Dynamic Large Strain Formulation for Nematic Liquid Crystal Elastomers

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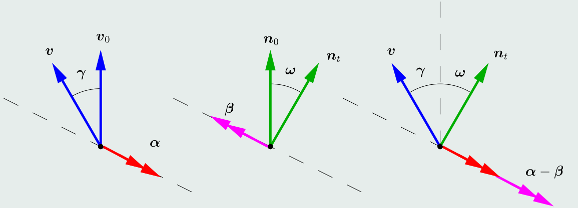
Introduction



motivated by [Warner and Terentjev (2007)]

- Orientation rate
  $\dot{\boldsymbol{\chi}} = \left(\dot{\boldsymbol{\alpha}} - \dot{\boldsymbol{\beta}}\right) \times \boldsymbol{\chi}$
- $\dot{\boldsymbol{\alpha}} = -\frac{1}{2}\boldsymbol{\epsilon} : \dot{\boldsymbol{F}}\boldsymbol{F}^{-1}$
- time evolution of $\boldsymbol{\beta}$ described as dissipative process

- distinct rotation degrees of freedom for the nematic director ($\boldsymbol{\beta}$) and the bulk elastomer ($\boldsymbol{\alpha}$), respectively
- distinct mappings for the deformation ($\boldsymbol{\varphi}$) of the bulk material and the orientation ($\boldsymbol{\chi}$) of the nematic director
- approach of widening the linear continuum theory [Warner and Terentjev (2007)] to large deformation and dynamic regime by considering invariants [Zheng (1994)] depending on $\boldsymbol{B}$, $\boldsymbol{n}_t$, $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$
- principle of virtual power for space-time discretization

Goals

- modeling the (isothermal) semisoft behavior of liquid crystal elastomer (LCE) films under dynamic stretch
- preserving mechanical balance laws, i.e. momentum and moment of momentum balances

Energy density formulation

cf. [De Gennes (1983), Anderson et al. (1999), Warner and Terentjev (2007)]

$$\psi = \underbrace{c_1\left(\boldsymbol{I}:\boldsymbol{C}-3-2\log(J)\right)+\frac{\lambda}{2}\left(\left[\log(J)\right]^2+(J-1)^2\right)+c_3\boldsymbol{n}_0\cdot\boldsymbol{C}\boldsymbol{n}_0}_{\text{elastic energy density}}$$

$$+\underbrace{c_3\left(\boldsymbol{I}:\left(\boldsymbol{n}_t\otimes\boldsymbol{n}_t\right)-1\right)+c_9\left|\boldsymbol{F}^T\boldsymbol{n}_t\right|^2+c_{10}\left(\boldsymbol{n}_0\cdot\boldsymbol{F}^T\boldsymbol{n}_t\right)^2}_{\text{translational interactive energy density}}$$

$$+\underbrace{\frac{c_{11}}{2}\operatorname{tr}\left[\boldsymbol{B}\boldsymbol{W}_{\alpha-\beta}\left(\boldsymbol{n}_t\otimes\boldsymbol{n}_t\right)\boldsymbol{W}_{\alpha-\beta}\right]+\frac{c_{12}}{2}\left[\left(\boldsymbol{\alpha}-\boldsymbol{\beta}\right)\times\boldsymbol{n}_t\right]^2}_{\text{rotational interactive energy density}}$$

- $\boldsymbol{W}_{\alpha-\beta}\boldsymbol{n}_t=\left[-\boldsymbol{\epsilon}\cdot(\boldsymbol{\alpha}-\boldsymbol{\beta})\right]\boldsymbol{n}_t=(\boldsymbol{\alpha}-\boldsymbol{\beta})\times\boldsymbol{n}_t$

Material parameters

cf. [Anderson et al. (1999), de Luca et al. (2013)]

- $c_1=\dfrac{\mu}{2}$
- $c_3=\dfrac{\mu\,(r-1)}{2}$
- $c_9=\dfrac{\mu}{2}\left(\dfrac{1}{r}-1\right)$
- $c_{10}=\dfrac{\mu}{2}\left(2-\dfrac{1}{r}-r\right)$
- $c_{11}=-0.05\mu$
- $c_{12}=0.05\mu$
- $\lambda=\dfrac{2}{3}\mu\left(\dfrac{1+\nu}{1-2\nu}-1\right)$
- $r=\dfrac{\ell_{\parallel}}{\ell_{\perp}}$

Translational interactive and nematic elastic energy density in the reference configuration

$$\psi\Big|_{\substack{\boldsymbol{C}=\boldsymbol{B}=\boldsymbol{I}\\ \boldsymbol{n}_t=\boldsymbol{n}_0}} =$$

$$= c_3\left[\boldsymbol{n}_0 \cdot \boldsymbol{C}\boldsymbol{n}_0 + \boldsymbol{I} : (\boldsymbol{n}_t \otimes \boldsymbol{n}_t) - 1\right] + c_9 \boldsymbol{B} : (\boldsymbol{n}_t \otimes \boldsymbol{n}_t) + c_{10}\left(\boldsymbol{n}_0 \boldsymbol{F}^T \boldsymbol{n}_t\right)^2\Big|_{\substack{\boldsymbol{C}=\boldsymbol{B}=\boldsymbol{I}\\ \boldsymbol{n}_t=\boldsymbol{n}_0}}$$

$$= \frac{\mu}{2}(r-1)\left[\boldsymbol{n}_0 \cdot \boldsymbol{n}_0 + \boldsymbol{n}_0 \cdot \boldsymbol{n}_0 - 1\right] + \frac{\mu}{2}\left(\frac{1}{r} - 1\right)\boldsymbol{n}_0 \cdot \boldsymbol{n}_0 + \frac{\mu}{2}\left(2 - \frac{1}{r} - r\right)(\boldsymbol{n}_0 \cdot \boldsymbol{n}_0)^2 = 0$$

1st Piola-Kirchhoff stress tensor

$$\frac{\partial \psi}{\partial \boldsymbol{F}}\Big|_{\substack{\boldsymbol{C}=\boldsymbol{B}=\boldsymbol{I}\\ \boldsymbol{n}_t=\boldsymbol{n}_0}} = 2c_3 \boldsymbol{F}(\boldsymbol{n}_0 \otimes \boldsymbol{n}_0) + 2c_9(\boldsymbol{n}_0 \otimes \boldsymbol{n}_0)\boldsymbol{F} + 2c_{10}\left(\boldsymbol{n}_0 \boldsymbol{F}^T \boldsymbol{n}_t\right)(\boldsymbol{n}_t \otimes \boldsymbol{n}_0)\Big|_{\substack{\boldsymbol{C}=\boldsymbol{B}=\boldsymbol{I}\\ \boldsymbol{n}_t=\boldsymbol{n}_0}}$$

$$= 2\frac{\mu}{2}(r-1)(\boldsymbol{n}_0 \otimes \boldsymbol{n}_0) + 2\frac{\mu}{2}\left(\frac{1}{r} - 1\right)(\boldsymbol{n}_0 \otimes \boldsymbol{n}_0)$$

$$+ 2\frac{\mu}{2}\left(2 - \frac{1}{r} - r\right)\boldsymbol{n}_0 \cdot \boldsymbol{n}_0 (\boldsymbol{n}_0 \otimes \boldsymbol{n}_0) = \boldsymbol{0}$$

Stress-free reference configuration

Translational interactive and nematic elastic energy density in the reference configuration

$$\psi\Big|_{\substack{\boldsymbol{C}=\boldsymbol{B}=\boldsymbol{I}\\ \boldsymbol{n}_t=\boldsymbol{n}_0}} =$$

$$= c_3\left[\boldsymbol{n}_0\cdot\boldsymbol{C}\boldsymbol{n}_0 + \boldsymbol{I} : (\boldsymbol{n}_t\otimes\boldsymbol{n}_t) - 1\right] + c_9\boldsymbol{B} : (\boldsymbol{n}_t\otimes\boldsymbol{n}_t) + c_{10}\left(\boldsymbol{n}_0\boldsymbol{F}^T\boldsymbol{n}_t\right)^2\Big|_{\substack{\boldsymbol{C}=\boldsymbol{B}=\boldsymbol{I}\\ \boldsymbol{n}_t=\boldsymbol{n}_0}}$$

$$= \frac{\mu}{2}(r-1)\left[\boldsymbol{n}_0\cdot\boldsymbol{n}_0 + \boldsymbol{n}_0\cdot\boldsymbol{n}_0 - 1\right] + \frac{\mu}{2}\left(\frac{1}{r}-1\right)\boldsymbol{n}_0\cdot\boldsymbol{n}_0 + \frac{\mu}{2}\left(2-\frac{1}{r}-r\right)(\boldsymbol{n}_0\cdot\boldsymbol{n}_0)^2 = 0$$

Stress vector work conjugated to $\boldsymbol{n}_t$

$$\frac{\partial\psi}{\partial\boldsymbol{n}_t}\Big|_{\substack{\boldsymbol{C}=\boldsymbol{B}=\boldsymbol{I}\\ \boldsymbol{n}_t=\boldsymbol{n}_0}} = 2c_3\boldsymbol{n}_t + 2c_9\boldsymbol{B}\boldsymbol{n}_t + 2c_{10}\left(\boldsymbol{n}_0\boldsymbol{F}^T\boldsymbol{n}_t\right)(\boldsymbol{F}\boldsymbol{n}_0)\Big|_{\substack{\boldsymbol{C}=\boldsymbol{B}=\boldsymbol{I}\\ \boldsymbol{n}_t=\boldsymbol{n}_0}}$$

$$= 2\frac{\mu}{2}(r-1)\boldsymbol{n}_0 + 2\frac{\mu}{2}\left(\frac{1}{r}-1\right)\boldsymbol{n}_0 + 2\frac{\mu}{2}\left(2-\frac{1}{r}-r\right)(\boldsymbol{n}_0\cdot\boldsymbol{n}_0)\boldsymbol{n}_0 = \boldsymbol{0}$$

Rotational interactive energy density in the reference configuration

$$\psi^{c_{11}}\Big|_{\substack{\boldsymbol{B}=\boldsymbol{I}\\ \boldsymbol{n}_t=\boldsymbol{n}_0\\ \boldsymbol{\alpha}=\boldsymbol{\beta}}} = \frac{c_{11}}{2}\operatorname{tr}\left[\boldsymbol{B}\boldsymbol{W}_{\alpha-\beta}\left(\boldsymbol{n}_t\otimes\boldsymbol{n}_t\right)\boldsymbol{W}_{\alpha-\beta}\right]\Big|_{\substack{\boldsymbol{B}=\boldsymbol{I}\\ \boldsymbol{n}_t=\boldsymbol{n}_0\\ \boldsymbol{\alpha}=\boldsymbol{\beta}}} = 0$$

$$\psi^{c_{12}}\Big|_{\substack{\boldsymbol{n}_t=\boldsymbol{n}_0\\ \boldsymbol{\alpha}=\boldsymbol{\beta}}} = \frac{c_{12}}{2}\left[(\boldsymbol{\alpha}-\boldsymbol{\beta})\times\boldsymbol{n}_t\right]^2\Big|_{\substack{\boldsymbol{n}_t=\boldsymbol{n}_0\\ \boldsymbol{\alpha}=\boldsymbol{\beta}}} = 0$$

- $\boldsymbol{W}_{\alpha-\beta}\big|_{\boldsymbol{\alpha}=\boldsymbol{\beta}} = [-\boldsymbol{\epsilon}\cdot(\boldsymbol{\beta}-\boldsymbol{\beta})] = \boldsymbol{0}$

Stress tensor and vectors work conjugated to $\boldsymbol{F}$, $\boldsymbol{n}_t$, $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ for $\psi^{c_{11}}$

$$\frac{\partial\psi^{c_{11}}}{\partial\boldsymbol{F}}\Big|_{\substack{\boldsymbol{B}=\boldsymbol{I}\\ \boldsymbol{n}_t=\boldsymbol{n}_0\\ \boldsymbol{\alpha}=\boldsymbol{\beta}}} = c_{11}\boldsymbol{W}_{\alpha-\beta}\left(\boldsymbol{n}_t\otimes\boldsymbol{n}_t\right)\boldsymbol{W}_{\alpha-\beta}\boldsymbol{F}\Big|_{\substack{\boldsymbol{B}=\boldsymbol{I}\\ \boldsymbol{n}_t=\boldsymbol{n}_0\\ \boldsymbol{\alpha}=\boldsymbol{\beta}}} = \boldsymbol{0}$$

$$\frac{\partial\psi^{c_{11}}}{\partial\boldsymbol{n}_t}\Big|_{\substack{\boldsymbol{B}=\boldsymbol{I}\\ \boldsymbol{n}_t=\boldsymbol{n}_0\\ \boldsymbol{\alpha}=\boldsymbol{\beta}}} = c_{11}\boldsymbol{W}_{\alpha-\beta}\boldsymbol{B}\boldsymbol{W}_{\alpha-\beta}\boldsymbol{n}_t\Big|_{\substack{\boldsymbol{B}=\boldsymbol{I}\\ \boldsymbol{n}_t=\boldsymbol{n}_0\\ \boldsymbol{\alpha}=\boldsymbol{\beta}}} = \boldsymbol{0}$$

$$\frac{\partial\psi^{c_{11}}}{\partial\boldsymbol{\alpha}}\Big|_{\substack{\boldsymbol{B}=\boldsymbol{I}\\ \boldsymbol{n}_t=\boldsymbol{n}_0\\ \boldsymbol{\alpha}=\boldsymbol{\beta}}} = -\frac{\partial\psi^{c_{11}}}{\partial\boldsymbol{\beta}}\Big|_{\substack{\boldsymbol{B}=\boldsymbol{I}\\ \boldsymbol{n}_t=\boldsymbol{n}_0\\ \boldsymbol{\alpha}=\boldsymbol{\beta}}} = c_{11}\left(\boldsymbol{\epsilon}\cdot\boldsymbol{n}_t\right)\boldsymbol{B}\left[(\boldsymbol{\epsilon}\cdot\boldsymbol{\beta})-(\boldsymbol{\epsilon}\cdot\boldsymbol{\alpha})\right]\boldsymbol{n}_t\Big|_{\substack{\boldsymbol{B}=\boldsymbol{I}\\ \boldsymbol{n}_t=\boldsymbol{n}_0\\ \boldsymbol{\alpha}=\boldsymbol{\beta}}} = \boldsymbol{0}$$

- as quadratic function of $(\boldsymbol{\alpha}-\boldsymbol{\beta})$, the condition is also fulfilled for $\psi^{c_{12}}$

Dissipative process for β

cf. [Oates and Wang (2009), Groß et al. (2023)]

- Clausius-Planck inequality
  - $\left(\boldsymbol{N} - \frac{\partial \psi}{\partial \boldsymbol{F}}\right) : \dot{\boldsymbol{F}} + \boldsymbol{\eta} \cdot \dot{\boldsymbol{\chi}} - \frac{\partial \psi}{\partial \boldsymbol{\chi}} \cdot \dot{\boldsymbol{\chi}} - \frac{\partial \psi}{\partial \boldsymbol{\alpha}} \cdot \dot{\boldsymbol{\alpha}} - \frac{\partial \psi}{\partial \boldsymbol{\beta}} \cdot \dot{\boldsymbol{\beta}} \geq 0$
- Continuum rotation mapping of the bulk elastomer
  - $\dot{\boldsymbol{\alpha}} = -\frac{1}{2}\boldsymbol{\epsilon} : \dot{\boldsymbol{F}}\boldsymbol{F}^{-1}$
- Coleman-Noll procedure
  - $\boldsymbol{N} = \frac{\partial \psi}{\partial \boldsymbol{F}} - \frac{1}{2}\frac{\partial \psi}{\partial \boldsymbol{\alpha}} \cdot \boldsymbol{\epsilon} \cdot \boldsymbol{F}^{-T}$
  - $\boldsymbol{\eta} = \frac{\partial \psi}{\partial \boldsymbol{\chi}}$
- Dissipation inequality

$$\mathcal{D}^{\text{int}} = -\frac{\partial \psi}{\partial \boldsymbol{\beta}} \cdot \dot{\boldsymbol{\beta}} \geq 0$$

$\mathcal{D}^{\text{int}} \stackrel{!}{=} \boldsymbol{\Sigma}_\beta \cdot \dot{\boldsymbol{\beta}}$ with $\boldsymbol{\Sigma}_\beta = V_\beta \dot{\boldsymbol{\beta}}$

Principle of virtual power

$$\delta_* \dot{\mathcal{T}}(\dot{\boldsymbol{\varphi}}, \dot{\mathbf{v}}, \dot{\mathbf{p}}) + \delta_* \dot{\mathcal{T}}_n(\dot{\boldsymbol{\chi}}, \dot{\mathbf{v}}_\chi, \dot{\mathbf{p}}_\chi) + \delta_* \dot{\Pi}^{\text{ext}}(\dot{\boldsymbol{\varphi}}, \boldsymbol{R}) + \delta_* \dot{\Pi}_n^{\text{ext}}(\dot{\boldsymbol{\chi}}) + \delta_* \dot{\Pi}^{\text{int}}\left(\dot{\boldsymbol{\varphi}}, \dot{\boldsymbol{\chi}}, \dot{\boldsymbol{\alpha}}, \dot{\boldsymbol{\beta}}, \boldsymbol{\tau}_\chi, \boldsymbol{w}_\tau\right) := 0$$

External deformational and orientational power

cf. [Anderson et al. (1999)]

- Functional of the external deformational power

$$\dot{\Pi}^{\text{ext}}(\dot{\boldsymbol{\varphi}}, \boldsymbol{R}) := -\int_{\mathscr{B}_0} \rho_0 \boldsymbol{B}_\varphi \cdot \dot{\boldsymbol{\varphi}} \, \mathrm{d}V - \int_{\partial_T \mathscr{B}_0} \boldsymbol{T} \cdot \dot{\boldsymbol{\varphi}} \, \mathrm{d}A - \int_{\partial_\varphi \mathscr{B}_0} \boldsymbol{R} \cdot \left(\dot{\boldsymbol{\varphi}} - \dot{\bar{\boldsymbol{\varphi}}}\right) \mathrm{d}A$$

- Virtual external deformational power

$$\delta_* \dot{\Pi}^{\text{ext}}(\dot{\boldsymbol{\varphi}}, \boldsymbol{R}) := -\int_{\mathscr{B}_0} \rho_0 \boldsymbol{B}_\varphi \cdot \delta_* \dot{\boldsymbol{\varphi}} \, \mathrm{d}V - \int_{\partial_T \mathscr{B}_0} \boldsymbol{T} \cdot \delta_* \dot{\boldsymbol{\varphi}} \, \mathrm{d}A - \int_{\partial_\varphi \mathscr{B}_0} \boldsymbol{R} \cdot \delta_* \dot{\boldsymbol{\varphi}} \, \mathrm{d}A - \int_{\partial_\varphi \mathscr{B}_0} \delta_* \boldsymbol{R} \cdot \left[\dot{\boldsymbol{\varphi}} - \dot{\bar{\boldsymbol{\varphi}}}\right] \mathrm{d}A$$

- Functional of the external orientational power

$$\dot{\Pi}_n^{\text{ext}}\left(\dot{\boldsymbol{\chi}}, \dot{\boldsymbol{\beta}}\right) := -\int_{\mathscr{B}_0} \rho_0 \boldsymbol{B}_\chi \cdot \dot{\boldsymbol{\chi}} \, \mathrm{d}V - \int_{\partial_W \mathscr{B}_0} \boldsymbol{W} \cdot \dot{\boldsymbol{\chi}} \, \mathrm{d}A + \int_{\mathscr{B}_0} \boldsymbol{\Sigma}_\beta \cdot \dot{\boldsymbol{\beta}} \, \mathrm{d}V$$

- Virtual external orientational power

$$\delta_* \dot{\Pi}_n^{\text{ext}}\left(\dot{\boldsymbol{\chi}}, \dot{\boldsymbol{\beta}}\right) := -\int_{\mathscr{B}_0} \rho_0 \boldsymbol{B}_\chi \cdot \delta_* \dot{\boldsymbol{\chi}} \, \mathrm{d}V - \int_{\partial_W \mathscr{B}_0} \boldsymbol{W} \cdot \delta_* \dot{\boldsymbol{\chi}} \, \mathrm{d}A + \int_{\mathscr{B}_0} \boldsymbol{\Sigma}_\beta \cdot \delta_* \dot{\boldsymbol{\beta}} \, \mathrm{d}V$$

Variational-based weak formulation (III)

Principle of virtual power

$$\delta_* \dot{\mathcal{T}}(\dot{\boldsymbol{\varphi}}, \dot{\mathbf{v}}, \dot{\mathbf{p}}) + \delta_* \dot{\mathcal{T}}_n\left(\dot{\boldsymbol{\chi}}, \dot{\mathbf{v}}_\chi, \dot{\mathbf{p}}_\chi\right) + \delta_* \dot{\Pi}^{\text{ext}}(\dot{\boldsymbol{\varphi}}, \boldsymbol{R}) + \delta_* \dot{\Pi}^{\text{ext}}_n(\dot{\boldsymbol{\chi}}) + \delta_* \dot{\Pi}^{\text{int}}\left(\dot{\boldsymbol{\varphi}}, \dot{\boldsymbol{\chi}}, \dot{\boldsymbol{\alpha}}, \dot{\boldsymbol{\beta}}, \boldsymbol{\tau}_\chi, \boldsymbol{w}_\tau\right) := 0$$

Internal power

- Functional of the internal power $\dot{\Pi}^{\text{int}}\left(\dot{\boldsymbol{\varphi}}, \dot{\boldsymbol{\chi}}, \dot{\boldsymbol{\alpha}}, \dot{\boldsymbol{\beta}}, \boldsymbol{\tau}_\chi, \boldsymbol{w}_\tau\right) := \mathcal{P}^{\text{int}}$

$$\mathcal{P}^{\text{int}} := \int_{\mathscr{B}_0} \left[\frac{\partial \psi}{\partial \boldsymbol{F}} : \dot{\boldsymbol{F}} + \frac{\partial \psi}{\partial \boldsymbol{\chi}} \cdot \dot{\boldsymbol{\chi}} + \frac{\partial \psi}{\partial \boldsymbol{\alpha}} \cdot \dot{\boldsymbol{\alpha}} + \frac{\partial \psi}{\partial \boldsymbol{\beta}} \cdot \dot{\boldsymbol{\beta}}\right] \mathrm{d}V$$
$$+ \int_{\mathscr{B}_0} \boldsymbol{\tau}_\chi \cdot \left[\dot{\boldsymbol{\chi}} - (\dot{\boldsymbol{\alpha}} \times \boldsymbol{\chi}) + \left(\dot{\boldsymbol{\beta}} \times \boldsymbol{\chi}\right)\right] \mathrm{d}V + \int_{\mathscr{B}_0} \boldsymbol{w}_\tau \cdot \left[\frac{1}{2}\boldsymbol{\epsilon} : \dot{\boldsymbol{F}}\boldsymbol{F}^{-1} + \dot{\boldsymbol{\alpha}}\right] \mathrm{d}V$$

- Virtual internal power

$$\delta_* \mathcal{P}^{\text{int}} := \int_{\mathscr{B}_0} \frac{\partial \psi}{\partial \boldsymbol{F}} : \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{\varphi}} \cdot \delta_* \dot{\boldsymbol{\varphi}} \, \mathrm{d}V + \int_{\mathscr{B}_0} \frac{1}{2} \boldsymbol{w}_\tau \cdot \boldsymbol{\epsilon} \cdot \boldsymbol{F}^{-t} : \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{\varphi}} \cdot \delta_* \dot{\boldsymbol{\varphi}} \, \mathrm{d}V + \int_{\mathscr{B}_0} \frac{\partial \psi}{\partial \boldsymbol{\chi}} \cdot \delta_* \dot{\boldsymbol{\chi}} \, \mathrm{d}V$$
$$+ \int_{\mathscr{B}_0} \boldsymbol{\tau}_\chi \cdot \delta_* \dot{\boldsymbol{\chi}} \, \mathrm{d}V - \int_{\mathscr{B}_0} \delta_* \dot{\boldsymbol{\alpha}} \cdot (\boldsymbol{\chi} \times \boldsymbol{\tau}_\chi) \, \mathrm{d}V + \int_{\mathscr{B}_0} \boldsymbol{w}_\tau \cdot \delta_* \dot{\boldsymbol{\alpha}} \, \mathrm{d}V$$
$$+ \int_{\mathscr{B}_0} \frac{\partial \psi}{\partial \boldsymbol{\alpha}} \cdot \delta_* \dot{\boldsymbol{\alpha}} \, \mathrm{d}V + \int_{\mathscr{B}_0} \delta_* \dot{\boldsymbol{\beta}} \cdot (\boldsymbol{\chi} \times \boldsymbol{\tau}_\chi) \, \mathrm{d}V + \int_{\mathscr{B}_0} \frac{\partial \psi}{\partial \boldsymbol{\beta}} \cdot \delta_* \dot{\boldsymbol{\beta}} \, \mathrm{d}V$$
$$+ \int_{\mathscr{B}_0} \delta_* \boldsymbol{\tau}_\chi \cdot \left[\dot{\boldsymbol{\chi}} - (\dot{\boldsymbol{\alpha}} \times \boldsymbol{\chi}) + \left(\dot{\boldsymbol{\beta}} \times \boldsymbol{\chi}\right)\right] \mathrm{d}V + \int_{\mathscr{B}_0} \delta_* \boldsymbol{w}_\tau \cdot \left[\frac{1}{2}\boldsymbol{\epsilon} : \dot{\boldsymbol{F}}\boldsymbol{F}^{-1} + \dot{\boldsymbol{\alpha}}\right] \mathrm{d}V$$

Space-time weak forms

Weak balance of linear momentum

$$\iint\limits_{\mathcal{T}_n \times \mathcal{B}_0} \delta_* \dot{\boldsymbol{\varphi}} \cdot [\dot{\mathbf{p}} - \rho_0 \boldsymbol{B}_\varphi] \, \mathrm{d}V \, \mathrm{d}t + \iint\limits_{\mathcal{T}_n \times \mathcal{B}_0} \frac{1}{2} \boldsymbol{w}_\tau \cdot \boldsymbol{\epsilon} \cdot \boldsymbol{F}^{-T} : \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{\varphi}} \cdot \delta_* \dot{\boldsymbol{\varphi}} \, \mathrm{d}V \, \mathrm{d}t$$
$$+ \iint\limits_{\mathcal{T}_n \times \mathcal{B}_0} \frac{\partial \psi}{\partial \boldsymbol{F}} : \frac{\partial \boldsymbol{F}}{\partial \boldsymbol{\varphi}} \cdot \delta_* \dot{\boldsymbol{\varphi}} \, \mathrm{d}V \, \mathrm{d}t - \iint\limits_{\mathcal{T}_n \times \partial_T \mathcal{B}_0} \delta_* \dot{\boldsymbol{\varphi}} \cdot \boldsymbol{T} \, \mathrm{d}A \, \mathrm{d}t - \iint\limits_{\mathcal{T}_n \times \partial_\varphi \mathcal{B}_0} \delta_* \dot{\boldsymbol{\varphi}} \cdot \boldsymbol{R} \, \mathrm{d}A \, \mathrm{d}t = 0$$

Weak balance of orientational momentum

$$\iint\limits_{\mathcal{T}_n \times \mathcal{B}_0} \delta_* \dot{\boldsymbol{\chi}} \cdot [\dot{\mathbf{p}}_\chi - \rho_0 \boldsymbol{\gamma}] \, \mathrm{d}V \, \mathrm{d}t + \iint\limits_{\mathcal{T}_n \times \mathcal{B}_0} \frac{\partial \psi}{\partial \boldsymbol{\chi}} \cdot \delta_* \dot{\boldsymbol{\chi}} \, \mathrm{d}V \, \mathrm{d}t$$
$$+ \iint\limits_{\mathcal{T}_n \times \mathcal{B}_0} \delta_* \dot{\boldsymbol{\chi}} \cdot \boldsymbol{\tau}_\chi \, \mathrm{d}V \, \mathrm{d}t - \iint\limits_{\mathcal{T}_n \times \partial_W \mathcal{B}_0} \delta_* \dot{\boldsymbol{\chi}} \cdot \boldsymbol{W} \, \mathrm{d}A \, \mathrm{d}t = 0$$

Weak balance of reorientation stress

$$\iint\limits_{\mathcal{T}_n \times \mathcal{B}_0} \delta_* \dot{\boldsymbol{\alpha}} \cdot \left[\boldsymbol{w}_\tau - (\boldsymbol{\chi} \times \boldsymbol{\tau}_\chi) + \frac{\partial \psi}{\partial \boldsymbol{\alpha}} \right] \mathrm{d}V \, \mathrm{d}t = 0$$

Weak balance of rotation stress

$$\iint\limits_{\mathcal{T}_n \times \mathcal{B}_0} \delta_* \dot{\boldsymbol{\beta}} \cdot \left[(\boldsymbol{\chi} \times \boldsymbol{\tau}_\chi) + \frac{\partial \psi}{\partial \boldsymbol{\beta}} + \boldsymbol{\Sigma}_\beta \right] \mathrm{d}V \, \mathrm{d}t = 0$$

Weak balance of orientation rates

$$\iint\limits_{\mathcal{T}_n \times \mathcal{B}_0} \delta_* \boldsymbol{\tau}_\chi \cdot \left[\dot{\boldsymbol{\chi}} - (\dot{\boldsymbol{\alpha}} \times \boldsymbol{\chi}) + (\dot{\boldsymbol{\beta}} \times \boldsymbol{\chi}) \right] \mathrm{d}V \, \mathrm{d}t = 0$$

Weak continuum rotation equation

$$\iint\limits_{\mathcal{T}_n \times \mathcal{B}_0} \delta_* \boldsymbol{w}_\tau \cdot \left[\dot{\boldsymbol{\alpha}} + \frac{1}{2} \boldsymbol{\epsilon} : \dot{\boldsymbol{F}} \boldsymbol{F}^{-1} \right] \mathrm{d}V \, \mathrm{d}t = 0$$

Linear momentum $\delta_* \dot{\boldsymbol{\varphi}} = \boldsymbol{c} = \text{const.}$

$$\boldsymbol{L}(t_{n+1}) - \boldsymbol{L}(t_n) = \iint_{\mathcal{T}_n \times \mathcal{B}_0} \rho_0 \boldsymbol{B}_\varphi \, \mathrm{d}V \, \mathrm{d}t + \iint_{\mathcal{T}_n \times \partial_T \mathcal{B}_0} \boldsymbol{T} \, \mathrm{d}A \, \mathrm{d}t + \iint_{\mathcal{T}_n \times \partial_\varphi \mathcal{B}_0} \boldsymbol{R} \, \mathrm{d}A \, \mathrm{d}t$$

Orientational momentum $\delta_* \dot{\boldsymbol{\chi}} = \boldsymbol{c} = \text{const.}$

$$\boldsymbol{L}_n(t_{n+1}) - \boldsymbol{L}_n(t_n) = \iint_{\mathcal{T}_n \times \mathcal{B}_0} \rho_0 \boldsymbol{B}_\chi \, \mathrm{d}V \, \mathrm{d}t + \iint_{\mathcal{T}_n \times \partial_W \mathcal{B}_0} \boldsymbol{W} \, \mathrm{d}A \, \mathrm{d}t - \iint_{\mathcal{T}_n \times \mathcal{B}_0} \left[\boldsymbol{\tau}_\chi + \frac{\partial \psi}{\partial \boldsymbol{\chi}} \right] \mathrm{d}V \, \mathrm{d}t$$

Moment of linear momentum $\delta_* \dot{\boldsymbol{\varphi}} = \boldsymbol{c} \times \boldsymbol{\varphi}$, $\delta_* \dot{\boldsymbol{\alpha}} = \boldsymbol{c}$, $\delta_* \dot{\boldsymbol{\beta}} = \boldsymbol{c}$

$$\begin{aligned}\boldsymbol{J}(t_{n+1}) - \boldsymbol{J}(t_n) = &- \iint_{\mathcal{T}_n \times \mathcal{B}_0} \left(\boldsymbol{F} \times \frac{\partial \psi}{\partial \boldsymbol{F}} \right) \mathrm{d}V \, \mathrm{d}t + \iint_{\mathcal{T}_n \times \mathcal{B}_0} [\boldsymbol{\varphi} \times \rho_0 \boldsymbol{B}_\varphi] \, \mathrm{d}V \, \mathrm{d}t \\ &+ \iint_{\mathcal{T}_n \times \partial_T \mathcal{B}_0} [\boldsymbol{\varphi} \times \boldsymbol{T}] \, \mathrm{d}A \, \mathrm{d}t + \iint_{\mathcal{T}_n \times \partial_\varphi \mathcal{B}_0} [\boldsymbol{\varphi} \times \boldsymbol{R}] \, \mathrm{d}A \, \mathrm{d}t \\ &+ \iint_{\mathcal{T}_n \times \mathcal{B}_0} \frac{\partial \psi}{\partial \boldsymbol{\beta}} \, \mathrm{d}V \, \mathrm{d}t + \iint_{\mathcal{T}_n \times \mathcal{B}_0} \boldsymbol{\Sigma}_\beta \, \mathrm{d}V \, \mathrm{d}t + \iint_{\mathcal{T}_n \times \mathcal{B}_0} \frac{\partial \psi}{\partial \boldsymbol{\alpha}} \, \mathrm{d}V \, \mathrm{d}t\end{aligned}$$

Moment of orientational momentum

$\delta_* \dot{\boldsymbol{\chi}} = \boldsymbol{c} \times \boldsymbol{\chi}$

$$\boldsymbol{J}_\chi(t_{n+1}) - \boldsymbol{J}_\chi(t_n) = -\iint\limits_{\mathscr{T}_n \times \mathscr{B}_0} \left(\boldsymbol{\chi} \times \frac{\partial \psi}{\partial \boldsymbol{\chi}}\right) \mathrm{d}V\,\mathrm{d}t - \iint\limits_{\mathscr{T}_n \times \mathscr{B}_0} (\boldsymbol{\chi} \times \boldsymbol{\tau}_\chi)\,\mathrm{d}V\,\mathrm{d}t + \iint\limits_{\mathscr{T}_n \times \mathscr{B}_0} [\boldsymbol{\chi} \times \rho_0 \boldsymbol{B}_\chi] + \mathrm{d}V\,\mathrm{d}t \iint\limits_{\mathscr{T}_n \times \partial_W \mathscr{B}_0} [\boldsymbol{\chi} \times \boldsymbol{W}]\,\mathrm{d}A\,\mathrm{d}t$$

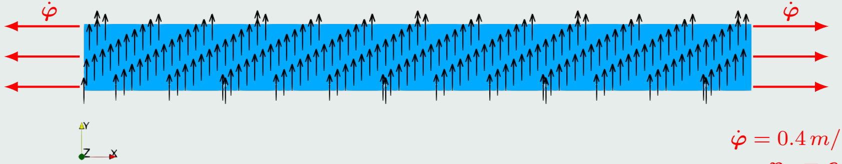
Total moment of momentum

$$\boldsymbol{J}(t_{n+1}) - \boldsymbol{J}(t_n) + \boldsymbol{J}_n(t_{n+1}) - \boldsymbol{J}_n(t_n) = -\iint\limits_{\mathscr{T}_n \times \mathscr{B}_0} \left(\boldsymbol{F} \times \frac{\partial \psi}{\partial \boldsymbol{F}}\right) \mathrm{d}V\,\mathrm{d}t - \iint\limits_{\mathscr{T}_n \times \mathscr{B}_0} \left(\boldsymbol{\chi} \times \frac{\partial \psi}{\partial \boldsymbol{\chi}}\right) \mathrm{d}V\,\mathrm{d}t + \iint\limits_{\mathscr{T}_n \times \mathscr{B}_0} \frac{\partial \psi}{\partial \boldsymbol{\alpha}}\,\mathrm{d}V\,\mathrm{d}t + \iint\limits_{\mathscr{T}_n \times \mathscr{B}_0} \frac{\partial \psi}{\partial \boldsymbol{\beta}}\,\mathrm{d}V\,\mathrm{d}t + \iint\limits_{\mathscr{T}_n \times \mathscr{B}_0} \boldsymbol{\Sigma}_\beta\,\mathrm{d}V\,\mathrm{d}t - \iint\limits_{\mathscr{T}_n \times \mathscr{B}_0} (\boldsymbol{\chi} \times \boldsymbol{\tau}_\chi)\,\mathrm{d}V\,\mathrm{d}t + \iint\limits_{\mathscr{T}_n \times \mathscr{B}_0} [\boldsymbol{\chi} \times \rho_0 \boldsymbol{B}_\chi] + \mathrm{d}V\,\mathrm{d}t \iint\limits_{\mathscr{T}_n \times \partial_W \mathscr{B}_0} [\boldsymbol{\chi} \times \boldsymbol{W}]\,\mathrm{d}A\,\mathrm{d}t + \iint\limits_{\mathscr{T}_n \times \mathscr{B}_0} [\boldsymbol{\varphi} \times \rho_0 \boldsymbol{B}_\varphi]\,\mathrm{d}V\,\mathrm{d}t + \iint\limits_{\mathscr{T}_n \times \partial_T \mathscr{B}_0} [\boldsymbol{\varphi} \times \boldsymbol{T}]\,\mathrm{d}A\,\mathrm{d}t + \iint\limits_{\mathscr{T}_n \times \partial_\varphi \mathscr{B}_0} [\boldsymbol{\varphi} \times \boldsymbol{R}]\,\mathrm{d}A\,\mathrm{d}t$$

Numerical test I: LCE film under tension

Boundary conditions

$0.0125 \times 0.125 \times 0.0005$ m, 10.000-em H1-standard



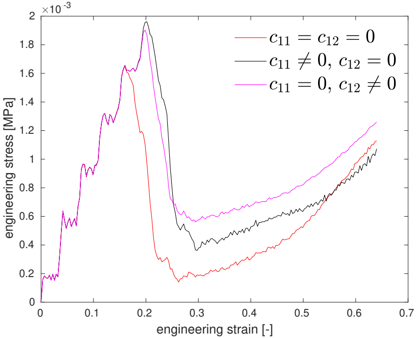
$\dot{\varphi} = 0.4\, m/s$

$\boldsymbol{n}_0 = \boldsymbol{e}_y$

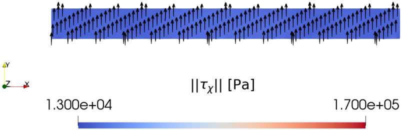
Parameters

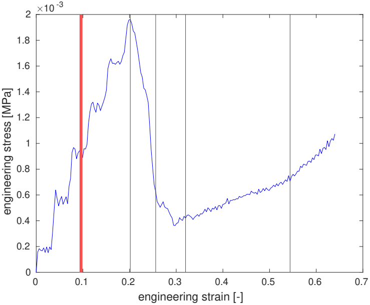
cf. [de Luca et al. (2013), Groß et al. (2022)]

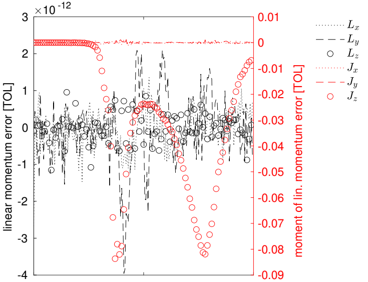
- $cG(k = 2)$
- $h_n = 0.0005\, s$ and $t_{end} = 0.1\, s$
- $TOL = 10^{-5}$
- convergence criterion: $\|\boldsymbol{R}\| < TOL$
- $E = 0.914\, MPa$
- $\nu = 0.49$
- $\rho = 1760\, kg/m^3$
- $r(T = 60°C) = 1.88$

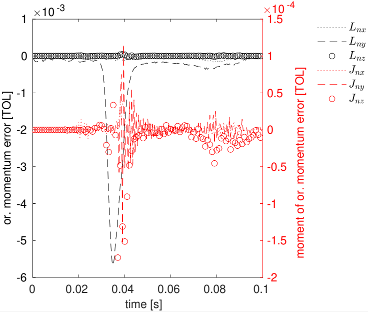


Numerical test I: LCE film under tension ($c_{11} \neq 0$, $c_{12} = 0$)









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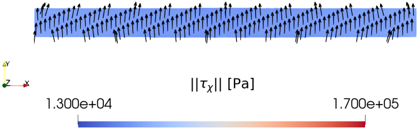

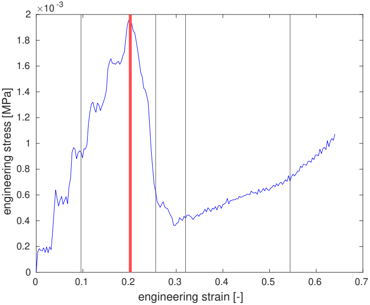

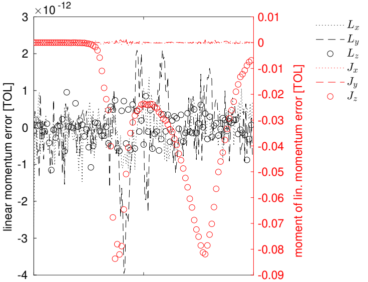

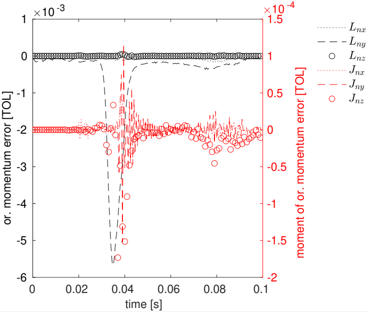

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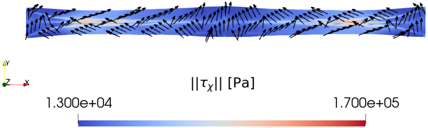

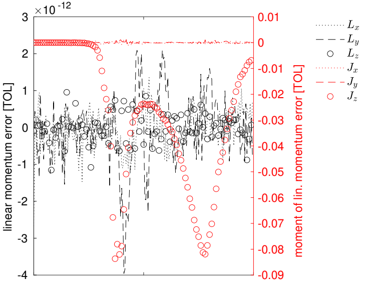

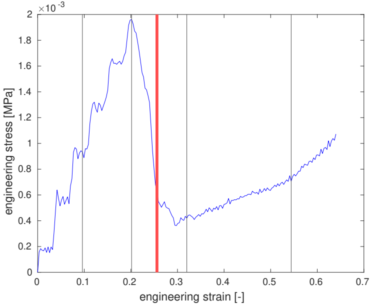

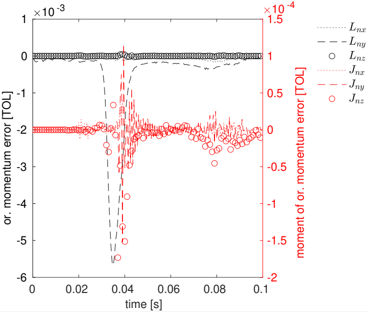

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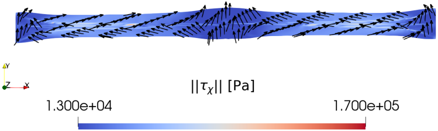

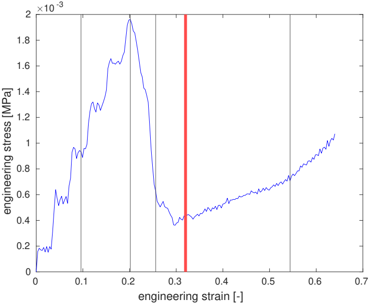

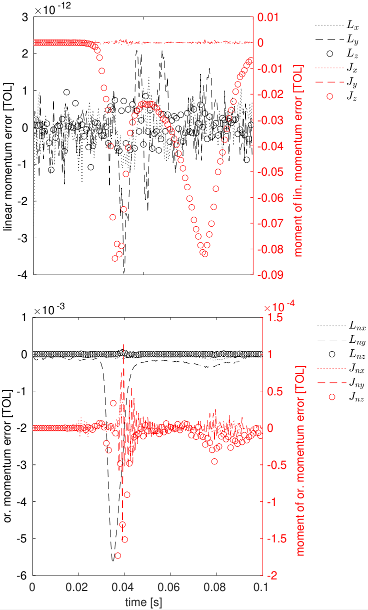

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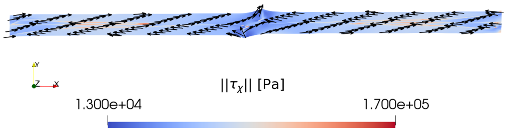

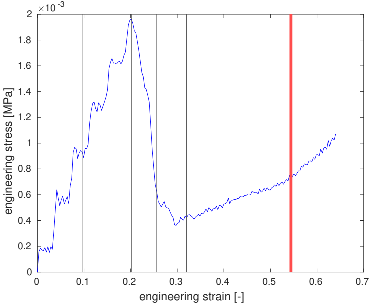

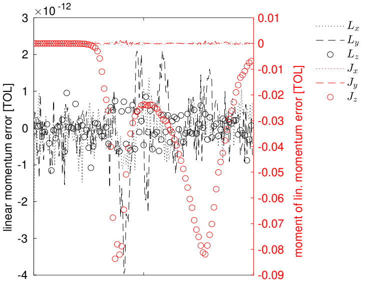

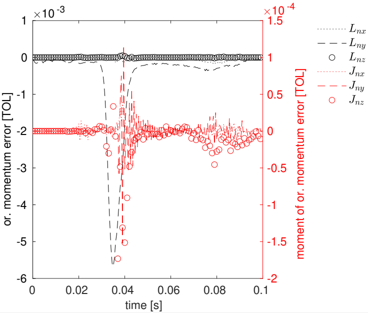

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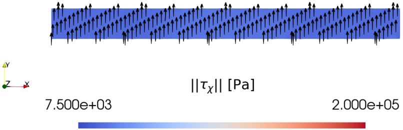

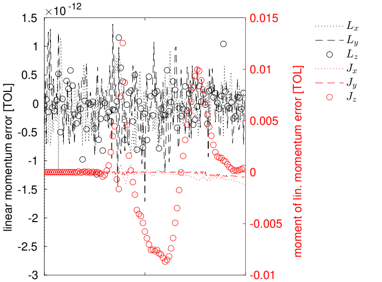

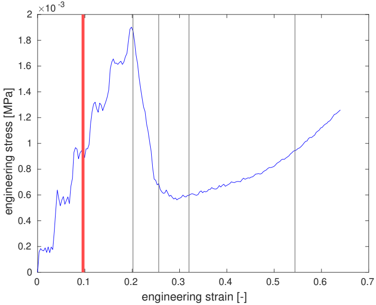

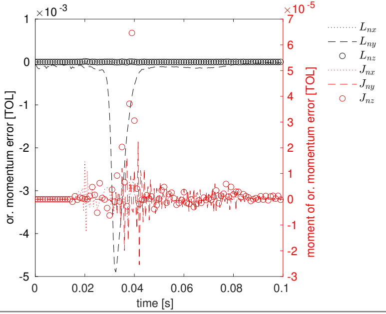

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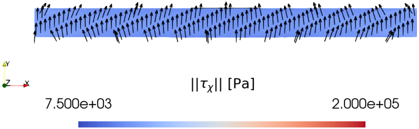

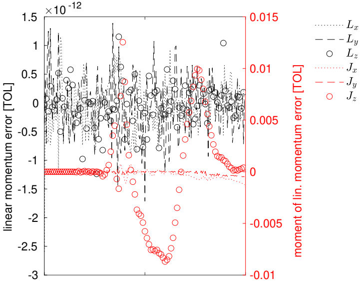

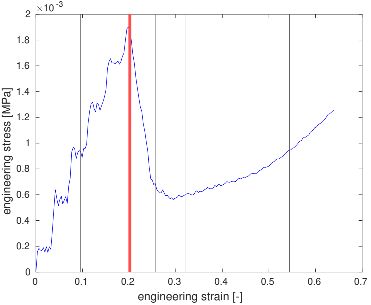

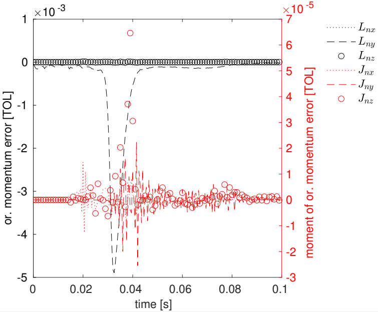

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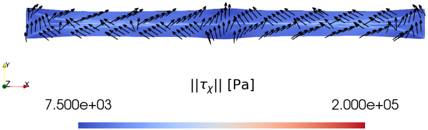

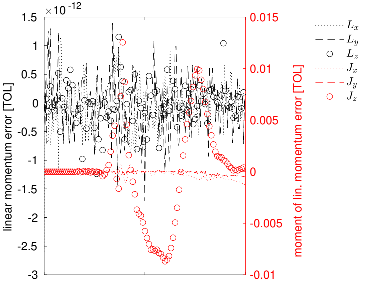

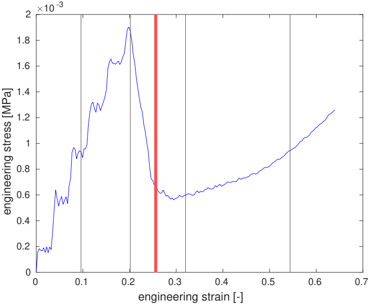

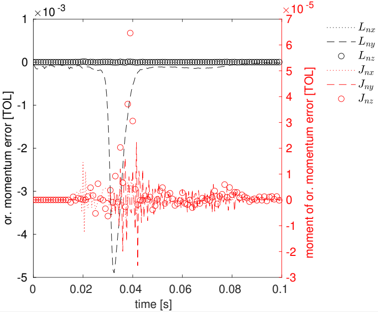

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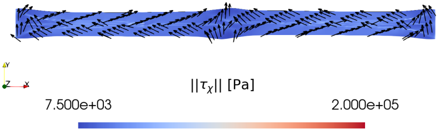

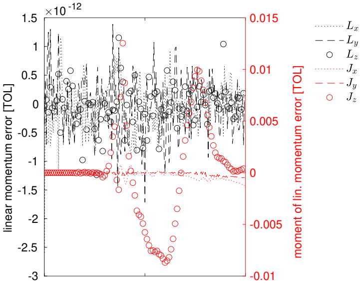

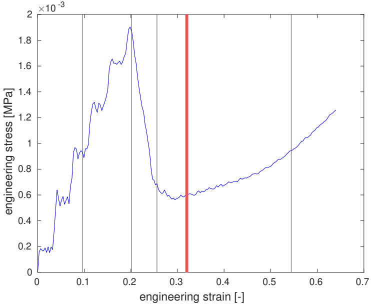

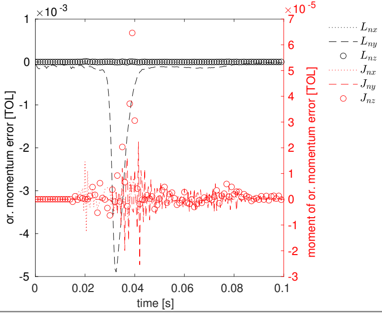

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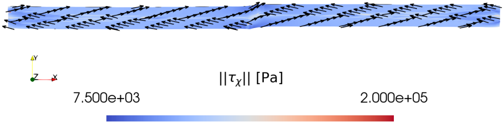

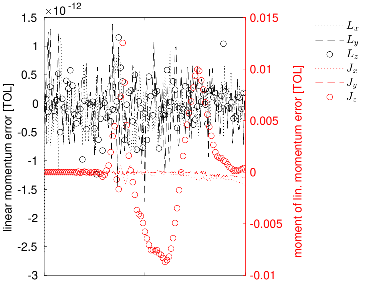

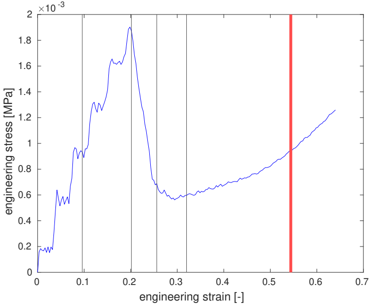

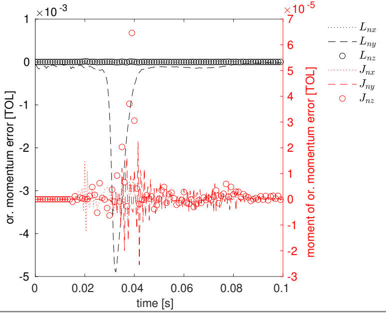

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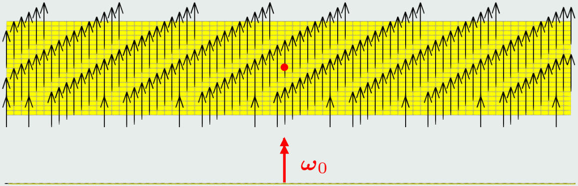
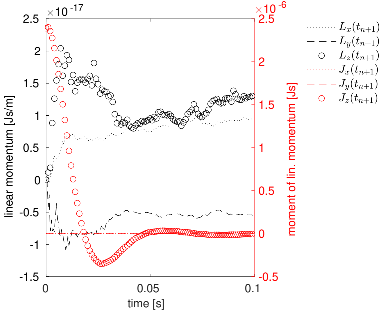
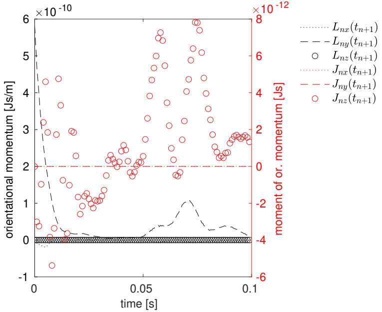
Numerical test II: LCE film under initial rotation

Mesh and boundary conditions $0.0125 \times 0.075 \times 0.0003$ m, 1.500-em H1-standard



$$\omega_0 = 20 \text{ rad/s } e_z$$
$$n_0 = e_y$$
no BC





Numerical test II: LCE film under initial rotation

Conclusions and future works

Conclusions

- numerical framework for including the semi-soft elastic behavior of LCEs in the context of dynamics
- semi-soft elastic response is obtained by describing the rotation of the nematic director as dissipative process
- strain energy densities from the linear elasticity theory have been chosen in order to keep invariance with respect to α and β as well
- rotational strain energy densities improve the plateau stage
- all momentum balances are preserved

Future work

- introduction of symmetry constraints for the orientational mapping in order to reduce the mesh size and thus the computational burden
- modelling based on experiments, e.g. arise of the striped pattern and rate-dependence
- modelling thermo-mechanical effects in the context of dynamic