



A New Mixed
FE-Formulation for
Liquid Crystal
Elastomer Films

Groß M., Concas
F. and Dietzsch J.

Introduction

Continuum model

Reorientation

Variational-based
weak formulation

Balance laws

Numerical studies

Initial rotation

Boundary load

Volume load

Summary

A New Mixed FE-Formulation for Liquid Crystal Elastomer Films

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Motivation and goals

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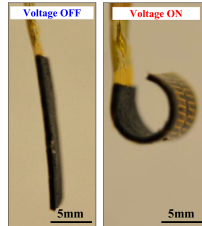
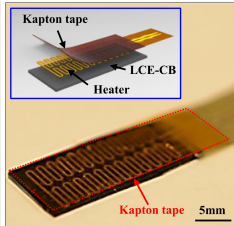
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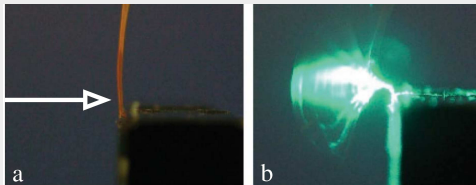
Summary

Goal 1: FE-simulation of thermal actuation of motion of LCE films



Introduction of Joule heat
energy by heating pads,
see Cui Y. et al. [2018]

Goal 2: FE-simulation of UV light acuation of motion of LCE films

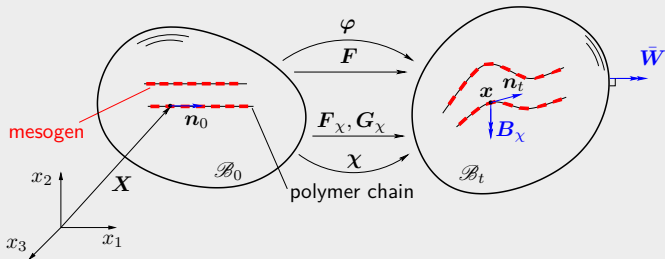


Using of UV light for
inducing vibration, see
Corbett & Warner [2009]

Step 1: FE formulation for actuation of continuum motions by boundary or volume loads

We design a dynamic mixed FE method for continuum motions with internal reorientation

Continuum configurations of a LCE with orientational loads



1 Orientation mapping

$$\chi : \mathcal{B}_0 \times \mathcal{T} \rightarrow \mathbb{R}^{n_{\text{dim}}} \text{ with}$$

$$\chi(\mathbf{X}, 0) = \mathbf{n}_0(\mathbf{X}) \text{ and } \mathbf{n}_0 \cdot \mathbf{n}_0 = 1$$

2 Orientation tensor

$$\mathbf{F}_\chi := \chi \otimes \mathbf{n}_0 \quad \mathbf{n}_t = \mathbf{F}_\chi \mathbf{n}_0$$

3 Orient. deformation tensor

$$\mathbf{C}_\chi := \mathbf{F}^t \mathbf{g} \mathbf{F}_\chi = \mathbf{F}^t \mathbf{g}_\chi \mathbf{F}$$

4 Distorsion tensor

$$\mathbf{K}_\chi := \mathbf{F}^t \mathbf{g} \mathbf{G}_\chi = \mathbf{F}^t \mathbf{g}_K \mathbf{F}$$

5 Orient. velocity vector

$$\mathbf{v}_\chi(\mathbf{X}, t) := \dot{\chi}(\mathbf{X}, t) = \dot{\mathbf{n}}_t$$

6 Orient. momentum vector

$$\mathbf{p}_\chi := \rho_0 [(l_\chi^2 - l_0^2) \mathbf{A}_0 + l_0^2 \mathbf{I}] \mathbf{v}_\chi$$

$$\mathbf{A}_0 := \mathbf{n}_0 \otimes \mathbf{n}_0$$

Free energy functions as stress potentials

(cp. Frank [1958], Leslie [1968], Warner et al. [1993], Anderson et al. [1999], Himpel et al. [2008], De Luca et al. [2013])

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Free energy associated with orientational deformations

- Interactive free energy (motivated by Anderson et al. [1999], Himpel et al. [2008])

$$\Psi_i(\mathbf{F}^t \mathbf{g} \chi) \equiv \Psi^{\text{ori}}(\mathbf{C}_\chi) := \hat{\Psi}^{\text{ori}}(I_1^{\text{ori}}, J_2^{\text{ori}})$$

- Oriental invariants

$$I_1^{\text{ori}} := \mathbf{C}_\chi \mathbf{A}_0 : \mathbf{G}^{-1} \qquad J_2^{\text{ori}} := \mathbf{C}_\chi \mathbf{A}_0 : \mathbf{C}_\chi \mathbf{A}_0$$

Free energy associated with distortions of the orientation field

- Frank free energy (motivated by Frank [1958], Leslie [1968], Anderson et al. [1999])

$$\Psi^{\text{dis}}(\mathbf{K}_\chi) := \hat{\Psi}^{\text{dis}}(I_1^{\text{dis}}, J_2^{\text{dis}})$$

- Distorsional invariants

$$I_1^{\text{dis}} := (\mathbf{K}_\chi - \text{Grad}[\mathbf{n}_0]) : \mathbf{G}^{-1} \qquad J_2^{\text{dis}} := (\mathbf{K}_\chi - \text{Grad}[\mathbf{n}_0]) : (\mathbf{K}_\chi - \text{Grad}[\mathbf{n}_0])$$

Free energy associated with non-isothermal elastic deformations

- Isotropic compressible free energy (see e.g. Warner et al. [1993], Anderson et al. [1999])

$$\Psi^{\text{ela}}(\mathbf{C}, \theta) := \hat{\Psi}^{\text{ela}}(I_1^{\text{ela}}, J_2^{\text{ela}}, I_3^{\text{ela}}, \theta)$$

- Deformation invariants

$$I_1^{\text{ela}} := \mathbf{C} : \mathbf{G}^{-1} \qquad J_2^{\text{ela}} := \mathbf{C} : \mathbf{C} \qquad I_3^{\text{ela}} := \det[\mathbf{C}]$$

Reorientation modelled as dissipative process

(cp. Garikipati et al. [2006])

- 1 Clausius-Planck inequality

$$D_{\chi}^{\text{int}} := \mathbf{N}_{\chi} : \mathbf{g} \dot{\mathbf{F}} - \dot{\Psi}^{\text{ori}}(\mathbf{C}_{\chi}) \equiv [\mathbf{N}_{\chi} - \mathbf{F}_{\chi} \mathbf{S}_{\chi}^t] : \mathbf{g} \dot{\mathbf{F}} - \mathbf{F} \mathbf{S}_{\chi} : \mathbf{g} \dot{\mathbf{F}}_{\chi} \geq 0$$

- 2 Normalized orientation vectors guaranteed by drilling degrees of freedom

$$\mathbb{I}^{\text{skw}} : \mathbf{g} \dot{\mathbf{F}}_{\chi} \mathbf{F}_{\chi}^{-1} = \epsilon \cdot \dot{\alpha} \quad \dot{\alpha} := \dot{\alpha}^k \mathbf{g}_k \circ \varphi(\mathbf{X}, t)$$

- 3 Reorientation dissipation

$$D_{\chi}^{\text{int}} := [\mathbf{N}_{\chi} - \mathbf{F}_{\chi} \mathbf{S}_{\chi}^t] : \mathbf{g} \dot{\mathbf{F}} - \boldsymbol{\tau}_{\chi} : \epsilon \cdot \dot{\alpha} \geq 0$$

- 4 Coleman-Noll procedure

$$\mathbf{N}_{\chi} := \mathbf{F}_{\chi} \mathbf{S}_{\chi}^t \quad \boldsymbol{\tau}_{\chi} := \mathbf{F} \mathbf{S}_{\chi} \mathbf{F}_{\chi}^t$$

Reorientation equations

- 1 Orientational non-equilibrium stress equation (solved on element level)

$$\boxed{-\frac{1}{2} \epsilon : \boldsymbol{\tau}_{\chi} = \boldsymbol{\Sigma}_{\chi}} \quad \boldsymbol{\Sigma}_{\chi} = V_{\chi} \dot{\alpha} \quad D_{\chi}^{\text{int}} := 2 \boldsymbol{\Sigma}_{\chi} \cdot \dot{\alpha} \geq 0$$

- 2 Global orientation equation with Dirichlet boundary conditions in general

$$\boxed{\dot{\chi} = -\epsilon \cdot \dot{\alpha} \cdot \chi}$$

Principle of virtual power extended to mixed fields

- 1 Incremental principle of virtual power

$$\int_{t_n}^{t_{n+1}} \delta_* \dot{\mathcal{H}}(\dot{\tilde{\mathbf{U}}}_1, \dots, \dot{\tilde{\mathbf{U}}}_s, \tilde{\mathbf{V}}_1, \dots, \tilde{\mathbf{V}}_p) dt = 0$$

- 2 Total virtual power of deformation φ , temperature Θ and orientation χ

$$\delta_* \dot{\mathcal{H}} := \delta_* \mathcal{P}_\varphi + \delta_* \mathcal{P}_\Theta + \delta_* \mathcal{P}_\chi \quad \mathcal{H} := \mathcal{T} + \Pi^{\text{int}} + \Pi^{\text{ext}}$$

Virtual power associated with the motion (I)

- 1 Virtual power of motion

$$\delta_* \mathcal{P}_\varphi := \delta_* \dot{\mathcal{T}}_\varphi(\dot{\varphi}, \dot{\mathbf{v}}, \dot{\mathbf{p}}) + \delta_* \dot{\Pi}_\varphi^{\text{ext}}(\dot{\varphi}, \tilde{\mathbf{R}}) + \delta_* \dot{\Pi}_\varphi^{\text{int}}(\dot{\varphi}, \dot{\tilde{\mathbf{F}}}, \dot{\tilde{\mathbf{C}}}, \tilde{\mathbf{P}}, \tilde{\mathbf{S}})$$

- 2 Path-independent virtual kinetic power

$$\delta_* \dot{\mathcal{T}}_\varphi(\dot{\varphi}, \dot{\mathbf{v}}, \dot{\mathbf{p}}) := \int_{\mathcal{B}_0} \delta_* \dot{\mathbf{v}} \cdot [\rho_0 \mathbf{v} - \mathbf{p}] dV + \int_{\mathcal{B}_0} \delta_* \dot{\mathbf{p}} \cdot [\dot{\varphi} - \mathbf{v}] dV + \int_{\mathcal{B}_0} \delta_* \dot{\varphi} \cdot \dot{\mathbf{p}} dV$$

- 3 Path-(in)dependent virtual external power

$$\begin{aligned} \delta_* \dot{\Pi}_\varphi^{\text{ext}}(\dot{\varphi}, \tilde{\mathbf{R}}) := & - \int_{\mathcal{B}_0} \delta_* \dot{\varphi} \cdot \mathbf{B} dV && - \int_{\partial_T \mathcal{B}_0} \delta_* \dot{\varphi} \cdot \tilde{\mathbf{T}} dA \\ & - \int_{\partial_\varphi \mathcal{B}_0} \delta_* \tilde{\mathbf{R}} \cdot [\dot{\varphi} - \dot{\tilde{\varphi}}] dA && - \int_{\partial_\varphi \mathcal{B}_0} \delta_* \dot{\varphi} \cdot \tilde{\mathbf{R}} dA \end{aligned}$$

Virtual power associated with the motion (II)

Path-independent virtual internal power $\delta_* \dot{I}^{\text{int}}(\dot{\varphi}, \dot{\bar{\mathbf{F}}}, \dot{\bar{\mathbf{C}}}, \dot{\bar{\mathbf{P}}}, \dot{\bar{\mathbf{S}}}) := \delta_* \mathcal{P}_\varphi^{\text{int}}$

$$\begin{aligned} \delta_* \mathcal{P}_\varphi^{\text{int}} := & \int_{\mathcal{B}_0} \delta_* \bar{\mathbf{P}} : \left[\text{Grad}[\dot{\varphi}] - \dot{\bar{\mathbf{F}}} \right] dV + \frac{1}{2} \int_{\mathcal{B}_0} \delta_* \bar{\mathbf{S}} : \left[\frac{\partial}{\partial t} (\bar{\mathbf{F}}^t \bar{\mathbf{F}}) - \dot{\bar{\mathbf{C}}} \right] dV \\ & + \int_{\mathcal{B}_0} \delta_* \dot{\bar{\mathbf{C}}} : \left[\frac{\partial \Psi}{\partial \bar{\mathbf{C}}} - \frac{1}{2} \bar{\mathbf{S}} \right] dV + \int_{\mathcal{B}_0} \delta_* \dot{\bar{\mathbf{F}}} : [\bar{\mathbf{F}} \bar{\mathbf{S}} - \bar{\mathbf{P}}] dV + \int_{\mathcal{B}_0} \bar{\mathbf{P}} : \text{Grad}[\delta_* \dot{\varphi}] dV \end{aligned}$$

Virtual power associated with the thermal evolution (I)

- Virtual power of thermal evolution

$$\delta_* \mathcal{P}_\Theta := \delta_* \dot{I}^{\text{ext}}(\dot{\Theta}, \tilde{\Theta}, \tilde{\lambda}, \tilde{h}) + \delta_* \dot{I}^{\text{int}}(\dot{\Theta}, \dot{\eta}, \tilde{\Theta})$$

- Path-dependent virtual external power

$$\begin{aligned} \delta_* \dot{I}^{\text{ext}}(\dot{\Theta}, \tilde{\Theta}, \tilde{\lambda}, \tilde{h}) := & \int_{\mathcal{B}_0} \delta_* \tilde{\Theta} \frac{D^{\text{tot}}}{\Theta} dV + \int_{\mathcal{B}_0} \frac{1}{\Theta} \text{Grad}[\delta_* \tilde{\Theta}] \cdot \mathbf{Q} dV \\ & + \int_{\partial_Q \mathcal{B}_0} \delta_* \tilde{\Theta} \frac{\bar{Q}}{\Theta} dA + \int_{\partial_\Theta \mathcal{B}_0} \delta_* \tilde{\Theta} \tilde{\lambda} dA - \int_{\partial_{\tilde{\Theta}} \mathcal{B}_0} \delta_* \tilde{\Theta} \tilde{h} dA \\ & + \int_{\partial_\Theta \mathcal{B}_0} \delta_* \tilde{\lambda} [\tilde{\Theta} - \Theta_\infty] dA - \int_{\partial_{\tilde{\Theta}} \mathcal{B}_0} \delta_* \tilde{h} [\dot{\Theta} - \dot{\tilde{\Theta}}] dA \end{aligned}$$

with

$$D^{\text{tot}} := -\frac{1}{\Theta} \text{Grad}[\tilde{\Theta}] \cdot \mathbf{Q} + 2 \dot{\alpha} \cdot \Sigma_\chi \quad \text{and} \quad \mathbf{Q} := -k_0 \det[\bar{\mathbf{F}}] \bar{\mathbf{C}}^{-1} \text{Grad}[\Theta]$$

Virtual power associated with the thermal evolution (II)

Path-independent virtual internal power

$$\delta_* \dot{I}_{\Theta}^{\text{int}}(\dot{\Theta}, \dot{\eta}, \dot{\Theta}) := \int_{\mathcal{B}_0} \delta_* \dot{\Theta} \left(\frac{\partial \Psi}{\partial \Theta} + \eta \right) dV + \int_{\mathcal{B}_0} \delta_* \dot{\eta} (\Theta - \tilde{\Theta}) dV - \int_{\mathcal{B}_0} \delta_* \tilde{\Theta} \dot{\eta} dV$$

Virtual power associated with the reorientation (I)

- Virtual power of reorientation

$$\delta_* \mathcal{P}_{\chi} := \delta_* \dot{\mathcal{T}}_{\chi}(\dot{\chi}, \dot{\mathbf{v}}_{\chi}, \dot{\mathbf{p}}_{\chi}) + \delta_* \mathcal{P}_{\chi}^{\text{ext}} + \delta_* \mathcal{P}_{\chi}^{\text{int}}$$

- Path-independent virtual kinetic power

$$\begin{aligned} \delta_* \dot{\mathcal{T}}_{\chi}(\dot{\chi}, \dot{\mathbf{v}}_{\chi}, \dot{\mathbf{p}}_{\chi}) := & \int_{\mathcal{B}_0} \delta_* \dot{\mathbf{v}}_{\chi} \cdot (\rho_0 [(l_{\chi}^2 - l_0^2) \mathbf{A}_0 + l_0^2 \mathbf{I}] \mathbf{v}_{\chi} - \mathbf{p}_{\chi}) dV \\ & + \int_{\mathcal{B}_0} \delta_* \dot{\mathbf{p}}_{\chi} \cdot [\dot{\chi} - \mathbf{v}_{\chi}] dV + \int_{\mathcal{B}_0} \delta_* \dot{\chi} \cdot \dot{\mathbf{p}}_{\chi} dV \end{aligned}$$

- Path-dependent virtual external power

$$\delta_* \dot{I}_{\chi}^{\text{ext}}(\dot{\alpha}, \dot{\chi}, \dot{\mathbf{Z}}, \dot{\tilde{\tau}}_n, \dot{\tilde{\nu}}) =: \delta_* \mathcal{P}_{\chi}^{\text{ext}}$$

where

$$\begin{aligned} \delta_* \mathcal{P}_{\chi}^{\text{ext}} := & - \int_{\mathcal{B}_0} \delta_* \dot{\chi} \cdot \mathbf{B}_{\chi} dV - \int_{\partial_W \mathcal{B}_0} \delta_* \dot{\chi} \cdot \bar{\mathbf{W}} dA - \int_{\partial_{\chi} \mathcal{B}_0} \delta_* \dot{\mathbf{Z}} \cdot [\dot{\chi} - \dot{\tilde{\chi}}] dA - \int_{\partial_{\chi} \mathcal{B}_0} \delta_* \dot{\chi} \cdot \bar{\mathbf{Z}} dA \\ & - \int_{\partial_{\chi} \mathcal{B}_0} 2 \delta_* \dot{\tilde{\tau}}_n \cdot \tilde{\nu} dA - \int_{\partial_{\chi} \mathcal{B}_0} 2 \delta_* \dot{\tilde{\nu}} \cdot \tilde{\tau}_n dA + \int_{\mathcal{B}_0} 2 \delta_* \dot{\alpha} \cdot \Sigma_{\chi} dV \end{aligned}$$

Variational-based weak formulation (IV)

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Virtual power associated with the reorientation (II)

Path-independent virtual internal power

$$\delta_* \dot{I}_\chi^{\text{int}}(\dot{\alpha}, \dot{\chi}, \dot{\mathbf{F}}, \dot{\mathbf{F}}_\chi, \dot{\mathbf{G}}_\chi, \dot{\mathbf{C}}_\chi, \dot{\mathbf{K}}_\chi, \tilde{\tau}_n, \tilde{\mathbf{P}}_\chi, \tilde{\mathbf{P}}_K, \tilde{\mathbf{S}}_\chi, \tilde{\mathbf{S}}_K) := \delta_* \mathcal{P}_\chi^{\text{int}}$$

where

$$\begin{aligned} \delta_* \mathcal{P}_\chi^{\text{int}} &:= \int_{\mathcal{B}_0} \delta_* \dot{\mathbf{F}} : [\tilde{\mathbf{F}}_\chi \tilde{\mathbf{S}}_\chi^t + \tilde{\mathbf{G}}_\chi \tilde{\mathbf{S}}_K^t] dV + \int_{\mathcal{B}_0} 2 \delta_* \tilde{\tau}_n \cdot [\dot{\chi} + \epsilon \cdot \dot{\alpha} \cdot \chi] dV \\ &+ \int_{\mathcal{B}_0} \delta_* \tilde{\mathbf{P}}_\chi : [\dot{\chi} \otimes \mathbf{n}_0 - \dot{\mathbf{F}}_\chi] dV + \int_{\mathcal{B}_0} \delta_* \tilde{\mathbf{P}}_K : [\text{Grad}[\dot{\chi}] - \dot{\mathbf{G}}_\chi] dV \\ &+ \int_{\mathcal{B}_0} \delta_* \tilde{\mathbf{S}}_\chi : \left[\frac{\partial}{\partial t} (\tilde{\mathbf{F}}^t \tilde{\mathbf{F}}_\chi) - \dot{\mathbf{C}}_\chi \right] dV + \int_{\mathcal{B}_0} \delta_* \tilde{\mathbf{S}}_K : \left[\frac{\partial}{\partial t} (\tilde{\mathbf{F}}^t \tilde{\mathbf{G}}_\chi) - \dot{\mathbf{K}}_\chi \right] dV \\ &+ \int_{\mathcal{B}_0} \delta_* \dot{\mathbf{C}}_\chi : \left[\frac{\partial \Psi}{\partial \tilde{\mathbf{C}}_\chi} - \tilde{\mathbf{S}}_\chi \right] dV + \int_{\mathcal{B}_0} \delta_* \dot{\mathbf{K}}_\chi : \left[\frac{\partial \Psi}{\partial \tilde{\mathbf{K}}_\chi} - \tilde{\mathbf{S}}_K \right] dV \\ &+ \int_{\mathcal{B}_0} \delta_* \dot{\mathbf{F}}_\chi : [\tilde{\mathbf{F}} \tilde{\mathbf{S}}_\chi - \tilde{\mathbf{P}}_\chi] dV + \int_{\mathcal{B}_0} \delta_* \dot{\mathbf{G}}_\chi : [\tilde{\mathbf{F}} \tilde{\mathbf{S}}_K - \tilde{\mathbf{P}}_K] dV \\ &+ \int_{\mathcal{B}_0} \tilde{\mathbf{P}}_\chi : [\delta_* \dot{\chi} \otimes \mathbf{n}_0] dV + \int_{\mathcal{B}_0} \tilde{\mathbf{P}}_K : \text{Grad}[\delta_* \dot{\chi}] dV + \int_{\mathcal{B}_0} \delta_* \tilde{\mathbf{S}}_\chi : \tilde{\mathbf{F}}^t (\epsilon \cdot \alpha) \tilde{\mathbf{F}}_\chi dV \\ &+ \int_{\mathcal{B}_0} \left[\frac{1}{2} \epsilon : \tau_\chi - \tilde{\tau}_n \cdot \epsilon \cdot \chi \right] \cdot 2 \delta_* \dot{\alpha} dV + \int_{\mathcal{B}_0} 2 \tilde{\tau}_n \cdot \delta_* \dot{\chi} dV \end{aligned}$$

Total virtual power in the incremental principle

$$\delta_* \dot{\mathcal{H}} := \delta_* \mathcal{P}_\varphi + \delta_* \mathcal{P}_\theta + \delta_* \dot{\mathcal{T}}_\chi(\dot{\chi}, \dot{\nu}_\chi, \dot{\mathbf{p}}_\chi) + \delta_* \mathcal{P}_\chi^{\text{ext}} + \delta_* \mathcal{P}_\chi^{\text{int}}$$

Weak balance of linear momentum

$$\int_{\mathcal{I}_n} \int_{\mathcal{B}_0} \delta_* \dot{\varphi} \cdot [\dot{\mathbf{p}} - \mathbf{B}] dV dt - \int_{\mathcal{I}_n} \int_{\partial_T \mathcal{B}_0} \delta_* \dot{\varphi} \cdot \bar{\mathbf{T}} dA dt$$

$$+ \int_{\mathcal{I}_n} \int_{\mathcal{B}_0} \text{Grad}[\delta_* \dot{\varphi}] : \tilde{\mathbf{P}} dV dt = \int_{\mathcal{I}_n} \int_{\partial_\varphi \mathcal{B}_0} \delta_* \dot{\varphi} \cdot \tilde{\mathbf{R}} dA dt$$

Weak balance of thermal momentum

(cf. Romero [2010])

$$\int_{\mathcal{I}_n} \int_{\mathcal{B}_0} \delta_* \tilde{\Theta} \left[\dot{\eta} - \frac{D^{\text{tot}}}{\Theta} \right] dV dt - \int_{\mathcal{I}_n} \int_{\partial_Q \mathcal{B}_0} \delta_* \tilde{\Theta} \frac{\bar{\mathbf{Q}}}{\Theta} dA dt$$

$$- \int_{\mathcal{I}_n} \int_{\mathcal{B}_0} \text{Grad}[\delta_* \tilde{\Theta}] \cdot \frac{1}{\Theta} \mathbf{Q} dV dt = \int_{\mathcal{I}_n} \int_{\partial_\Theta \mathcal{B}_0} \delta_* \tilde{\Theta} \tilde{\lambda} dA dt$$

Weak balance of orientational momentum

$$\int_{\mathcal{I}_n} \int_{\mathcal{B}_0} \delta_* \dot{\chi} \cdot [\dot{\mathbf{p}}_\chi + 2 \tilde{\boldsymbol{\tau}}_n - \mathbf{B}_\chi] dV dt - \int_{\mathcal{I}_n} \int_{\partial_W \mathcal{B}_0} \bar{\mathbf{W}} \cdot \delta_* \dot{\chi} dA dt$$

$$+ \int_{\mathcal{I}_n} \int_{\mathcal{B}_0} \tilde{\mathbf{P}}_K : \text{Grad}[\delta_* \dot{\chi}] dV dt + \int_{\mathcal{I}_n} \int_{\mathcal{B}_0} \tilde{\mathbf{P}}_\chi : [\delta_* \dot{\chi} \otimes \mathbf{n}_0] dV dt = \int_{\mathcal{I}_n} \int_{\partial_\chi \mathcal{B}_0} \tilde{\mathbf{Z}} \cdot \delta_* \dot{\chi} dA dt$$

Weak balance of orientation rate

$$\int_{\mathcal{I}_n} \int_{\mathcal{B}_0} 2 \delta_* \tilde{\boldsymbol{\tau}}_n \cdot [\dot{\chi} + \boldsymbol{\epsilon} \cdot \dot{\boldsymbol{\alpha}} \cdot \chi] dV dt = \int_{\mathcal{I}_n} \int_{\partial_\chi \mathcal{B}_0} 2 \delta_* \tilde{\boldsymbol{\tau}}_n \cdot \tilde{\boldsymbol{\nu}} dA dt$$



Balance laws of the weak formulation (I)

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Energy and momentum functions of the LCE extended continuum

Kinetic energy $\mathcal{T}(t) := \int_{\mathcal{B}_0} \frac{1}{2} \mathbf{v} \cdot \mathbf{p} \, dV$	Kinetic energy of orientation $\mathcal{T}_\chi(t) := \int_{\mathcal{B}_0} \frac{1}{2} \mathbf{v}_\chi \cdot \mathbf{p}_\chi \, dV$	Potential energy $\Pi^{\text{int}}(t) := \int_{\mathcal{B}_0} \Psi \, dV$
Linear momentum $\mathbf{L}(t) := \int_{\mathcal{B}_0} \mathbf{p} \, dV$	Angular momentum $\mathbf{J}(t) := \int_{\mathcal{B}_0} \boldsymbol{\varphi} \times \mathbf{p} \, dV$	Momentum of orientation $\mathbf{L}_\chi(t) := \int_{\mathcal{B}_0} \mathbf{p}_\chi \, dV$
Moment of momentum $\mathbf{J}_\chi(t) := \int_{\mathcal{B}_0} \boldsymbol{\chi} \times \mathbf{p}_\chi \, dV$	Reorientation function $\mathcal{C}^{\text{ori}}(t) := \int_{\mathcal{B}_0} [\ \boldsymbol{\chi}\ ^2 - 1] \, dV$	Thermal energy $\Pi^{\text{the}}(t) := \int_{\mathcal{B}_0} \Theta \eta \, dV$
Entropy $\mathcal{S}(t) := \int_{\mathcal{B}_0} \eta \, dV$	Total energy $\mathcal{H} := \mathcal{T} + \mathcal{T}_\chi + \Pi^{\text{int}} + \Pi^{\text{the}} + \Pi^{\text{ext}}$	Lyapunov function $\mathcal{F} := \mathcal{H} - \Theta_\infty \mathcal{S}$

Linear momentum

(symmetry of virtual translations)

$$\mathbf{L}(t_{n+1}) - \mathbf{L}(t_n) = \int_{\mathcal{I}_n} \int_{\mathcal{B}_0} \mathbf{B} \, dV dt + \int_{\mathcal{I}_n} \int_{\partial_T \mathcal{B}_0} \bar{\mathbf{T}} \, dA dt + \int_{\mathcal{I}_n} \int_{\partial_\varphi \mathcal{B}_0} \tilde{\mathbf{R}} \, dA dt$$

Orientalational momentum

(symmetry of virtual orientations)

$$\mathbf{L}_\chi(t_{n+1}) - \mathbf{L}_\chi(t_n) = \int_{\mathcal{I}_n} \int_{\mathcal{B}_0} [\mathbf{B}_\chi - 2\tilde{\boldsymbol{\tau}}_n - \tilde{\mathbf{P}}_\chi \mathbf{n}_0] \, dV dt + \int_{\mathcal{I}_n} \int_{\partial_W \mathcal{B}_0} \bar{\mathbf{W}} \, dA dt + \int_{\mathcal{I}_n} \int_{\partial_\chi \mathcal{B}_0} \tilde{\mathbf{Z}} \, dA dt$$

Balance laws of the weak formulation (II)

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Thermal momentum

(cf. Romero [2010])

$$\mathcal{S}(t_{n+1}) - \mathcal{S}(t_n) = \int_{\mathcal{I}_n} \int_{\mathcal{B}_0} \frac{D^{\text{tot}}}{\Theta} dV dt + \int_{\mathcal{I}_n} \int_{\partial_Q \mathcal{B}_0} \frac{\bar{Q}}{\Theta} dA dt + \int_{\mathcal{I}_n} \int_{\partial_\Theta \mathcal{B}_0} \tilde{\lambda} dA dt$$

Angular momentum

(symmetry of virtual rotations)

$$\begin{aligned} \mathbf{J}(t_{n+1}) - \mathbf{J}(t_n) &= \int_{\mathcal{I}_n} \int_{\mathcal{B}_0} \boldsymbol{\varphi} \times \mathbf{B} dV dt + \int_{\mathcal{I}_n} \int_{\partial_T \mathcal{B}_0} \boldsymbol{\varphi} \times \bar{\mathbf{T}} dA dt + \int_{\mathcal{I}_n} \int_{\partial_\varphi \mathcal{B}_0} \boldsymbol{\varphi} \times \tilde{\mathbf{R}} dA dt \\ &+ \int_{\mathcal{I}_n} \int_{\mathcal{B}_0} [\tilde{\mathbf{F}}_\chi \tilde{\mathbf{S}}_\chi + \tilde{\mathbf{G}}_\chi \tilde{\mathbf{S}}_K] \times \tilde{\mathbf{F}} dV dt \end{aligned}$$

Moment of orientational momentum

(symmetry of virtual reorientations)

$$\begin{aligned} \mathbf{J}_\chi(t_{n+1}) - \mathbf{J}_\chi(t_n) &= \int_{\mathcal{I}_n} \int_{\mathcal{B}_0} \boldsymbol{\chi} \times \mathbf{B}_\chi dV dt + \int_{\mathcal{I}_n} \int_{\partial_W \mathcal{B}_0} \boldsymbol{\chi} \times \bar{\mathbf{W}} dA dt + \int_{\mathcal{I}_n} \int_{\partial_\chi \mathcal{B}_0} \boldsymbol{\chi} \times \tilde{\mathbf{Z}} dA dt \\ &- \int_{\mathcal{I}_n} \int_{\mathcal{B}_0} [\tilde{\mathbf{F}}_\chi \tilde{\mathbf{S}}_\chi + \tilde{\mathbf{G}}_\chi \tilde{\mathbf{S}}_K] \times \tilde{\mathbf{F}} dV dt - \int_{\mathcal{I}_n} \int_{\mathcal{B}_0} \boldsymbol{\chi} \times 2 \tilde{\boldsymbol{\tau}}_n dV dt \end{aligned}$$

Kinetic energy of motion

(symmetry of virtual time shifts)

$$\begin{aligned} \mathcal{T}(t_{n+1}) - \mathcal{T}(t_n) &= \int_{\mathcal{I}_n} \int_{\mathcal{B}_0} \mathbf{B} \cdot \dot{\boldsymbol{\varphi}} dV dt + \int_{\mathcal{I}_n} \int_{\partial_T \mathcal{B}_0} \bar{\mathbf{T}} \cdot \dot{\boldsymbol{\varphi}} dA dt + \int_{\mathcal{I}_n} \int_{\partial_\varphi \mathcal{B}_0} \tilde{\mathbf{R}} \cdot \dot{\boldsymbol{\varphi}} dA dt \\ &- \int_{\mathcal{I}_n} \int_{\mathcal{B}_0} [\tilde{\mathbf{S}} : \dot{\tilde{\mathbf{F}}} \tilde{\mathbf{F}} + \tilde{\mathbf{S}}_\chi : \dot{\tilde{\mathbf{F}}} \tilde{\mathbf{F}}_\chi + \tilde{\mathbf{S}}_K : \dot{\tilde{\mathbf{F}}} \tilde{\mathbf{G}}_\chi] dV dt \end{aligned}$$

Balance laws of the weak formulation (III)

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Kinetic energy of orientation

(symmetry of virtual time shifts)

$$\begin{aligned} \mathcal{T}_\chi(t_{n+1}) - \mathcal{T}_\chi(t_n) &= \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} \mathbf{B}_\chi \cdot \dot{\chi} \, dV dt + \int_{\mathcal{T}_n} \int_{\partial_\varphi \mathcal{B}_0} \bar{\mathbf{W}} \cdot \dot{\chi} \, dA dt + \int_{\mathcal{T}_n} \int_{\partial_\varphi \mathcal{B}_0} \bar{\mathbf{Z}} \cdot \dot{\chi} \, dA dt \\ &\quad - \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} [\tilde{\mathbf{S}}_\chi : \dot{\bar{\mathbf{F}}}^t (\dot{\bar{\mathbf{F}}}_\chi + \epsilon \cdot \dot{\alpha} \cdot \bar{\mathbf{F}}_\chi) + \tilde{\mathbf{S}}_K : \dot{\bar{\mathbf{F}}}^t \dot{\bar{\mathbf{G}}}_\chi + D_\chi^{\text{int}}] \, dV dt \end{aligned}$$

Thermal energy

(symmetry of virtual time shifts)

$$\begin{aligned} \Pi^{\text{the}}(t_{n+1}) - \Pi^{\text{the}}(t_n) &= \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} \left[-\frac{\partial \Psi}{\partial \Theta} \dot{\Theta} + D_\chi^{\text{int}} \right] \, dV dt + \int_{\mathcal{T}_n} \int_{\partial_\Theta \mathcal{B}_0} \dot{\Theta} \bar{h} \, dA dt \\ &\quad + \int_{\mathcal{T}_n} \int_{\partial_\Theta \mathcal{B}_0} \Theta \bar{\lambda} \, dA dt + \int_{\mathcal{T}_n} \int_{\partial_Q \mathcal{B}_0} \bar{Q} \, dA dt \end{aligned}$$

Potential energy

(symmetry of virtual time shifts)

$$\begin{aligned} \Pi(t_{n+1}) - \Pi(t_n) &= \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} [\tilde{\mathbf{S}}_\chi : \frac{\partial}{\partial t} (\dot{\bar{\mathbf{F}}}^t \bar{\mathbf{F}}_\chi) + \tilde{\mathbf{S}}_K : \frac{\partial}{\partial t} (\dot{\bar{\mathbf{F}}}^t \bar{\mathbf{G}}_\chi) + \tilde{\mathbf{S}}_\chi : \dot{\bar{\mathbf{F}}}^t (\epsilon \cdot \dot{\alpha}) \bar{\mathbf{F}}_\chi] \, dV dt \\ &\quad + \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} [\tilde{\mathbf{S}} : \dot{\bar{\mathbf{F}}}^t \bar{\mathbf{F}} - \mathbf{B} \cdot \dot{\varphi} - \mathbf{B}_\chi \cdot \dot{\chi}] \, dV dt \end{aligned}$$

Path-independent volume dead loads

$$\Pi^{\text{ext}}(t) := - \int_{\mathcal{B}_0} \mathbf{B} \cdot \varphi \, dV dt - \int_{\mathcal{B}_0} \mathbf{B}_\chi \cdot \chi \, dV$$

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Total energy

(cf. Romero [2010])

$$\begin{aligned} \mathcal{H}(t_{n+1}) - \mathcal{H}(t_n) &= \int_{\mathcal{T}_n} \int_{\partial_\varphi \mathcal{B}_0} \tilde{\mathbf{R}} \cdot \dot{\boldsymbol{\varphi}} \, dA \, dt + \int_{\mathcal{T}_n} \int_{\partial_\varphi \mathcal{B}_0} \tilde{\mathbf{Z}} \cdot \dot{\boldsymbol{\chi}} \, dA \, dt \\ &\quad - \int_{\mathcal{T}_n} \int_{\partial_T \mathcal{B}_0} \tilde{\mathbf{T}} \cdot \dot{\boldsymbol{\varphi}} \, dA \, dt + \int_{\mathcal{T}_n} \int_{\partial_\varphi \mathcal{B}_0} \tilde{\mathbf{W}} \cdot \dot{\boldsymbol{\chi}} \, dA \, dt \\ &\quad - \int_{\mathcal{T}_n} \int_{\partial_\Theta \mathcal{B}_0} \tilde{\lambda} \Theta \, dA \, dt + \int_{\mathcal{T}_n} \int_{\partial_\Theta \mathcal{B}_0} \tilde{h} \dot{\Theta} \, dA \, dt + \int_{\mathcal{T}_n} \int_{\partial_Q \mathcal{B}_0} \bar{Q} \, dA \, dt \end{aligned}$$

Lyapunov function

(cf. Romero [2010])

$$\begin{aligned} \mathcal{F}(t_{n+1}) - \mathcal{F}(t_n) &= \int_{\mathcal{T}_n} \int_{\partial_T \mathcal{B}_0} \tilde{\mathbf{T}} \cdot \dot{\boldsymbol{\varphi}} \, dA \, dt + \int_{\mathcal{T}_n} \int_{\partial_\varphi \mathcal{B}_0} \tilde{\mathbf{R}} \cdot \dot{\boldsymbol{\varphi}} \, dA \, dt \\ &\quad + \int_{\mathcal{T}_n} \int_{\partial_\varphi \mathcal{B}_0} \tilde{\mathbf{W}} \cdot \dot{\boldsymbol{\chi}} \, dA \, dt + \int_{\mathcal{T}_n} \int_{\partial_\varphi \mathcal{B}_0} \tilde{\mathbf{Z}} \cdot \dot{\boldsymbol{\chi}} \, dA \, dt + \int_{\mathcal{T}_n} \int_{\partial_\Theta \mathcal{B}_0} \tilde{h} \dot{\Theta} \, dA \, dt \\ &\quad - \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} \frac{\Theta_\infty}{\Theta} D^{\text{tot}} \, dV \, dt + \int_{\mathcal{T}_n} \int_{\partial_Q \mathcal{B}_0} \frac{\Theta - \Theta_\infty}{\Theta} \bar{Q} \, dA \, dt \end{aligned}$$

Reorientation function

$$\mathcal{C}^{\text{ori}}(t_{n+1}) - \mathcal{C}^{\text{ori}}(t_n) \equiv \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} 2 \boldsymbol{\chi} \cdot \dot{\boldsymbol{\chi}} \, dV \, dt = \int_{\mathcal{T}_n} \int_{\partial_{\boldsymbol{\chi}} \mathcal{B}_0} 2 \boldsymbol{\chi} \cdot \tilde{\boldsymbol{\nu}} \, dA \, dt$$

Thin LCE film subject to initial rotation

Boundary and initial conditions

121-em with H2O-mixed-Bbar

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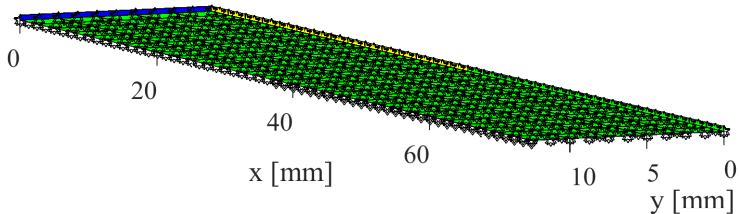
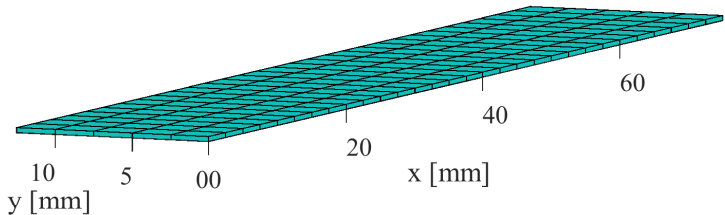
Boundary load

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Mesh and boundary conditions

$$n_0^A = e_y, \omega_0^A = 32 e_z [1/s]$$



Activated Dirichlet and Neumann boundaries

Green bottom patches as boundary $\partial_x \mathcal{B}_0$: Fixed orientation $n_z^A = 0$

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Isothermal dynamical effects of the reorientation

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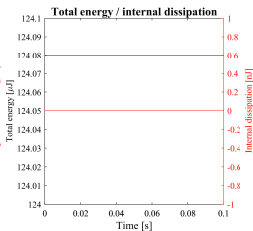
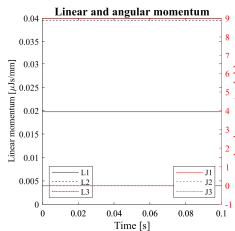
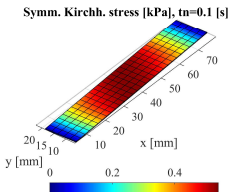
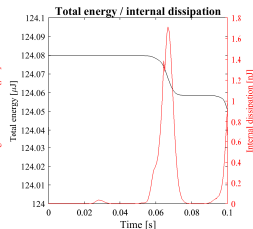
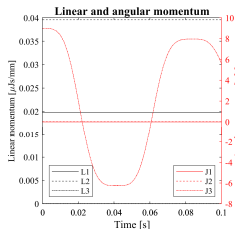
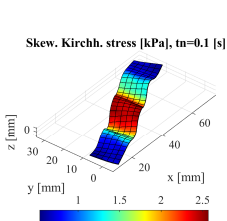
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Balance laws with/without reorientation ($E \approx 0.914$ [MPa], $\nu \approx 0.493$)



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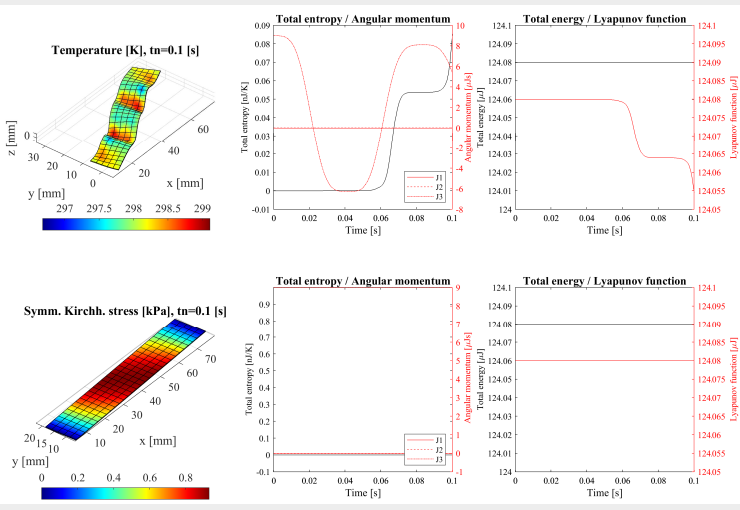
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Balance laws with/without reorientation ($E \approx 0.914$ [MPa], $\nu \approx 0.493$)





Thin LCE film subject to initial rotation

Unsteady right-left-rotation due to reorientation

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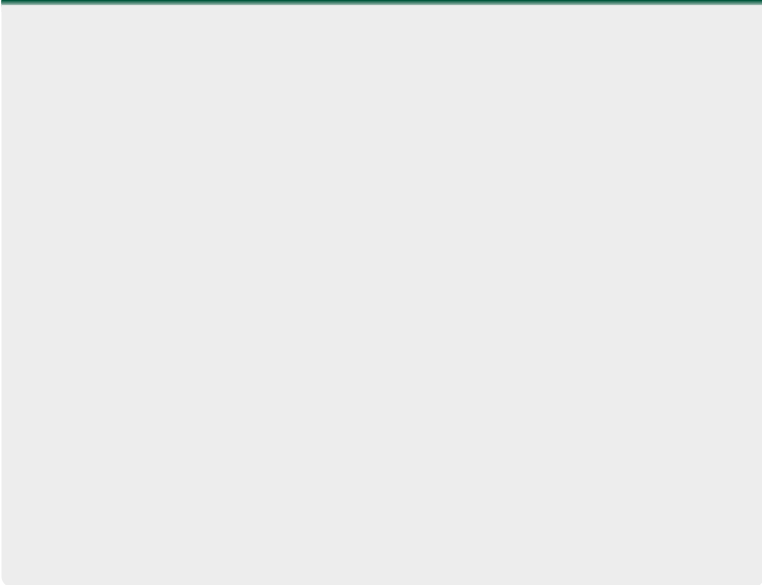
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Movie I of a **soft** film

($E \approx 0.914$ [MPa], $\nu \approx 0.493$)





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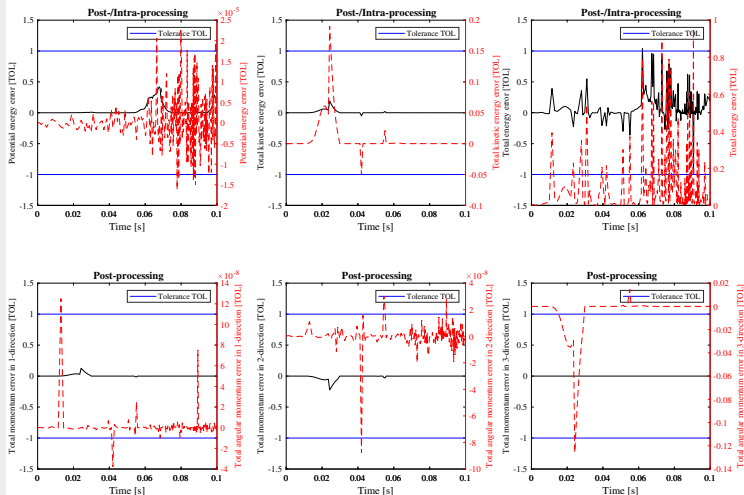
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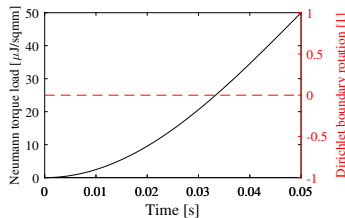
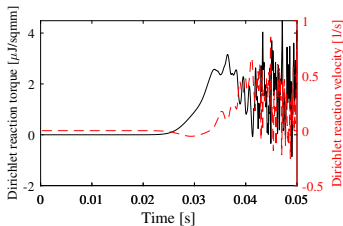
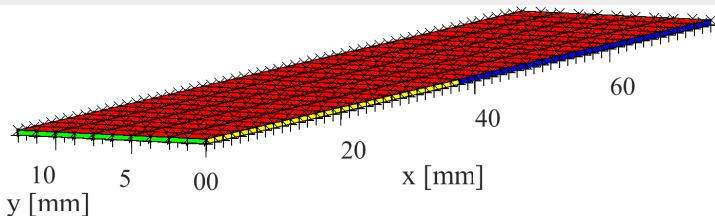
Balance laws versus time

($E \approx 0.914$ [MPa], $\nu \approx 0.493$)



Boundary conditions and loads

$$n_0 = (e_x + e_y)/\sqrt{2}$$



Activated Dirichlet and Neumann boundaries

Red top as $\partial_W \mathcal{B}_0$: $W_y^A = -\hat{W}^A(t)$ Green bottom as $\partial_X \mathcal{B}_0$: Fixed orientation $n_z^A = 0$



Thin LCE film subject to boundary load

Contraction with folding motion

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($E \approx 9.140$ [MPa], $\nu \approx 0.493$)



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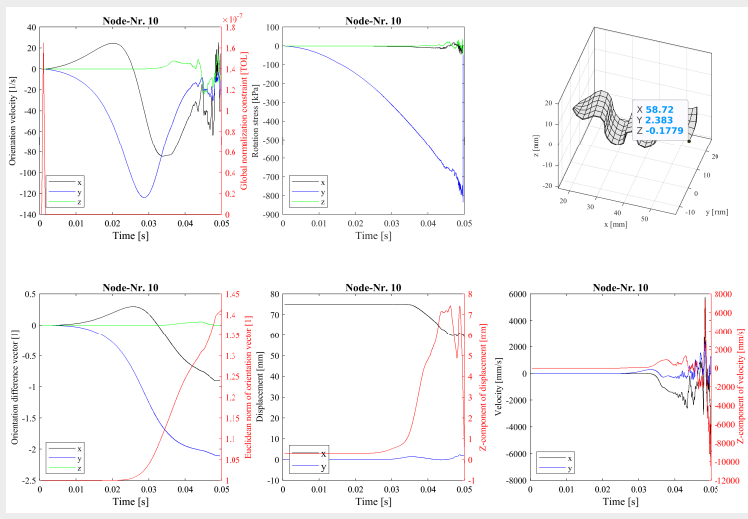
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Nodal time evolutions

($E \approx 9.140$ [MPa], $\nu \approx 0.493$)





Thin LCE film subject to boundary load

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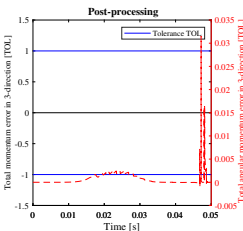
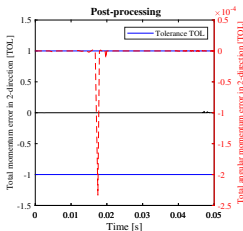
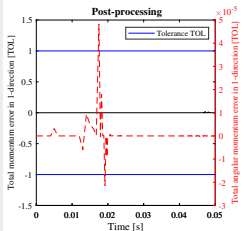
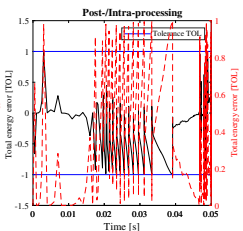
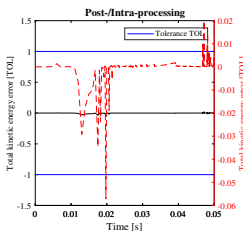
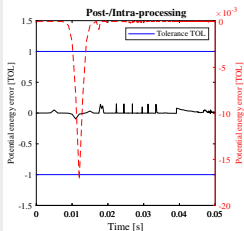
Boundary load

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Time adaptivity based on balance laws

($E \approx 9.140$ [MPa], $\nu \approx 0.493$)





Thin LCE film subject to volume load

Boundary and initial conditions

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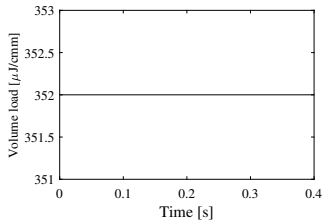
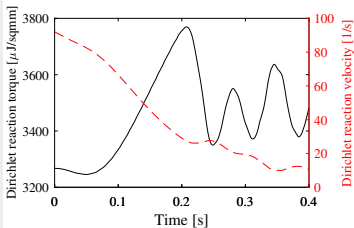
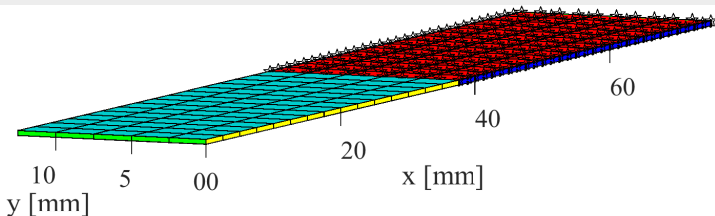
Boundary load

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Boundary conditions and loads

$$n_0 = e_x$$



Activated Dirichlet and Neumann boundaries

Red top as $\partial_\chi \mathcal{B}_0$: Orientation $n^A = n_0^A$ Blue sides as $\partial_\theta \mathcal{B}_0$: Temperature $\theta^A = \theta_\infty$



Thin LCE film subject to volume load

Steady clockwise rotation due to reorientation

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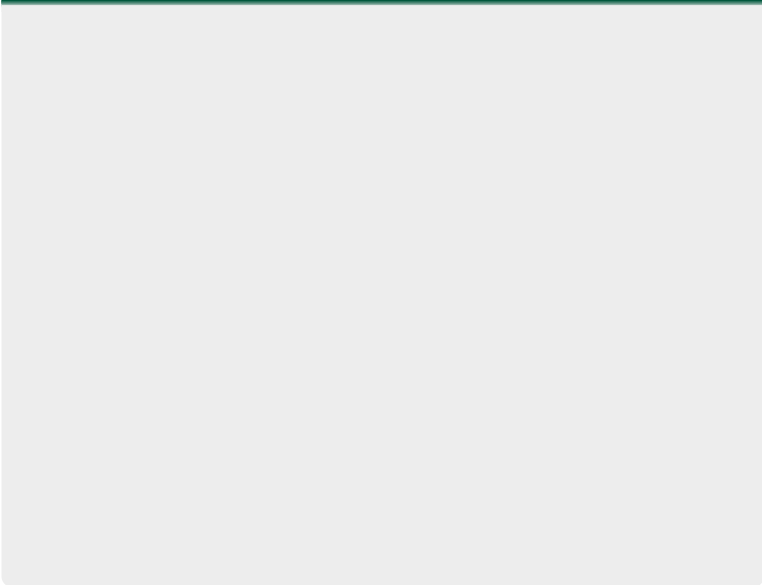
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Movie I of the **stiff** film

($E \approx 9.140$ [MPa], $\nu \approx 0.493$)





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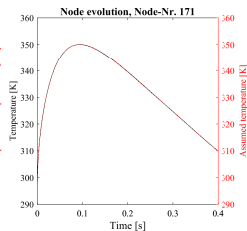
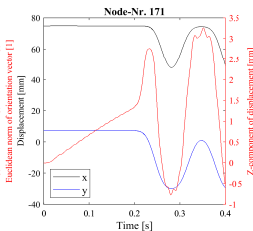
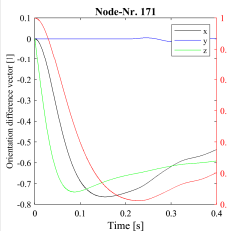
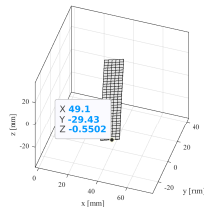
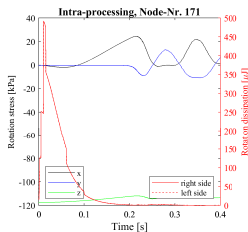
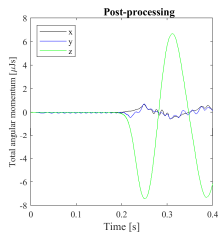
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Nodal time evolutions and balance laws ($E \approx 9.140$ [MPa], $\nu \approx 0.493$)





- 1 Motivation: **Non-isothermal simulations of motion actuations**
 - ▶ with **liquid crystal elastomers** as actuator material by using of
 - ▶ **boundary** and **volume** loads (thermal and photochemical fields).
- 2 Numerical goals: **Dynamic finite element simulations**
 - ▶ with the approach of a **mixed finite element** method and
 - ▶ **reorientations** by using of drilling degrees of freedom.
- 3 Numerical strategy: **Boundary and volume actuation by**
 - ▶ introducing an **independent global orientation field**,
 - ▶ formulating local rotations by **drilling degrees of freedom**,
 - ▶ using of **local evolution equations** for stress-induced motions.
- 4 Numerical results: **Motion actuation with**
 - ▶ **Neumann boundary** loads and **volume-specific** loads
 - ▶ activates **deformation modes** and **rigid-body modes**.
- 5 Next step:
 - ▶ **Adapting orientation loads** for simulating **thermal actuations**