# Energy-momentum time integration of gradient-based models for fiber-bending stiffness in anisotropic thermo-mechanical continua

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# Motivation

- Dynamic simulations of fiber-reinforced materials in lightweight structures
- Keywords:
  - Nearly-incompressible material behavior
  - Thermo-elastic material behavior
  - Anisotropic material behavior
    - Fiber stretch stiffness
    - Fiber bending stiffness
  - Long term simulations
- Solution strategy:
  1. Extend the Cauchy-Boltzmann continuum by higher order gradients to capture fiber bending stiffness
  2. Mixed finite elements to reduce locking effects
  3. Extension to a thermo-mechanical coupling
  4. Higher-order energy-momentum conserving time integrator for stable and accurate dynamic simulations

## Continuum mechanics and material formulation

- Strain energy function (thermoelastic matrix part $\Psi_\mathrm{M}$, thermoelastic fiber part $\Psi_\mathrm{F}$ and the higher order gradient part $\Psi^\mathrm{X}_\mathrm{HOG}$)
$$\Psi(\boldsymbol{C}, \Theta, \boldsymbol{a}_0) = \Psi_\mathrm{M}(\boldsymbol{C}, \Theta) + \Psi_\mathrm{F}(\boldsymbol{C}, \Theta, \boldsymbol{a}_0) + \Psi^\mathrm{X}_\mathrm{HOG}(\dots, \boldsymbol{a}_0)$$
$\boldsymbol{C}$ - right Cauchy-Green tensor, $\Theta$ - absolute temperature, $\boldsymbol{a}_0$ - fiber direction
- Components and specific dependencies ($J(\boldsymbol{C}) = \sqrt{\det[\boldsymbol{C}]}$)
$$\Psi_\mathrm{M}(\boldsymbol{C}, J, \Theta) = \Psi^\mathrm{iso}_\mathrm{M}(\boldsymbol{C}, J) + \Psi^\mathrm{vol}_\mathrm{M}(J) + \Psi^\mathrm{cap}_\mathrm{M}(\Theta) + \Psi^\mathrm{coup}_\mathrm{M}(\Theta, J)$$
$$\Psi_\mathrm{F}(\boldsymbol{C}, \Theta, \boldsymbol{a}_0) = \Psi^\mathrm{ela}_\mathrm{F}(\boldsymbol{C}, \boldsymbol{a}_0) + \Psi^\mathrm{cap}_\mathrm{F}(\Theta) + \Psi^\mathrm{coup}_\mathrm{F}(\Theta, \boldsymbol{C}, \boldsymbol{a}_0)$$
- Thermo-mechanical coupling [Groß 18] with $\boldsymbol{M} = \boldsymbol{a}_0 \otimes \boldsymbol{a}_0$
$$\Psi^\mathrm{coup}_\mathrm{M} = -2 n_\mathrm{dim} \beta_\mathrm{M} (\Theta - \Theta_\infty) J \frac{\partial \Psi^\mathrm{vol}_\mathrm{M}(J)}{\partial J} \qquad \Psi^\mathrm{coup}_\mathrm{F} = -2 \beta_\mathrm{F} (\Theta - \Theta_\infty) \sqrt{I_4} \frac{\partial \Psi^\mathrm{ela}_\mathrm{F}(I_4 \dots)}{\partial I_4}$$
$\Theta_\infty$ - ambient temperature, $I_4 = \mathrm{tr}[\boldsymbol{C}\boldsymbol{M}]$
- Polyconvex material formulation for the hyperelastic parts

## Higher order gradient part $\Psi^{\mathrm{F}}_{\mathrm{HOG}}$ regarding $\boldsymbol{F}$ [Asmanoglo 17]

- Referential Representation: $\boldsymbol{\Lambda}^{\mathrm{F}}(\boldsymbol{F}, \nabla\boldsymbol{F}) = \boldsymbol{F}^T \cdot \boldsymbol{a}_0 \cdot \nabla\boldsymbol{F}^T \; \boldsymbol{\kappa}^{\mathrm{F}}_0 = \boldsymbol{\Lambda}^{\mathrm{F}} \cdot \boldsymbol{a}_0$
- Invariants given by
$$I^{\mathrm{F}}_6(\boldsymbol{F}, \nabla\boldsymbol{F}) = \boldsymbol{\kappa}^{\mathrm{F}}_0 \cdot \boldsymbol{\kappa}^{\mathrm{F}}_0 \qquad I^{\mathrm{F}}_7(\boldsymbol{F}, \nabla\boldsymbol{F}, \boldsymbol{C}) = \boldsymbol{\kappa}^{\mathrm{F}}_0 \cdot \boldsymbol{C} \cdot \boldsymbol{\kappa}^{\mathrm{F}}_0$$
- Dependencies
$$\Psi^{\mathrm{F}}_{\mathrm{HOG}}(\boldsymbol{\Lambda}^{\mathrm{F}}, \boldsymbol{C}, \boldsymbol{a}_0) = \hat{f}(I^{\mathrm{F}}_6(\boldsymbol{\Lambda}^{\mathrm{F}}), I^{\mathrm{F}}_7(\boldsymbol{\Lambda}^{\mathrm{F}}, \boldsymbol{C}))$$

## Higher order gradient part $\Psi^{\mathrm{C}}_{\mathrm{HOG}}$ regarding $\boldsymbol{C}$ [Ferretti 14]

- Sixth Invariant: $I^{C}_6(\nabla\boldsymbol{C}) = (\boldsymbol{a}_0 \cdot \nabla\boldsymbol{C} \cdot \boldsymbol{a}_0) \cdot (\boldsymbol{a}_0 \cdot \nabla\boldsymbol{C} \cdot \boldsymbol{a}_0)$
- Set $\boldsymbol{\Lambda}^{\mathrm{C}}(\nabla\boldsymbol{C}) = \boldsymbol{a}_0 \cdot \nabla\boldsymbol{C}$ and $\boldsymbol{\kappa}^{\mathrm{C}}_0 = \boldsymbol{\Lambda}^{\mathrm{C}} \cdot \boldsymbol{a}_0$
- Invariants given by
$$I^{\mathrm{C}}_6(\nabla\boldsymbol{C}) = \boldsymbol{\kappa}^{\mathrm{C}}_0 \cdot \boldsymbol{\kappa}^{\mathrm{C}}_0 \qquad I^{\mathrm{C}}_7(\boldsymbol{C}, \nabla\boldsymbol{C}) = \boldsymbol{\kappa}^{\mathrm{C}}_0 \cdot \boldsymbol{C} \cdot \boldsymbol{\kappa}^{\mathrm{C}}_0$$
- Dependencies
$$\Psi^{\mathrm{C}}_{\mathrm{HOG}}(\boldsymbol{\Lambda}^{\mathrm{C}}, \boldsymbol{C}, \boldsymbol{a}_0) = \hat{f}(I^{\mathrm{C}}_6(\boldsymbol{\Lambda}^{\mathrm{C}}), I^{\mathrm{C}}_7(\boldsymbol{\Lambda}^{\mathrm{C}}, \boldsymbol{C}))$$

## Total internal energy $\Pi^{\text{int}}$ for the mixed principle of virtual power [Groß 18]

$$\begin{aligned}\Pi^{\text{int}} = &\int_{\mathcal{B}_0} \Psi_{\mathrm{M}}(\tilde{\boldsymbol{C}}, \tilde{J}, \Theta)\mathrm{d}V + \int_{\mathcal{B}_0} \Psi_{\mathrm{F}}(\tilde{\boldsymbol{C}}_A, \Theta, \boldsymbol{a}_0)\mathrm{d}V + \int_{\mathcal{B}_0} \frac{1}{2}\boldsymbol{S} : (\boldsymbol{C}(\boldsymbol{q}) - \tilde{\boldsymbol{C}})\mathrm{d}V + \int_{\mathcal{B}_0} \tilde{\boldsymbol{S}} : \tilde{\boldsymbol{C}}\mathrm{d}V \\ &+ \int_{\mathcal{B}_0} \eta\,(\Theta - \tilde{\Theta})\mathrm{d}V + \int_{\mathcal{B}_0} \Psi^{\mathrm{X}}_{\mathrm{HOG}}(\boldsymbol{\Lambda}^{\mathrm{X}}(\dots), \tilde{\boldsymbol{C}}_A, \boldsymbol{a}_0)\mathrm{d}V + \Pi^{\mathrm{X}}_{\mathrm{HOG}} + \int_{\mathcal{B}_0} \tilde{\boldsymbol{H}} : \tilde{\boldsymbol{\Lambda}}\mathrm{d}V \\ &+ \int_{\mathcal{B}_0} p\,(J(\tilde{\boldsymbol{C}}) - \tilde{J})\mathrm{d}V + \int_{\mathcal{B}_0} \tilde{p}\tilde{J}\mathrm{d}V + \int_{\mathcal{B}_0} \frac{1}{2}\boldsymbol{S}_A : (\tilde{\boldsymbol{C}} - \tilde{\boldsymbol{C}}_A)\mathrm{d}V + \int_{\mathcal{B}_0} \tilde{\boldsymbol{S}}_A : \tilde{\boldsymbol{C}}_A\mathrm{d}V\end{aligned}$$

- Independent mixed field $\tilde{\boldsymbol{C}}$ and corresponding Lagrangian multiplier $\boldsymbol{S}$
- Assumed temperature field $\tilde{\Theta}$ and the entropy density field $\eta$
- Superimposed stress tensor $\tilde{\boldsymbol{S}}$ to derive energy–momentum scheme [Groß 18]
- Independent mixed fields for the volumetric dilatation $\tilde{J}$ and $\tilde{\boldsymbol{C}}_A$ for the anisotropic part of the strain energy function [Simo 85] [Schr 16]

## Internal energy for $\Pi^{\mathrm{F}}_{\mathrm{HOG}}$ regarding $\boldsymbol{F}$

$$\Pi^{\mathrm{F}}_{\mathrm{HOG}} = \int_{\mathcal{B}_0} \tilde{\boldsymbol{P}} : (\boldsymbol{F}(\boldsymbol{q}) - \tilde{\boldsymbol{F}})\mathrm{d}V + \int_{\mathcal{B}_0} \boldsymbol{B} \odot_3 (\nabla(\tilde{\boldsymbol{F}}) - \tilde{\boldsymbol{\Gamma}})\mathrm{d}V + \int_{\mathcal{B}_0} \boldsymbol{H} : (\boldsymbol{\Lambda}_{\mathrm{F}}(\tilde{\boldsymbol{F}}, \tilde{\boldsymbol{\Gamma}}) - \tilde{\boldsymbol{\Lambda}})\mathrm{d}V$$

- Independent mixed fields $\tilde{\boldsymbol{F}}$, $\tilde{\boldsymbol{\Gamma}}$ for $\boldsymbol{F}$, $\nabla(\boldsymbol{F})$ $\Big(\boldsymbol{\Lambda}_{\mathrm{F}}(\boldsymbol{F}, \nabla(\boldsymbol{F})) \rightarrow \boldsymbol{\Lambda}_{\mathrm{F}}(\tilde{\boldsymbol{F}}, \tilde{\boldsymbol{\Gamma}})\Big)$
- Independent mixed field $\tilde{\boldsymbol{\Lambda}}$ for $\boldsymbol{\Lambda}_{\mathrm{F}}(\tilde{\boldsymbol{F}}, \tilde{\boldsymbol{\Gamma}})$ and corresponding superimposed field $\tilde{\boldsymbol{H}}$ for energy–momentum scheme

## Internal energy for $\Pi^{\mathrm{C}}_{\mathrm{HOG}}$ regarding $\boldsymbol{C}$

$$\Pi^{\mathrm{C}}_{\mathrm{HOG}} = \int_{\mathcal{B}_0} \frac{1}{2} \boldsymbol{S}_G : (\boldsymbol{C}(\boldsymbol{q}) - \tilde{\boldsymbol{C}}_G) + \int_{\mathcal{B}_0} \boldsymbol{B} \odot_3 (\nabla(\tilde{\boldsymbol{C}}_G) - \tilde{\boldsymbol{\Gamma}})\mathrm{d}V + \int_{\mathcal{B}_0} \boldsymbol{H} : (\boldsymbol{\Lambda}_{\mathrm{C}}(\tilde{\boldsymbol{\Gamma}}) - \tilde{\boldsymbol{\Lambda}})\mathrm{d}V$$

- Independent mixed fields $\tilde{\boldsymbol{\Gamma}}$ for $\nabla(\tilde{\boldsymbol{C}}_G)$ $\Big(\boldsymbol{\Lambda}_{\mathrm{C}}(\nabla(\boldsymbol{C})) \rightarrow \boldsymbol{\Lambda}_{\mathrm{C}}(\tilde{\boldsymbol{\Gamma}})\Big)$
- Independent mixed field $\tilde{\boldsymbol{\Lambda}}$ for $\boldsymbol{\Lambda}_{\mathrm{C}}(\tilde{\boldsymbol{\Gamma}})$ and corresponding superimposed field $\tilde{\boldsymbol{H}}$ for energy–momentum scheme

## Superimposed fields

[Groß 18] [Groß 20]

$$\tilde{\boldsymbol{S}} = \frac{\tilde{\Psi}(1) - \tilde{\Psi}(0) - \int \frac{\partial \Psi_{\mathrm{M}}^{\mathrm{iso}}}{\partial \tilde{\boldsymbol{C}}} : \dot{\tilde{\boldsymbol{C}}} - \int \frac{\partial (\Psi_{\mathrm{M}}^{\mathrm{cap}} + \Psi_{\mathrm{F}}^{\mathrm{cap}})}{\partial \Theta} \dot{\Theta}}{\dot{\tilde{\boldsymbol{C}}} : \dot{\tilde{\boldsymbol{C}}}} \dot{\tilde{\boldsymbol{C}}}$$

$$\tilde{p} = \frac{\tilde{\Psi}(1) - \tilde{\Psi}(0) - \int \frac{\partial (\Psi_{\mathrm{M}}^{\mathrm{iso}} + \Psi_{\mathrm{M}}^{\mathrm{vol}})}{\partial \tilde{J}} \dot{\tilde{J}} - \int \frac{\partial \Psi_{\mathrm{M}}^{\mathrm{coup}}}{\partial \Theta} \dot{\Theta}}{\dot{\tilde{J}} \dot{\tilde{J}}} \dot{\tilde{J}}$$

$$\tilde{\boldsymbol{S}}_A = \frac{\tilde{\Psi}(1) - \tilde{\Psi}(0) - \int \frac{\partial (\Psi_{\mathrm{F}}^{\mathrm{ela}})}{\partial \tilde{\boldsymbol{C}}_A} : \dot{\tilde{\boldsymbol{C}}}_A - \int \frac{\partial \Psi_{\mathrm{F}}^{\mathrm{coup}}}{\partial \Theta} \dot{\Theta}}{\dot{\tilde{\boldsymbol{C}}}_A : \dot{\tilde{\boldsymbol{C}}}_A} \dot{\tilde{\boldsymbol{C}}}_A$$

$$\tilde{\boldsymbol{H}} = \frac{\tilde{\Psi}(1) - \tilde{\Psi}(0) - \int \frac{\partial \Psi_{\mathrm{HOG}}^{\mathrm{X}}}{\partial \tilde{\boldsymbol{\Lambda}}} : \dot{\tilde{\boldsymbol{\Lambda}}}}{\dot{\tilde{\boldsymbol{\Lambda}}} : \dot{\tilde{\boldsymbol{\Lambda}}}} \dot{\tilde{\boldsymbol{\Lambda}}}$$

## Mixed principle of virtual power $\dot{\mathcal{H}} = \dot{T} + \dot{\Pi}^{\mathrm{ext}} + \dot{\Pi}^{\mathrm{int}}$

- Kinetic power functional

$$\dot{T}(\dot{\boldsymbol{q}}, \dot{\boldsymbol{v}}, \dot{\boldsymbol{p}}) = \int_{\mathcal{B}_0} (\rho_0 \boldsymbol{v} - \boldsymbol{p}) \cdot \dot{\boldsymbol{v}} \mathrm{d}V + \int_{\mathcal{B}_0} \dot{\boldsymbol{p}} \cdot (\dot{\boldsymbol{q}} - \boldsymbol{v}) \mathrm{d}V + \int_{\mathcal{B}_0} \boldsymbol{p} \cdot \ddot{\boldsymbol{q}} \mathrm{d}V$$

- External power functional

$$\dot{\Pi}^{\text{ext}} = -\int_{\partial \mathcal{B}_0} \boldsymbol{\lambda}_q \cdot (\dot{\boldsymbol{q}} - \dot{\boldsymbol{q}}^{\text{ref}}) \mathrm{d}A - \int_{\mathcal{B}_0} \rho_0 \boldsymbol{g} \cdot \dot{\boldsymbol{q}} \mathrm{d}V + \int_{\mathcal{B}_0} \nabla \left( \frac{\tilde{\Theta}}{\Theta} \right) \cdot \boldsymbol{Q}$$

$$\boldsymbol{Q} = -\left[ J(\tilde{\boldsymbol{C}}_A) \frac{k_{\mathrm{F}} - k_{\mathrm{M}}}{\tilde{\boldsymbol{C}}_A : \boldsymbol{M}} \boldsymbol{M} + k J(\tilde{\boldsymbol{C}}) \tilde{\boldsymbol{C}}^{-1} \right] \nabla \Theta$$

- Variation with respect to the variables in the arguments of the total energy balance $\int_T \dot{\mathcal{H}} \mathrm{d}t = \int_T [\delta_* \dot{T} + \delta_* \dot{\Pi}^{\mathrm{ext}} + \delta_* \dot{\Pi}^{\mathrm{int}}] \mathrm{d}t = 0$ with the dependencies:

$$\dot{\mathcal{H}} = \dot{T}(\dot{\boldsymbol{q}}, \dot{\boldsymbol{v}}, \dot{\boldsymbol{p}}) + \dot{\Pi}^{\text{ext}}(\dot{\boldsymbol{q}}, \boldsymbol{\lambda}_q, \tilde{\Theta}, \dot{\Theta})$$

$$+ \dot{\Pi}^{\text{int}}(\dot{\boldsymbol{q}}, \tilde{\Theta}, \dot{\eta}, \dot{\tilde{\boldsymbol{C}}}, \dot{\tilde{J}}, \dot{\tilde{\boldsymbol{C}}}_A, \boldsymbol{S}, p, \boldsymbol{S}_A, \dot{\tilde{\boldsymbol{\Gamma}}}, \dot{\tilde{\boldsymbol{\Lambda}}}, \boldsymbol{B}, \boldsymbol{H}, \dots)$$

## Weak forms for both fomulations

$$\int_T \int_{\mathcal{B}_0} \left[\frac{1}{\rho_0}\boldsymbol{p} - \dot{\boldsymbol{q}}\right] \cdot \delta\dot{\boldsymbol{v}} \mathrm{d}V \mathrm{d}t = 0 \quad \int_T \int_{\partial\mathcal{B}_0} [-\boldsymbol{\lambda}_q] \cdot \delta\dot{\boldsymbol{q}} \mathrm{d}A \mathrm{d}t = 0 \quad \int_T \int_{\partial\mathcal{B}_0} \left[\dot{\tilde{\boldsymbol{q}}} - \dot{\boldsymbol{q}}^{\mathrm{ref}}(t)\right] \cdot \delta\boldsymbol{\lambda}_q \mathrm{d}A \mathrm{d}t = 0$$

$$\int_T \int_{\mathcal{B}_0} \left[\eta + \frac{\partial\Psi}{\partial\Theta}\right] \delta\dot{\Theta} \mathrm{d}V \mathrm{d}t = 0 \quad \int_T \int_{\mathcal{B}_0} \left[\frac{\mathrm{Div}[\boldsymbol{Q}]}{\Theta} + \dot{\eta}\right] \delta\tilde{\Theta} \mathrm{d}V \mathrm{d}t = 0$$

$$\int_T \int_{\mathcal{B}_0} \frac{1}{2}\left[\dot{\tilde{\boldsymbol{C}}} - \dot{\boldsymbol{C}}\right] : \delta\boldsymbol{S} \mathrm{d}V \mathrm{d}t = 0 \quad \int_T \int_{\mathcal{B}_0} \left[\Theta - \tilde{\Theta}\right] \delta\dot{\eta} \mathrm{d}V \mathrm{d}t = 0$$

$$\int_T \int_{\mathcal{B}_0} \left[\dot{\tilde{J}} - \dot{J}\right] \delta p \mathrm{d}V \mathrm{d}t = 0 \quad \int_T \int_{\mathcal{B}_0} \left[p - \left[\frac{\partial\Psi}{\partial\tilde{J}} + \tilde{p}\right]\right] \delta\dot{\tilde{J}} \mathrm{d}V \mathrm{d}t = 0$$

$$\int_T \int_{\mathcal{B}_0} \frac{1}{2}\left[\dot{\tilde{\boldsymbol{C}}}_A - \dot{\tilde{\boldsymbol{C}}}\right] : \delta\boldsymbol{S}_A \mathrm{d}V \mathrm{d}t = 0 \quad \int_T \int_{\mathcal{B}_0} \left[\frac{1}{2}\boldsymbol{S}_A - \left[\frac{\partial\Psi}{\partial\tilde{\boldsymbol{C}}_A} + \tilde{\boldsymbol{S}}_A\right]\right] : \delta\dot{\tilde{\boldsymbol{C}}}_A \mathrm{d}V \mathrm{d}t = 0$$

$$\int_T \int_{\mathcal{B}_0} \left[\frac{1}{2}\boldsymbol{S} - \left(\frac{\partial\Psi}{\partial\tilde{\boldsymbol{C}}} + \frac{p}{2J(\tilde{\boldsymbol{C}})}\mathrm{cof}[\tilde{\boldsymbol{C}}] + \frac{1}{2}\boldsymbol{S}_A + \tilde{\boldsymbol{S}}\right)\right] : \delta\dot{\tilde{\boldsymbol{C}}} \mathrm{d}V \mathrm{d}t = 0$$

$$\int_T \int_{\mathcal{B}_0} \left[\boldsymbol{\Lambda}^{\mathrm{X}}(\ldots) - \tilde{\boldsymbol{\Lambda}}\right] : \delta_*\boldsymbol{H} \mathrm{d}V \mathrm{d}t = 0 \quad \int_T \int_{\mathcal{B}_0} \left[\boldsymbol{H} - \left[\frac{\partial\Psi}{\partial\tilde{\Lambda}} + \tilde{\boldsymbol{H}}\right]\right] : \delta_*\dot{\tilde{\boldsymbol{\Lambda}}} \mathrm{d}V \mathrm{d}t = 0$$

$$\int_T \int_{\mathcal{B}_0} \left[\boldsymbol{B} - \boldsymbol{H} : \frac{\partial\boldsymbol{\Lambda}^{\mathrm{X}}}{\partial\dot{\tilde{\boldsymbol{\Gamma}}}}\right] \odot_3 \delta_*\dot{\tilde{\boldsymbol{\Gamma}}} \mathrm{d}V \mathrm{d}t = 0$$

## Weak forms of $\boldsymbol{F}$ fomulations

$$\int_T \int_{\mathcal{B}_0} \left[ \boldsymbol{S} : \frac{1}{2} \frac{\partial \dot{\boldsymbol{C}}}{\partial \dot{\boldsymbol{q}}} + \boldsymbol{P} : \frac{\partial \dot{\boldsymbol{F}}}{\partial \dot{\boldsymbol{q}}} - \dot{\boldsymbol{p}} \right] \cdot \delta_* \dot{\boldsymbol{q}} \mathrm{d}V \mathrm{d}t = 0 \qquad \int_T \int_{\mathcal{B}_0} \left[ \dot{\tilde{\boldsymbol{F}}} - \dot{\boldsymbol{F}} \right] : \delta_* \boldsymbol{P} \mathrm{d}V \mathrm{d}t = 0$$

$$\int_T \int_{\mathcal{B}_0} \left[ \boldsymbol{P} - \left( \boldsymbol{H} : \frac{\partial \boldsymbol{\Lambda}^{\mathrm{F}}}{\partial \dot{\tilde{\boldsymbol{F}}}} + \boldsymbol{B} \odot_3 \frac{\partial \nabla \dot{\tilde{\boldsymbol{F}}}}{\partial \dot{\tilde{\boldsymbol{F}}}} \right) \right] : \delta_* \dot{\tilde{\boldsymbol{F}}} \mathrm{d}V \mathrm{d}t \quad \int_T \int_{\mathcal{B}_0} \left[ \nabla(\dot{\tilde{\boldsymbol{F}}}) - \dot{\tilde{\boldsymbol{\Gamma}}} \right] \odot_3 \delta_* \boldsymbol{B} \mathrm{d}V \mathrm{d}t = 0$$

## Weak forms of $\boldsymbol{C}$ fomulations

$$\int_T \int_{\mathcal{B}_0} \left[ \boldsymbol{S} : \frac{1}{2} \frac{\partial \dot{\boldsymbol{C}}}{\partial \dot{\boldsymbol{q}}} + \boldsymbol{S}_G : \frac{1}{2} \frac{\partial \dot{\boldsymbol{C}}}{\partial \dot{\boldsymbol{q}}} - \dot{\boldsymbol{p}} \right] \cdot \delta_* \dot{\boldsymbol{q}} \mathrm{d}V \mathrm{d}t = 0 \qquad \int_T \int_{\mathcal{B}_0} \left[ \dot{\boldsymbol{C}} - \dot{\tilde{\boldsymbol{C}}}_G \right] : \delta_* \boldsymbol{S}_G \mathrm{d}V \mathrm{d}t = 0$$

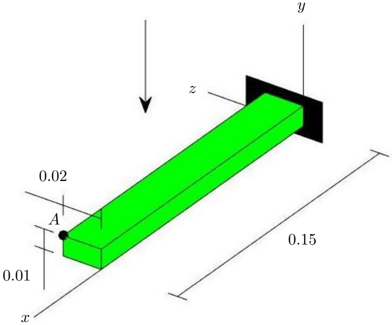
$$\int_T \int_{\mathcal{B}_0} \left[ \boldsymbol{S}_G - \boldsymbol{B} \odot_3 \frac{\partial \nabla \dot{\tilde{\boldsymbol{C}}}_G}{\partial \dot{\tilde{\boldsymbol{C}}}_G} \right] : \delta_* \dot{\tilde{\boldsymbol{C}}}_G \mathrm{d}V \mathrm{d}t \qquad \int_T \int_{\mathcal{B}_0} \left[ \nabla(\dot{\tilde{\boldsymbol{C}}}_G) - \dot{\tilde{\boldsymbol{\Gamma}}} \right] \odot_3 \delta_* \boldsymbol{B} \mathrm{d}V \mathrm{d}t = 0$$

## Angular momentum balance law regarding $\boldsymbol{F}$ formulation

$$\boldsymbol{\mathcal{J}}_{n+1} - \boldsymbol{\mathcal{J}}_n = \int_{t_n}^{t_n+1} \int_{\mathcal{B}_0} \left[ \left( \boldsymbol{H} : \frac{\partial \boldsymbol{\Lambda}^{\mathrm{F}}}{\partial \dot{\tilde{\boldsymbol{F}}}} + \boldsymbol{B} \odot_3 \frac{\partial \nabla \dot{\tilde{\boldsymbol{F}}}}{\partial \dot{\tilde{\boldsymbol{F}}}} \right) \times \tilde{\boldsymbol{F}} \right] \mathrm{d}V \mathrm{d}t + \int_{t_n}^{t_n+1} \int_{\partial \mathcal{B}_0} [\boldsymbol{q} \times \boldsymbol{\lambda}_q] \mathrm{d}A \mathrm{d}t + \int_{t_n}^{t_n+1} \int_{\mathcal{B}_0} [\boldsymbol{q} \times \rho_0 \boldsymbol{g}] \mathrm{d}V \mathrm{d}t$$

## Angular momentum balance law regarding $\boldsymbol{C}$ formulation

$$\boldsymbol{\mathcal{J}}_{n+1} - \boldsymbol{\mathcal{J}}_n = \int_{t_n}^{t_n+1} \int_{\mathcal{B}_0} \left[ \boldsymbol{B} \odot_3 \frac{\partial \nabla \dot{\tilde{\boldsymbol{C}}}_G}{\partial \dot{\tilde{\boldsymbol{C}}}_G} \times \tilde{\boldsymbol{F}} \right] \mathrm{d}V \mathrm{d}t + \int_{t_n}^{t_n+1} \int_{\partial \mathcal{B}_0} [\boldsymbol{q} \times \boldsymbol{\lambda}_q] \mathrm{d}A \mathrm{d}t + \int_{t_n}^{t_n+1} \int_{\mathcal{B}_0} [\boldsymbol{q} \times \rho_0 \boldsymbol{g}] \mathrm{d}V \mathrm{d}t$$

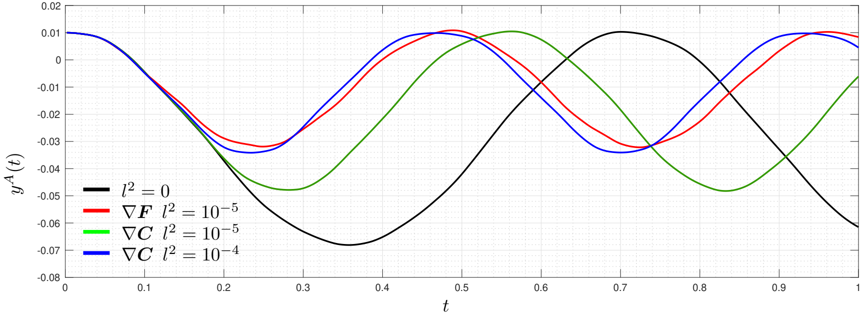



- Strain energy function of elastic matrix and fiber part

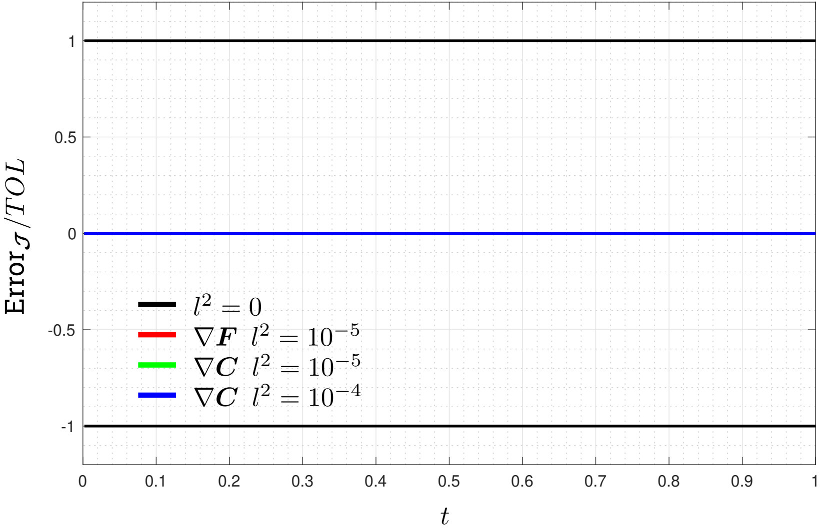
$$\Psi^{\mathrm{ISO}} = \frac{\epsilon_1}{2}(\mathrm{tr}[\boldsymbol{C}] - 3 - 2\ln(J)) \quad \Psi^{\mathrm{VOL}} = \frac{\epsilon_2}{2}\left(\ln(J)^2 + (J-1)^2\right) \quad \Psi_{\mathrm{F}}^{\mathrm{ela}} = \frac{\epsilon_3}{2}(\mathrm{tr}[\boldsymbol{CM}] - 1)^2$$

- Anisotropic direction $(\boldsymbol{a}_0)^T = [1\ 0\ 0]$
- $T = 1.0$, $h_n = 0.002$ and $g = [0\ \ -2\ 0]^T$
- Quadratic serendipity mesh (20 nodes) with $n_{el} = 24$
- Linear approximation for $\tilde{J}$ and constant approximation for $\tilde{C}_A$
- Introducing length scale $l^2$ with $c = \epsilon_1 l^2$ for material parameter of $\Psi_{\mathrm{HOG}}$
- Strain energy function of higher order gradient part $\Psi_{\mathrm{HOG}}^{\mathrm{X}} = l^2\left(I_6^{\mathrm{X}}\right)^2$

# Numerical example
## Trajectory $\epsilon_1 = 0.1e6 \quad \epsilon_2 = 100e6 \quad \epsilon_3 = 0$

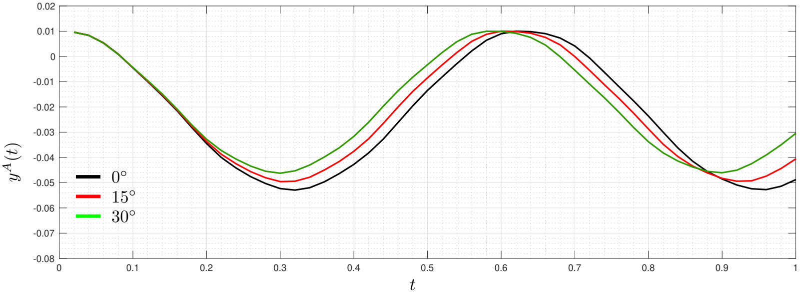


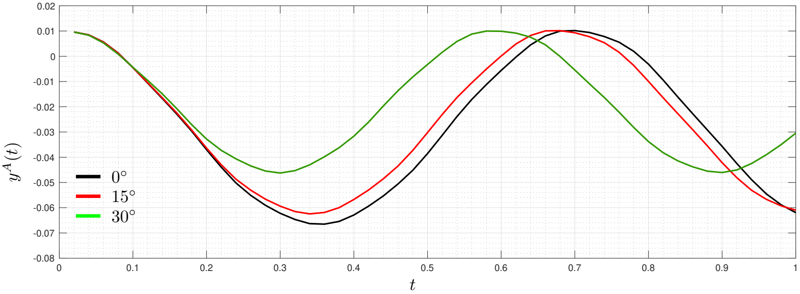
## Numerical example
## Angular momentum conservation $\epsilon_1 = 0.1e6$ $\epsilon_2 = 100e6$ $\epsilon_3 = 0$



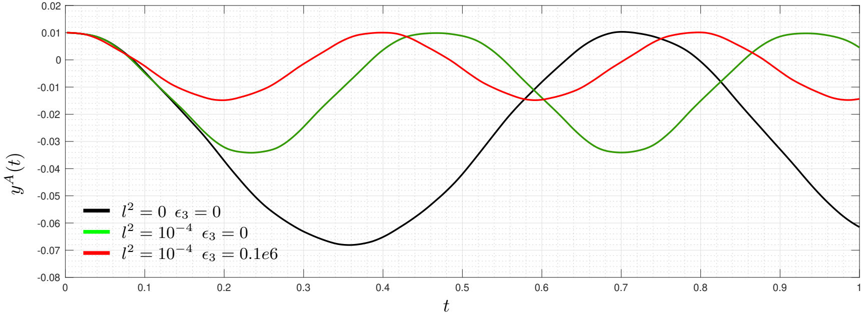
# Numerical example

## Trajectory for different fiber angles $\epsilon_1 = 0.1e6$ $\epsilon_2 = 100e6$ $\epsilon_3 = 0$



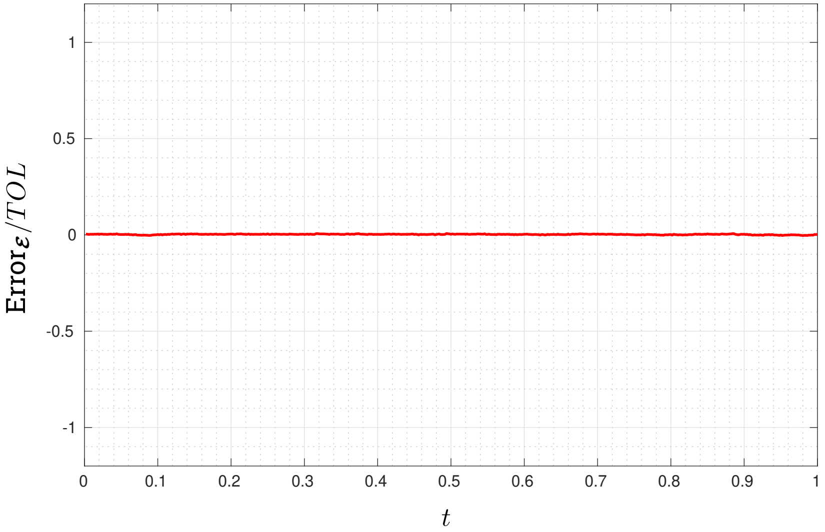



# Numerical example
## Trajectory for $\nabla C$ $\quad \epsilon_1 = 0.1e6 \qquad \epsilon_2 = 100e6$



# Numerical example

## Energy conservation $\epsilon_1 = 0.1e6 \quad \epsilon_2 = 100e6 \quad \epsilon_3 = 0.1e6 \quad l^2 = 10^{-4}$



# Conclusion

- Motivation:
  - Dynamic simulations of fiber-reinforced materials in light-weight structures
- Important results:
  - Higher-order gradients capture the fiber-bending stiffness
  - Achieve similar effects for a higher order gradient based material formulation expressd in terms of the right Cauchy-Green tensor
  - Higher-order energy-momentum time integrators conserve total energy
- Outlook:
  - Extension of the material formulation to a thermo-viscoelastic formulation
  - Investigation of locking effects
  - Formulate the superimposed field directly in terms of $\nabla C$ and thus achieve a fiber roving independence.

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