

Groß M., Dietzsch J., Kalaimani I. and Saleh T.

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Variational computational modelling of dynamical behaviour of fiber roving composites with inelastic anisotropic continua and thermomechanical coupling

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# Motivation: roving-matrix composite simulation

Variational computational modelling of dynamical behaviour of fiber roving composites with inelastic anisotropic continua and thermomechanical coupling

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## Background: Roving-matrix composite parts in rotordynamics



### Modelling: The need for macroscopic formulations with length scales



Goal: FE simulations taking into account length scales in anisotropic continuum formulations

We design dynamic mixed FE methods for higher gradient materials with length scales



# Overview about gradient material formulations

(see e.g. Spencer & Soldatos [2007], Askes & Aifantes [2011], Madeo et al. [2015], Asmanoglo & Menzel [2017], Ferretti et al. [2014])





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## Principle of virtual power and time integration Application example: Quasi-static analysis with dynamic load

## Path-independent time integration (motivated by Betsch & Steinmann [2002], Armero [2008])

Preservation of balance law of potential energy  $\mathcal{H}_t := \Pi^{\text{int}}(\mathbf{C}_t) + \Pi^{\text{ext}}(\varphi_t, \mathbf{C}_t)$  $\mathcal{H}_{t_{n+1}} - \mathcal{H}_{t_n} = \int_{t_n}^{t_{n+1}} \left\{ \int_{\mathscr{B}_0} \frac{\partial \Psi}{\partial \mathbf{C}_t} : \dot{\mathbf{C}}_t \, \mathrm{d}V \, \mathrm{d}t + \left[ \int_{\partial_T \mathscr{B}_0} \bar{\mathbf{T}}(t) \cdot \dot{\varphi}_t \, \mathrm{d}A + \frac{1}{2} \int_{\mathscr{B}_0} \bar{\mathbf{S}}(t) : \dot{\mathbf{C}}_t \, \mathrm{d}V \right] \right\} \mathrm{d}t$ 

Algorithmic stress  $ar{m{S}}(t)$  corrects material non-linearity

Independent time evolution variables corrects geometric non-linearity

$$\begin{split} \Pi_{t_{n+1}}^{\text{int}} &- \Pi_{t_n}^{\text{int}} = \int_{t_n}^{t_{n+1}} \dot{\Pi}^{\text{int}} \left( \dot{\boldsymbol{Y}}_1, \dots, \dot{\boldsymbol{Y}}_n \right) \, \mathrm{d}t \\ &= \int_{t_n}^{t_{n+1}} \dot{\Pi}^{\text{int}} \left( \dot{\boldsymbol{Y}}_1, \dots, \dot{\boldsymbol{Y}}_n \right) \, \mathrm{d}t - \sum_{i=1}^n \int_{t_n}^{t_{n+1}} \int_{\mathscr{B}_0} \tilde{\boldsymbol{Z}}_i \odot \left[ \dot{\boldsymbol{Y}}_i - \dot{\boldsymbol{Y}}_i \right] \, \mathrm{d}V \, \mathrm{d}t \end{split}$$

Mixed principle of virtual power

(cf. Schröder & Kuhl [2015])

$$\int_{t_n}^{t_{n+1}} \delta_* \dot{\mathcal{H}} \left( \dot{\boldsymbol{\varphi}}_t, \dot{\tilde{\boldsymbol{C}}}_t, \tilde{\boldsymbol{S}}_t \right) \, \mathrm{d}t = 0 \quad \text{with} \quad \dot{\boldsymbol{\varPi}}^{\mathrm{int}} := \int_{\mathscr{B}_0} \left\{ \dot{\boldsymbol{\varPsi}}(\tilde{\boldsymbol{C}}_t) - \frac{1}{2} \dot{\boldsymbol{S}}_t : \left[ \dot{\tilde{\boldsymbol{C}}}_t - \overline{\boldsymbol{F}_t^T} \overline{\boldsymbol{F}}_t \right] \right\} \mathrm{d}\boldsymbol{V}$$

#### Space-time weak forms

$$\begin{split} \int_{t_n}^{t_{n+1}} & \int_{\mathscr{B}_0} \delta_* \dot{\tilde{\boldsymbol{C}}}_t : \left[ 2 \, \frac{\partial \Psi}{\partial \tilde{\boldsymbol{C}}_t} + \tilde{\boldsymbol{S}}(t) - \tilde{\boldsymbol{S}}_t \right] \mathrm{d}V \, \mathrm{d}t = 0 = \int_{t_n}^{t_{n+1}} & \int_{\mathscr{B}_0} \delta_* \tilde{\boldsymbol{S}}_t : \frac{1}{2} \left[ \dot{\tilde{\boldsymbol{C}}}_t - \overline{\boldsymbol{F}_t^T \boldsymbol{F}}_t \right] \mathrm{d}V \, \mathrm{d}t \\ & \int_{t_n}^{t_{n+1}} & \int_{\mathscr{B}_0} \boldsymbol{F}_t \, \tilde{\boldsymbol{S}}_t : \operatorname{Grad}[\delta_* \dot{\boldsymbol{\varphi}}_t] \, \mathrm{d}V \, \mathrm{d}t = \int_{t_n}^{t_{n+1}} & \int_{\partial_T \mathscr{B}_0} \bar{\boldsymbol{T}}(t) \cdot \delta_* \dot{\boldsymbol{\varphi}}_t \, \mathrm{d}A \, \mathrm{d}t \end{split}$$



# Anisotropy with rotational degrees of freedom



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## Local rotational degrees of freedom

Roving rotation from vorticity vector (perfect roving-matrix interface)

$$2\,\mathbb{I}^{\mathrm{skw}} := \boldsymbol{\epsilon}\cdot\boldsymbol{\epsilon} \qquad \qquad \mathbb{I}^{\mathrm{skw}}: \boldsymbol{l}_t = -\boldsymbol{\epsilon}\cdot\boldsymbol{\omega}_t \qquad \qquad \boldsymbol{l}_t := \dot{\boldsymbol{F}}_t \boldsymbol{F}_t^{-1} \qquad \dot{\boldsymbol{\gamma}}_t := \boldsymbol{\omega}_t$$

Variational setting by a rotational energy functional

$$\dot{H}_{\rm rot}(\dot{\boldsymbol{\varphi}}_t,\dot{\boldsymbol{\alpha}}_t,\dot{\boldsymbol{C}}_t,\tilde{\boldsymbol{S}}_t,\tilde{\boldsymbol{\tau}}_{\rm skw}) \coloneqq \dot{H}_{\rm rot}^{\rm int}(\dot{\boldsymbol{C}},\dot{\boldsymbol{\alpha}}_t) + \int_{\mathscr{B}_0} \tilde{\boldsymbol{\tau}}_{\rm skw}^T : \boldsymbol{\epsilon} \cdot \left[\frac{1}{2}\,\boldsymbol{\epsilon}:\dot{\boldsymbol{F}}_t\boldsymbol{F}_t^{-1} + \dot{\boldsymbol{\alpha}}_t\right] \mathrm{d}\boldsymbol{V}$$

Modified/additional space-time weak forms in the quasi-static case

$$\begin{split} \int_{t_n}^{t_{n+1}} & \int_{\mathscr{B}_0} \left[ \boldsymbol{F}_t \, \tilde{\boldsymbol{S}}_t(\boldsymbol{\varphi}_t, \boldsymbol{\alpha}_t) + \tilde{\boldsymbol{\tau}}_{\mathsf{skw}}^T : \mathbb{F}_t^{\mathsf{skw}} \cdot \boldsymbol{F}_t^{-T} \right] : \operatorname{Grad}[\delta_* \dot{\boldsymbol{\varphi}}_t] \, \mathrm{d}\boldsymbol{V} \, \mathrm{d}t &= \int_{t_n}^{t_{n+1}} \int_{\partial \mathcal{T}} \tilde{\boldsymbol{\mathcal{T}}}(t) \cdot \delta_* \dot{\boldsymbol{\varphi}}_t \, \mathrm{d}\boldsymbol{A} \, \mathrm{d}t \\ & \int_{t_n}^{t_{n+1}} \int_{\mathscr{B}_0} \delta_* \tilde{\boldsymbol{\tau}}_{\mathsf{skw}}^T : \boldsymbol{\epsilon} \cdot \left[ \frac{1}{2} \boldsymbol{\epsilon} : \dot{\boldsymbol{F}}_t \boldsymbol{F}_t^{-1} + \dot{\boldsymbol{\alpha}}_t \right] \, \mathrm{d}\boldsymbol{V} \, \mathrm{d}t = 0 = \int_{t_n}^{t_{n+1}} \int_{\mathscr{B}_0} \left[ \frac{\partial \boldsymbol{\Psi}}{\partial \boldsymbol{\alpha}_t} + \tilde{\boldsymbol{\tau}}_{\mathsf{skw}}^T : \boldsymbol{\epsilon} \right] \cdot \delta_* \dot{\boldsymbol{\alpha}}_t \, \mathrm{d}\boldsymbol{V} \, \mathrm{d}t \end{split}$$



# Kinematics with rotational degrees of freedom

Curvilinear setting Configurations (motivated by Wriggers [2008]) Variational computational modelling of Deformation mapping dynamical φ, behaviour of fiber  $\frac{\partial \varphi(\boldsymbol{X}(\boldsymbol{\xi}), t)}{\partial \varepsilon_{i}} =: \boldsymbol{g}_{j}$ roving composites with inelastic Rotation mapping anisotropic continua and  $\frac{\partial \boldsymbol{\alpha}(\boldsymbol{X}(\boldsymbol{\xi}),t)}{\partial \boldsymbol{\xi}^{j}} =: \boldsymbol{\gamma}_{\boldsymbol{j}}$ thermomechanical coupling Groß M., Dietzsch  $\boldsymbol{\gamma}_i := \alpha_{i}^k \boldsymbol{g}_k$ J., Kalaimani I and Saleh T. Covariant formulation (cf. Eringen [1967]) Metric coefficients for translations and local rotations  $g_{ij} := \boldsymbol{g}_i \cdot \boldsymbol{g}_j \quad \boldsymbol{g}_j = g_{ij} \, \boldsymbol{g}^i \qquad K_{ij} := \boldsymbol{g}_i \cdot \boldsymbol{\gamma}_j \quad \boldsymbol{\gamma}_j = K_{ij} \, \boldsymbol{g}^i$ Metric tensors  $\boldsymbol{g} := \frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{z}} \equiv \boldsymbol{g}_j \otimes \boldsymbol{g}^j = g_{ij} \, \boldsymbol{g}^i \otimes \boldsymbol{g}^j$  $\boldsymbol{g}_{\alpha} := \frac{\partial \boldsymbol{\alpha}}{\partial \boldsymbol{\sigma}} \equiv \boldsymbol{\gamma}_{j} \otimes \boldsymbol{g}^{j} = K_{ij} \, \boldsymbol{g}^{i} \otimes \boldsymbol{g}^{j}$ Covariant formulation Deformation/rotation gradient  $\boldsymbol{F} = \frac{\partial \boldsymbol{\varphi}}{\partial \boldsymbol{Y}} = \boldsymbol{g}_{j} \otimes \boldsymbol{G}^{j} \qquad \boldsymbol{g}_{j} = \boldsymbol{F} \boldsymbol{G}_{j} \qquad \boldsymbol{G}_{\alpha} = \frac{\partial \boldsymbol{\alpha}}{\partial \boldsymbol{Y}} = \boldsymbol{\gamma}_{j} \otimes \boldsymbol{G}^{j} \qquad \boldsymbol{\gamma}_{j} = \boldsymbol{G}_{\alpha} \boldsymbol{G}_{j}$ Line stretch and local curvature-twist  $\mathrm{d} \boldsymbol{x} \cdot \boldsymbol{g} \cdot \mathrm{d} \boldsymbol{x} = \boldsymbol{d} \boldsymbol{X} \cdot \boldsymbol{C} \cdot \mathrm{d} \boldsymbol{X} \quad \boldsymbol{C} = \boldsymbol{F}^T \boldsymbol{g} \boldsymbol{F}$  $\mathrm{d}\boldsymbol{x} \cdot \boldsymbol{g}_{\alpha} \cdot \mathrm{d}\boldsymbol{x} = \boldsymbol{d}\boldsymbol{X} \cdot \boldsymbol{K} \cdot \mathrm{d}\boldsymbol{X} \quad \boldsymbol{K} = \boldsymbol{F}^{T} \boldsymbol{g}_{\alpha} \boldsymbol{F}$ 6



# Covariant kinematics of roving deformations

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#### Tensor invariants as roving deformation indicators

Translational deformation indicators for stretch and distorsion  $I_1(C_A) := C_A : G^{-1} \equiv I_4(C, a_0)$   $J_2(C_A) := C_A : C_A \equiv J_5(C, a_0)$ 

Rotational deformation indicators for twist and curvature (bending)  $I_1(\mathbf{K}_F) := \mathbf{K}_F : \mathbf{G}^{-1} =: T_F$   $J_2(\mathbf{K}_F) := \mathbf{K}_F : \mathbf{K}_F =: \frac{B_F}{2}$ 



# Consistent time integration of the local rotations

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Path-independence with linear stress (geometric non-linearity)  

$$\dot{\Pi}_{rot}^{con} := \dot{\Pi}_{rot} + \int_{\mathscr{B}_0} \frac{\partial \Psi_K}{\partial \vec{K}_t} : \dot{\vec{K}}_t \, dV - \int_{\mathscr{B}_0} \tilde{\vec{S}}_{K_t} : \left[\dot{\vec{K}}_t - \overline{F_t^T G}_{\alpha_t}\right] dV$$
Path-independence with non-linear stress (material non-linearity)  

$$\dot{\Pi}_{rot}^{ext}(\dot{\alpha}_t, \dot{K}_t) := \int_{\partial_W} \bar{\vec{W}}(t) \cdot \dot{\alpha} \, dA + \int_{\mathscr{B}_0} \bar{\vec{S}}_K(t) : \dot{\vec{K}}_t \, dV$$
Modified/additional weak forms in the quasi-static case  

$$\int_{t_n}^{t_{n+1}} \int_{\mathscr{B}_0} \left[F_t \tilde{\vec{S}}_t + G_{\alpha_t} \tilde{\vec{S}}_{K_t}^T + \tilde{\tau}_{skw}^T : \mathbb{I}^{skw} \cdot F_t^{-T}\right] : \operatorname{Grad}[\delta_* \dot{\varphi}_t] \, dV \, dt = \int_{t_n}^{t_{n+1}} \int_{\partial_T \mathcal{B}_0} \bar{T}(t) \cdot \delta_* \dot{\varphi}_t \, dA \, dt$$

$$\int_{t_n}^{t_{n+1}} \int_{\mathscr{B}_0} \delta_* \dot{\vec{K}}_t : \left[\frac{\partial \Psi_K}{\partial \vec{K}_t} + \bar{\vec{S}}_K(t) - \tilde{\vec{S}}_{K_t}\right] \, dV \, dt = 0 = \int_{t_n}^{t_{n+1}} \int_{\mathscr{B}_0} \delta_* \tilde{\vec{S}}_{K_t} : \left[\dot{\vec{K}}_t - \overline{F_t^T G}_{\alpha_t}\right] \, dV \, dt$$

$$\int_{t_n}^{t_{n+1}} \int_{\mathscr{B}_0} F_t \tilde{\vec{S}}_{K_t} : \operatorname{Grad}[\delta_* \dot{\alpha}_t] \, dV \, dt + \int_{t_n}^{t_{n+1}} \int_{\widetilde{\mathcal{B}}_0} \tilde{\vec{T}}_{skw} : \epsilon \cdot \delta_* \dot{\alpha}_t \, dV \, dt = \int_{t_n}^{t_{n+1}} \int_{\partial w} \bar{\vec{W}}(t) \cdot \delta_* \dot{\alpha}_t \, dA \, dt$$
Material and two-point stress tensors

 $\boldsymbol{\tau}_{K}^{T} := \boldsymbol{F} \boldsymbol{N}_{K}^{T} \quad \boldsymbol{\mu}_{K} := \boldsymbol{P}_{K} \boldsymbol{F}^{T}$ 

$$oldsymbol{S}_K := rac{\partial arPsi_K}{\partial oldsymbol{K}} \quad oldsymbol{N}_K := oldsymbol{G}_lpha oldsymbol{S}_K^T \quad oldsymbol{P}_K := oldsymbol{F} oldsymbol{S}_K$$



# Path-independence couple stress approximation

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Path-independence relation for local rotations  

$$\Psi_{K}(\tilde{K}_{t_{n+1}}) - \Psi_{K}(\tilde{K}_{t_{n}}) = \int_{t_{n}}^{t_{n+1}} \dot{\Psi}_{K}(\tilde{K}_{t}) dt \equiv \int_{0}^{1} \overset{\circ}{\Psi}_{K}(\tilde{K}_{\alpha}) d\alpha$$
Separate constrained variational problem for 'system input'  $\bar{S}_{K}(\alpha)$   

$$\mathcal{F}_{K}(\bar{S}_{K}(\alpha), \lambda_{K}) := \lambda_{K} \mathcal{G}_{K}(\bar{S}_{K}(\alpha)) + \int_{0}^{1} F_{K}(\bar{S}_{K}(\alpha)) d\alpha \stackrel{!}{=} \text{extr}$$
Path independence relation as local stress constraint  

$$\mathcal{G}_{K}(\bar{S}_{K}(\alpha)) := \Psi_{K}(\tilde{K}_{t_{n+1}}) - \Psi_{K}(\tilde{K}_{t_{n}}) - \int_{0}^{1} \left[ \bar{S}_{K}(\alpha) + \frac{\partial \Psi_{K}(\tilde{K}_{\alpha})}{\partial \tilde{K}_{\alpha}} \right] : \mathring{K}_{\alpha}^{\circ} d\alpha$$
Minimization function  

$$F_{K}(\bar{S}_{K}(\alpha)) := \frac{1}{2} g \, \bar{\mu}_{K} : \bar{\mu}_{K} g \equiv \frac{1}{2} C_{\alpha} \, \bar{S}_{K}(\alpha) : \bar{S}_{K}(\alpha) C_{\alpha}$$
Algorithmic couple stress tensor  

$$\bar{S}_{K}(\alpha) := \lambda_{K} \, \tilde{C}_{\alpha}^{-1} \, \mathring{K}_{\alpha} \, \tilde{C}_{\alpha}^{-1}$$

$$\lambda_{K} = \frac{\mathcal{G}_{K}(O)}{1 - 1^{\frac{2}{2}} - \frac{2}{2}} \sum_{\alpha = 1}^{2} - \frac{1}{2} \sum_{\alpha = 1}^{2} -$$

 $\int_{\alpha} \tilde{\boldsymbol{C}}_{\alpha}^{-1} \, \check{\boldsymbol{K}}_{\alpha} : \check{\boldsymbol{K}}_{\alpha} \, \tilde{\boldsymbol{C}}_{\alpha}^{-1} \, \mathrm{d}\alpha$ 



# Dynamical formulation with inertia effects

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Total energy with kinetic energy from local rotations  $\mathcal{H} := \mathcal{T}^{\mathrm{tra}} + \mathcal{T}^{\mathrm{rot}} + \Pi^{\mathrm{int}}$ Total kinetic energy Translational kinetic energy  $\mathcal{T}^{\mathrm{tra}}(\dot{\boldsymbol{\varphi}}, \boldsymbol{v}, \boldsymbol{p}) := \frac{1}{2} \int_{\mathscr{M}} \boldsymbol{v} \cdot \left[ \rho_0 \, \boldsymbol{I} \right] \boldsymbol{v} \, \mathrm{d}V - \int_{\mathscr{M}} \left[ \boldsymbol{v} - \dot{\boldsymbol{\varphi}} \right] \cdot \boldsymbol{p} \, \mathrm{d}V$ 2 Rotational kinetic energy  $\mathcal{T}^{\mathrm{rot}}(\dot{\boldsymbol{lpha}}, \boldsymbol{\omega}, \boldsymbol{\pi}) := rac{1}{2} \int_{\mathscr{R}} \boldsymbol{\omega} \cdot \boldsymbol{J} \boldsymbol{\omega} \, \mathrm{d}V - \int_{\mathscr{R}} [\boldsymbol{\omega} - \dot{\boldsymbol{lpha}}] \cdot \boldsymbol{\pi} \, \mathrm{d}V$ 

## **RVE with roving** Inertia density tensor of a roving (cf. Zhilin [2000]) Inertia density in the RVE coordinate system $J = J_F a_0 \otimes a_0 + J_1 a_1 \otimes a_1 + J_2 a_2 \otimes a_2$ Transverse isotropy $(J_1 = J_2 =: \rho_0 (l_0)^2)$ $\boxed{J = \rho_0 (l_F)^2 A_0 + \rho_0 (l_0)^2 [I - A_0]}$ $a_1 \otimes a_1 + a_2 \otimes a_2 = I - A_0$ $J_F := \rho_0 (l_F)^2$



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Turbomolecular pump rotor under dynamic loads (Boundary and initial conditions I; 121-em with H8-mixed-Bbar)

## Boundary conditions on the top side



## Dirichlet and Neumann boundaries on the top side

Yellow patches: cooling with fixed temperature  $\Theta = \Theta_{\infty} = 298.15$ Green patches: insulation  $\bar{Q}^A := 0$  and torque load  $W_z^A = -\hat{W}^A(t)$ 



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Turbomolecular pump rotor under dynamic loads (Boundary and initial conditions II; 121-em with H8-mixed-Bbar)

Boundary conditions on the bottom side



## Dirichlet and Neumann boundaries on the bottom side

#### Initial conditions

$$\boldsymbol{\omega}_0^A = \boldsymbol{X}^A \quad \boldsymbol{\alpha}_0^A = \boldsymbol{0} \quad \boldsymbol{v}_0^A = \boldsymbol{0} \quad \boldsymbol{\omega}_0^A = \boldsymbol{0} \quad \boldsymbol{\Theta}_0^A = \boldsymbol{\Theta}_{\infty} \quad \boldsymbol{\eta}_0^A = \boldsymbol{0} \quad \boldsymbol{\tau}_{\mathrm{skw}}^A = \boldsymbol{O}$$



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Turbomolecular pump rotor under dynamic loads (Roving distribution; 121-em with H8-mixed-Bbar)

Roving direction field at Gauss points in space



#### Roving direction fields

Rotor blades: two layers with diagonal rovings (crossed) Rotor hub : rovings in tangential direction (see motivation)



## Turbomolecular pump rotor under dynamic loads (Loads and generalized reactions; 121-em with H8-mixed-Bbar)

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0

1

Time [s]

Time evolutions of applied loads and generalized reactions 20 70 ocity [1/s] E Neumann heat load [kW/sqm] 15 Dirichlet reaction Dirichlet 0 n 1 2 3 0 1 2 3 Time [s] Time [s]  $\times 10^{6}$ 3 2 Dirichlet boundary heat flux [J/Ks] entropy [kJ/K] Neumann traction load [kN/sqm] Neumann pressure load [kN/sqm] 0.5 0.5 boundary -3 Dirichlet -0.5 -0.5 -4 -5 -1 2 3

n

1

2

Time [s]

3



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Turbomolecular pump rotor under dynamic loads (Current configurations I; 121-em with H8-mixed-Bbar)

Movie of simulated motion with circumferential elongation as color



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Turbomolecular pump rotor under dynamic loads (Current configurations II; 121-em with H8-mixed-Bbar)

Current temperature and heat load arrows at  $t_n = 3.0 \,\mathrm{s}$ 





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Turbomolecular pump rotor under dynamic loads (Current configurations III; 121-em with H8-mixed-Bbar)

Rate of roving bending and torque load arrows at  $t_n = 2.2 \,\mathrm{s}$ 





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Turbomolecular pump rotor under dynamic loads (Current configurations IV; 121-em with H8-mixed-Bbar)

Twist rate of roving and pressure load arrows at  $t_n = 2.2\,\mathrm{s}$ 





# Turbomolecular pump rotor under dynamic loads (Time evolutions I; 121-em with H8-mixed-Bbar)

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## Solutions over time at space node A=295





# Turbomolecular pump rotor under dynamic loads (Time evolutions II; 121-em with H8-mixed-Bbar)

Post-processing

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Fotal/Kinetic

4

0

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### Energies and momenta over time













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# Turbomolecular pump rotor under dynamic loads (Time evolutions III; 121-em with H8-mixed-Bbar)

### Mechanical balance laws over time





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Motivation:

- Dynamic finite element simulations of fiber roving composites
- Extension of transverse isotropy with length scale parameters
- Goals: FE simulations which
  - take into account the roving diameter and spacing,
  - roving stiffness with respect to curvature and twist.
- Strategy:
  - Introduction of a mixed field for the gradient of rotation
  - Discretization by using a mixed principle of virtual power
- Important results: Length scales for
  - roving diameter/spacing in the kinetic energy density
  - roving torsional/flexural stiffness in the strain energy
- Next steps:
  - Implementation of algorithms for virtual parameter identification
  - Identification of length scale parameters using mesoscale models