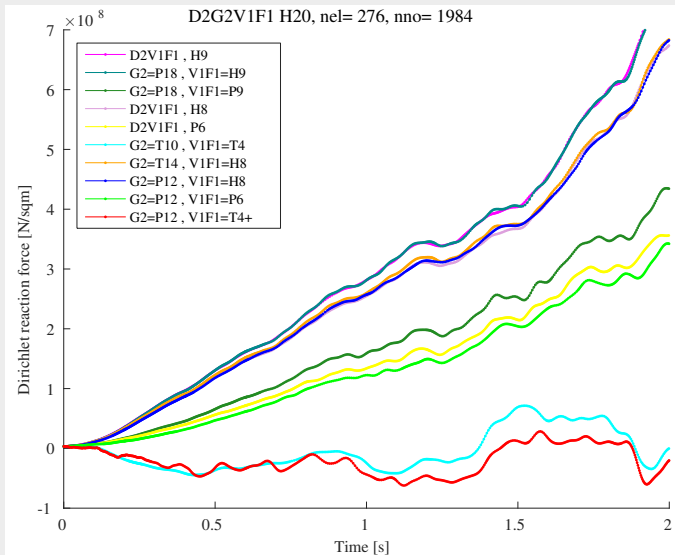
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Time evolutions of reaction force in the clamping

(cf. Kasper & Taylor [2004])





Fiber-reinforced air beam with two cells (H20)

(Comparison of $\tilde{N}_B$ (III); $k_{\text{mec}} = 1, k_{\text{the}} = 2, k_{\text{vis}} = 1$)

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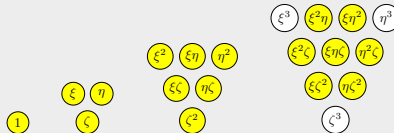
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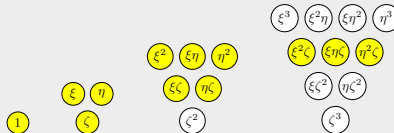
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Monomials of the H20-derivative (Layers 0,1,2,3 of Pascal's pyramid)



Monomials of the P12 element (Layers 0,1,2,3 of Pascal's pyramid)



► Missing monomials: $\zeta^2, \xi^2\eta, \xi\eta^2, \xi\zeta^2, \eta\zeta^2$

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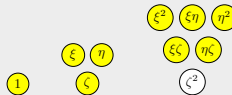
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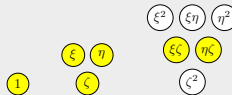
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Monomials of the P12-derivative (Layers 0,1,2 of Pascal's pyramid)



Monomials of the P6 element (Layers 0,1,2 of Pascal's pyramid)



► Missing monomials: ξ^2 , $\xi\eta$, η^2

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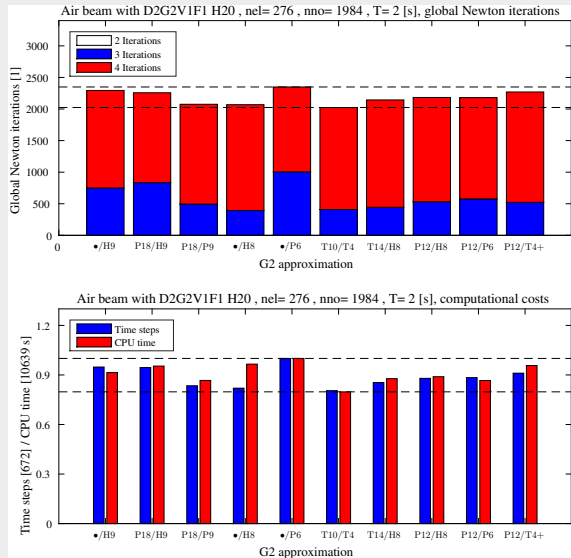
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Number of time steps / Total cpu time / Number of global iterations





Fiber-reinforced air beam with two cells (H27)

(Comparison of $\tilde{N}_B$ (I); $k_{\text{mec}} = 1$, $k_{\text{the}} = 2$, $k_{\text{vis}} = 1$)

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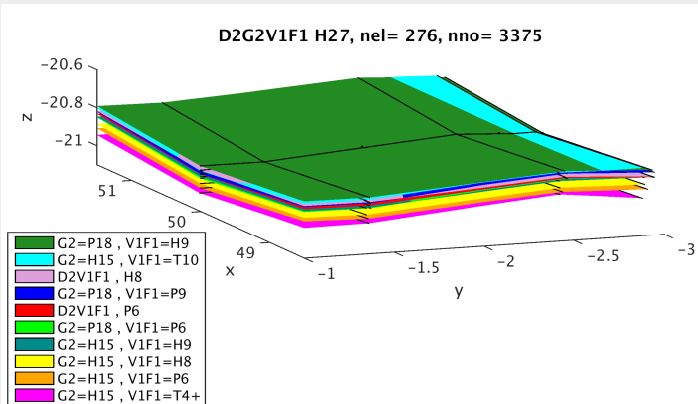
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Fiber-reinforced air beam with two cells (H27)

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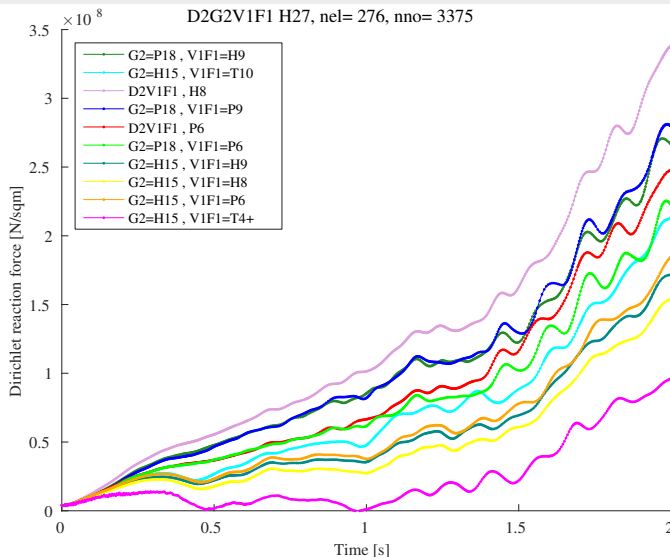
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Time evolutions of reaction force in the clamping

(cf. Kasper & Taylor [2004])





Fiber-reinforced air beam with two cells (H27)

(Comparison of $\tilde{N}_B$ (III); $k_{\text{mec}} = 1, k_{\text{the}} = 2, k_{\text{vis}} = 1$)

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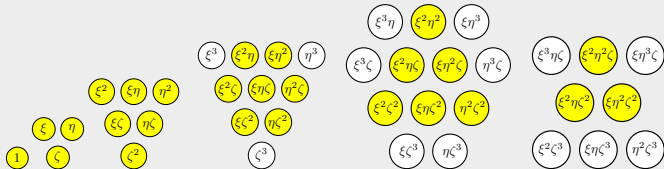
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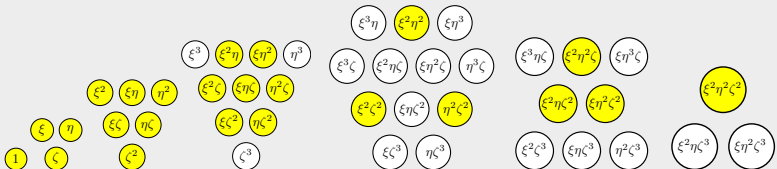
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Monomials of the H27-derivative (Layers 0,1,2,3,4,5 of Pascal's pyramid)



Monomials of the H15 element (Layers 0,1,2,3,4,5,6 of Pascal's pyramid)





Fiber-reinforced air beam with two cells (H27)

(Comparison of $\tilde{N}_B$ (IV); $k_{\text{mec}} = 1$, $k_{\text{the}} = 2$, $k_{\text{vis}} = 1$)

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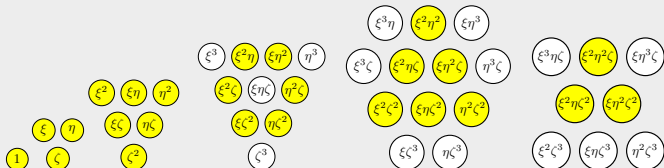
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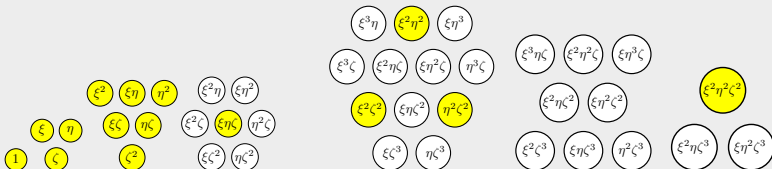
Monomials of the H15-derivative (Layers 0,1,2,3,4,5 of Pascal's pyramid)



Monomials of the H8 element (Layers 0,1,2,3 of Pascal's pyramid)



Monomials of the H9 element (Layers 0,1,2,3,4,5,6 of Pascal's pyramid)





Fiber-reinforced air beam with two cells (H27)

(Computational costs; $k_{\text{mec}} = 1, k_{\text{the}} = 2, k_{\text{vis}} = 1$)

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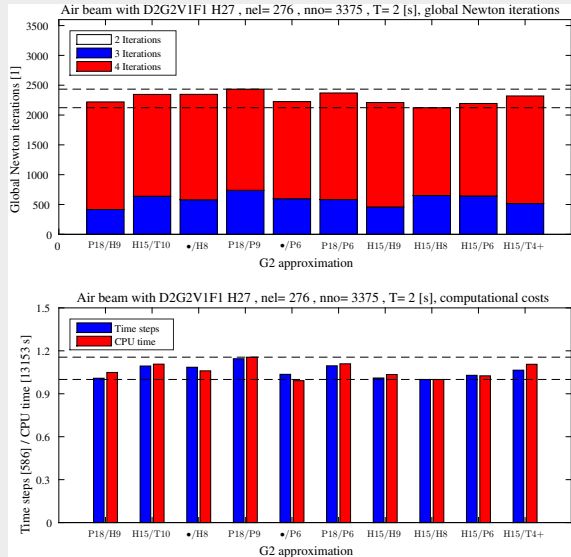
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Fiber-reinforced spherical shell with a slit

(Thermodynamical convergence (I); $k_{\text{mec}} = 1, k_{\text{the}} = 2, k_{\text{vis}} = 1$)

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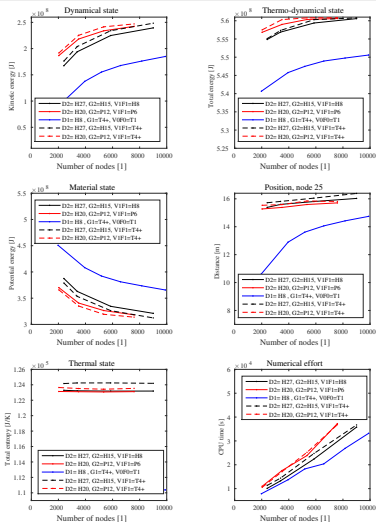
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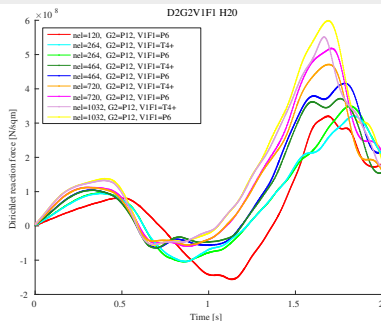
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Reaction force, D2G2V1F1 H20





Fiber-reinforced spherical shell with a slit

(Thermodynamical convergence (II); $k_{mec} = 1, k_{the} = 2, k_{vis} = 1$)

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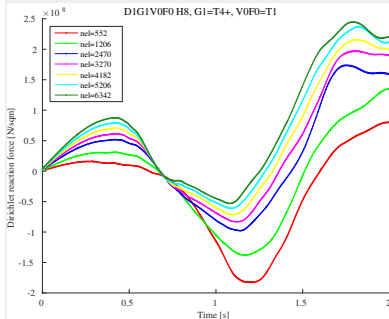
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Reaction force, D1=H8, G1=T4+, V0F0=T1



Reaction force, D2G2V1F1 H27

