

# A New Mixed FE-Formulation for Liquid Crystal Elastomer Films

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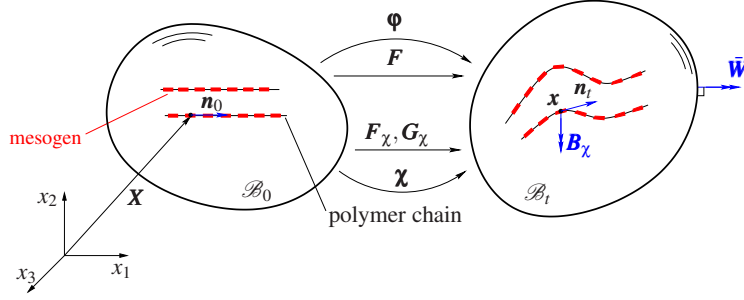
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**Abstract.** Liquid crystal elastomers (LCEs) are soft materials, which are capable of large deformations induced by temperature changes and ultraviolet irradiation [1]. Therefore, since many years, these materials are under investigation in experimental researches as actuator materials. LCEs arise from a nematic polymer melt, consisting of long and flexible polymer chains as well as oriented and rigid rod-like molecules, the so-called mesogens, by crosslinking. After this process, the flow ability and the orientation of the mesogens is retained. To date, the alignment of LCEs is primarily achieved in thin films. When the orientational order in the film is lost due to temperature changes or ultraviolet irradiation, the LCE film is capable of length changes of 400 percent. In order to numerically simulate LCE materials as actuators in multibody system models by using the finite element method, a continuum formulation is necessary, which include in a thermo-viscoelastic material formulation of the polymer chains the orientation effects of the mesogens. This can be performed by introducing a normalized direction vector as an independent field, and deriving from additional (orientational) balance laws independent differential equations [2]. These differential equations describe the independent rotation of the rigid mesogens connected with the flexible polymer chains. The orientation-dependent stress law of LCEs arises from an anisotropic free energy, comparable with fibre-reinforced materials. But, the direction vector of a LCE model has to be independent. In contrast to [2], we apply a variational principle for deriving a new mixed finite element (FE) formulation, which is based on drilling degrees of freedom for describing the mesogens rotation [3]. This principle leads to balance laws, preserved by an energy-momentum scheme.

## 1 INTRODUCTION

Liquid crystals are liquids with regularly arranged or oriented molecules. Since this is not a crystal phase nor an isotropic liquid phase, liquid crystals are in the so-called mesophase. The simplest form of a mesophase is the nematic phase, because here the mesogens are arranged almost in parallel. In LCE, a change of temperature can lead to a transition from the nematic orientation to a disordered (isotropic) orientation, and vice versa. The mesogens of a LCE can be described by an orientation vector  $\mathbf{n}_0$ , with  $\mathbf{n}_0 \cdot \mathbf{n}_0 = 1$  (see Fig. 1), in the initial configuration  $\mathcal{B}_0$ . Hence, the temperature increase causes the rotation of the orientation vector at the material point  $\mathbf{X} \in \mathcal{B}_0$  into the orientation  $\mathbf{n}_t$  at the position  $\mathbf{x} \in \mathcal{B}_t$  of the current configuration  $\mathcal{B}_t$ . First constitutive laws for liquid crystals are presented in [4], wherein a free energy function in dependence on  $\mathbf{n}_t$  is derived. This Frank free energy increases with the distortion of the orientation vector field  $\mathbf{n}_t(\mathbf{x})$ . It is based on a quadratic form with respect to the spatial gradient  $\text{grad}[\mathbf{n}_t]$ , where  $\text{grad}[\bullet]$  denotes the partial derivative with respect to  $\mathbf{x} \in \mathcal{B}_t$ . Reference [5] is a



**Figure 1:** Configurations of a LCE with orientational volume and surface loads.

first one about a continuum theory for LCE, in which  $\mathbf{n}_t$  is considered with boundary conditions. This theory defines balance laws with a kinetic energy with respect to the partial time derivative  $\dot{\mathbf{n}}_t$  as well as volume and surface forces acting on  $\mathbf{n}_t$ . In this way, the linear momentum balance law defines the motion, and an orientational momentum balance law the time evolution of  $\mathbf{n}_t$ . In [2], this approach is extended by the dynamical constraint  $\mathbf{n}_t \cdot \mathbf{n}_t = 1$  in the sense of a differential-algebraic system. Here, the balance laws are formulated in a Lagrangian description based on the material gradient  $\text{Grad}[\mathbf{n}_t \circ \boldsymbol{\varphi}]$ , where  $\text{Grad}[\bullet]$  denotes the partial derivative with respect to  $\mathbf{X} \in \mathcal{B}_0$  and  $\boldsymbol{\varphi}$  the deformation mapping (see Fig. 1). Reference [6] satisfies the constraint  $\|\mathbf{n}_t\| = 1$  by means of the rotation tensor. A special mixed FE-formulation with respect to  $\mathbf{n}_t$  is able to avoid a differential-algebraic equation system or a rotation tensor equation, respectively, because the pure rotation of  $\mathbf{n}_t$  can be formulated by local drilling degrees of freedom [3]. Therefore, in this paper, we present a non-isothermal mixed finite element formulation with energy-momentum scheme based on drilling degrees of freedom for rotating the orientation vector.

## 2 CONTINUUM MODEL

We consider a LCE material, moving in the  $n_{\text{dim}}$ -dimensional ambient space  $\mathbb{R}^{n_{\text{dim}}}$  with temperature  $\Theta_\infty$ , as a continuum in the configuration  $\mathcal{B}_0$  with the orientation vector  $\mathbf{n}_0(\mathbf{X})$  in the material point  $\mathbf{X} \in \mathcal{B}_0$  at initial time  $t = 0$ . The deformation mapping  $\boldsymbol{\varphi} : \mathcal{B}_0 \times \mathcal{T} \rightarrow \mathcal{B}_t$  describes the motion in the time interval  $\mathcal{T} = [0, T]$  into the deformed configuration  $\mathcal{B}_t$  at time  $t \in \mathcal{T}$ , and satisfies the identity  $\boldsymbol{\varphi}(\mathbf{X}, 0) = \mathbf{X}$  at each point  $\mathbf{X} \in \mathcal{B}_0$ . The *temperature mapping*  $\Theta : \mathcal{B}_0 \times \mathcal{T} \rightarrow \mathbb{R}_+$  maps the initial value  $\Theta(\mathbf{X}, 0) = \Theta_0(\mathbf{X})$  of the absolute temperature to the temperature  $\theta(\mathbf{x})$  in  $\mathbf{x} = \boldsymbol{\varphi}(\mathbf{X}) \in \mathcal{B}_t$ . The time evolution of the temperature follows from the time rate  $\dot{\Theta}(\mathbf{X}, t) = \dot{\theta}$ , where the superposed dot denotes the partial derivative with respect to time  $t$ . The *orientation mapping*  $\boldsymbol{\chi} : \mathcal{B}_0 \times \mathcal{T} \rightarrow \mathbb{R}^{n_{\text{dim}}}$ , satisfying  $\boldsymbol{\chi}(\mathbf{X}, 0) = \mathbf{n}_0(\mathbf{X})$  at each point  $\mathbf{X} \in \mathcal{B}_0$ , gives the orientation vector  $\mathbf{n}_t(\mathbf{x})$  in the point  $\mathbf{x} \in \mathcal{B}_t$ . The deformation  $\boldsymbol{\varphi}$  results by time integration from the material velocity vector  $\mathbf{v}(\mathbf{X}, t) := \dot{\boldsymbol{\varphi}}(\mathbf{X}, t) = \dot{\mathbf{x}}$ . The orientation  $\boldsymbol{\chi}$  arises from the *orientational velocity vector*  $\mathbf{v}_\chi(\mathbf{X}, t) := \dot{\boldsymbol{\chi}}(\mathbf{X}, t) = \dot{\mathbf{n}}_t$ . Denoting by  $\rho_0$  the mass density in  $\mathcal{B}_0$ , we then obtain the linear momentum vector  $\mathbf{p} := \rho_0 \mathbf{v}$ . As in [2, 3], we assume a *radius of gyration*  $l_\chi$  associated with the mesogens in direction  $\mathbf{n}_0$  within the representative volume element of the edge length  $l_0$  at each point  $\mathbf{X} \in \mathcal{B}_0$ . We arrive at the *orientational momentum vector*

$$\mathbf{p}_\chi := \mathbf{A}_\chi \mathbf{v}_\chi = \rho_0 \left[ (l_\chi^2 - l_0^2) \mathbf{A}_0 + l_0^2 \mathbf{I} \right] \mathbf{v}_\chi \quad (1)$$

where  $\mathbf{A}_0 := \mathbf{n}_0 \otimes \mathbf{n}_0$  denotes the second-order structural tensor of the mesophase and  $\mathbf{I}$  the second-order identity tensor. The infinitesimal line element  $d\mathbf{x} = \mathbf{F} d\mathbf{X}$  at the position  $\mathbf{x} \in \mathcal{B}_t$  is given by the defor-

mation gradient  $\mathbf{F} := \text{Grad}[\boldsymbol{\varphi}]$ . Analogously, we introduce the *orientation tensor*  $\mathbf{F}_\chi := \boldsymbol{\chi} \otimes \mathbf{n}_0$ , which maps the initial orientation  $\mathbf{n}_0$  to the current orientation  $\mathbf{n}_t$  (see Fig. 1). The stretch of the material line element  $d\mathbf{x}$  is measured by the right Cauchy-Green tensor  $\mathbf{C} := \mathbf{F}^t \mathbf{g} \mathbf{F}$  with respect to the *translational metric tensor*  $\mathbf{g} := \text{grad}[\mathbf{x}]$ . We denote by the superscript  $t$  the transposition of a second-order tensor. In the same way, the stretch of the material line element  $d\mathbf{x}$  due to the rotation of the orientation vector  $\mathbf{n}_t$  is determined by the *orientational deformation tensor*  $\mathbf{C}_\chi := \mathbf{F}^t \mathbf{g} \mathbf{F}_\chi = \mathbf{F}^t \mathbf{g}_\chi \mathbf{F}$ , where  $\mathbf{g}_\chi$  designates the *orientational metric tensor*. The orientational invariants in Reference [2] for describing an isothermal *interactive free energy density*  $\Psi_i(\mathbf{F}^t \mathbf{g} \boldsymbol{\chi}) := \hat{\Psi}^{\text{ori}}(I_1^{\text{ori}}, J_2^{\text{ori}})$  can be written as

$$I_1^{\text{ori}} := \mathbf{C}_\chi \mathbf{A}_0 : \mathbf{G}^{-1} \quad J_2^{\text{ori}} := \mathbf{C}_\chi \mathbf{A}_0 : \mathbf{C}_\chi \mathbf{A}_0 \quad (2)$$

where the symbol  $:$  indicates double contraction and the translational metric tensor  $\mathbf{G} := \text{Grad}[\mathbf{X}]$  belongs to the initial configuration  $\mathcal{B}_0$ . Hence, we consider the interactive free energy  $\Psi^{\text{ori}}(\mathbf{C}_\chi)$ . The considered non-isothermal *elastic free energy density*  $\Psi^{\text{ela}}(\mathbf{C}, \Theta) := \hat{\Psi}^{\text{ela}}(I_1^{\text{ela}}, J_2^{\text{ela}}, I_3^{\text{ela}}, \Theta)$  depends on the invariants

$$I_1^{\text{ela}} := \mathbf{C} : \mathbf{G}^{-1} \quad J_2^{\text{ela}} := \mathbf{C} : \mathbf{C} \quad I_3^{\text{ela}} := \det[\mathbf{C}] \quad (3)$$

In order to quantify the increase of the Frank free energy density caused by distortions with respect to the initial configuration  $\mathcal{B}_0$ , we introduce the *distorsion tensor*  $\mathbf{K}_\chi := \mathbf{F}^t \mathbf{g} \mathbf{G}_\chi = \mathbf{F}^t \mathbf{g}_K \mathbf{F}$  with the metric tensor  $\mathbf{g}_K := \text{grad}[\mathbf{n}_t]$ . We refer to  $\mathbf{G}_\chi := \text{Grad}[\boldsymbol{\chi}]$  as the *orientation gradient*. Motivated by [3], the distorsion can be then measured by the invariants

$$I_1^{\text{dis}} := (\mathbf{K}_\chi - \text{Grad}[\mathbf{n}_0]) : \mathbf{G}^{-1} \quad J_2^{\text{dis}} := (\mathbf{K}_\chi - \text{Grad}[\mathbf{n}_0]) : (\mathbf{K}_\chi - \text{Grad}[\mathbf{n}_0]) \quad (4)$$

which vanish in the initial configuration. Thus, we assume a general form of the free energy, given by

$$\Psi(\mathbf{C}, \mathbf{C}_\chi, \mathbf{K}_\chi, \Theta) := \Psi^{\text{ela}}(\mathbf{C}, \Theta) + \Psi^{\text{ori}}(\mathbf{C}_\chi) + \Psi^{\text{dis}}(\mathbf{K}_\chi) \quad (5)$$

In a LCE, the rotation of the orientation vector  $\mathbf{n}_t$  is directly connected with the deformation  $\boldsymbol{\varphi}$ . Stretching the LCE, we obtain a stress field rotating  $\mathbf{n}_t$ . Such a dissipative *reorientation* can be introduced by a evolution equation [7]. Analogous to finite viscoelasticity, we start with the Clausius-Planck inequality

$$D_\chi^{\text{int}} := \mathbf{N}_\chi : \mathbf{g} \dot{\mathbf{F}} - \dot{\Psi}^{\text{ori}}(\mathbf{C}_\chi) \equiv \left[ \mathbf{N}_\chi - \mathbf{F}_\chi \mathbf{S}_\chi^t \right] : \mathbf{g} \dot{\mathbf{F}} - \mathbf{F} \mathbf{S}_\chi : \mathbf{g} \dot{\mathbf{F}}_\chi \geq 0 \quad (6)$$

for the *reorientation dissipation*  $D_\chi^{\text{int}}$ . From now on, we require that the orientation vector  $\mathbf{n}_t$  has unit length  $\|\mathbf{n}_t\| = 1$  at each  $t \in \mathcal{T}$ . Hence, the velocity rate tensor  $\mathbf{g} \dot{\mathbf{F}}_\chi \mathbf{F}_\chi^{-1}$  is skew-symmetric and given by

$$\mathbf{g} \dot{\mathbf{F}}_\chi \mathbf{F}_\chi^{-1} = \boldsymbol{\varepsilon} \cdot \dot{\boldsymbol{\alpha}} \quad \text{with} \quad \dot{\boldsymbol{\alpha}} := \dot{\alpha}^k \mathbf{g}_k \circ \boldsymbol{\varphi}(\mathbf{X}, t) \quad (7)$$

We denote by  $\boldsymbol{\varepsilon}$  the third-order Levi-Civita tensor. We herewith introduce a *rotation mapping*  $\boldsymbol{\alpha} : \mathcal{B}_0 \times \mathcal{T} \rightarrow \mathbb{R}^{n_{\text{dim}}}$ , which satisfies the condition  $\boldsymbol{\alpha}(\mathbf{X}, 0) = \mathbf{0}$  at each point  $\mathbf{X} \in \mathcal{B}_0$ , where  $\mathbf{0}$  designates the zero vector. We arrive at the reorientation dissipation

$$D_\chi^{\text{int}} := \left[ \mathbf{N}_\chi - \mathbf{F}_\chi \mathbf{S}_\chi^t \right] : \mathbf{g} \dot{\mathbf{F}} - \boldsymbol{\tau}_\chi : \boldsymbol{\varepsilon} \cdot \dot{\boldsymbol{\alpha}} \geq 0 \quad (8)$$

We denote with  $\boldsymbol{\tau}_\chi := \mathbf{F} \mathbf{S}_\chi \mathbf{F}_\chi^t$  a two-point orientational stress tensor, which we refer to as *orientational Kirchhoff stress tensor*. According to the Coleman-Noll procedure, we define the two-point *Piola*

reorientation stress tensor  $\mathbf{N}_\chi := \mathbf{F}_\chi \mathbf{S}_\chi^t$ , where the *orientational stress tensor*  $\mathbf{S}_\chi := \partial\Psi^{\text{ori}}/\partial\mathbf{C}_\chi$  is energy-conjugated to  $\mathbf{C}_\chi$ . Consequently,  $D_\chi^{\text{int}}$  is always non-negative with the local evolution equation

$$-\frac{1}{2}\boldsymbol{\varepsilon} : \boldsymbol{\tau}_\chi = \boldsymbol{\Sigma}_\chi \quad \text{with} \quad \boldsymbol{\Sigma}_\chi = V_\chi \dot{\boldsymbol{\alpha}} \quad (9)$$

and takes the form of the bilinear form  $D_\chi^{\text{int}} := 2\boldsymbol{\Sigma}_\chi \cdot \dot{\boldsymbol{\alpha}} \geq 0$  with respect to the *rotational viscosity parameter*  $V_\chi$ . The rotation of  $\mathbf{n}_t$  due to the reorientation in the LCE is then given by the global equation

$$\dot{\boldsymbol{\chi}} = -\boldsymbol{\varepsilon} \cdot \dot{\boldsymbol{\alpha}} \cdot \boldsymbol{\chi} \quad (10)$$

The natural constraint  $\|\mathbf{n}_t\| = 1$  for the orientation vector at each point  $\mathbf{x} \in \mathcal{B}_t$  is satisfied by the identity  $\dot{\boldsymbol{\chi}} \cdot \boldsymbol{\chi} = 0$  at each time  $t \in \mathcal{T}$  due to the initial condition  $\mathbf{n}_0 \cdot \mathbf{n}_0 = 1$ .

### 3 MIXED FINITE ELEMENT FORMULATION

We aim at a weak formulation with mixed fields  $\tilde{\mathbf{U}}_i$ ,  $i = 1, \dots, s$ , whose time evolutions have to be continuous, and remainder fields  $\tilde{\mathbf{V}}_j$ ,  $j = 1, \dots, p$ , which are temporally discontinuous, in general. Thus, a space-time discretization will be energy-consistent, if we use the *mixed principle of virtual power*

$$\int_{t_n}^{t_{n+1}} \delta_* \mathcal{H}(\dot{\tilde{\mathbf{U}}}_1, \dots, \dot{\tilde{\mathbf{U}}}_s, \tilde{\mathbf{V}}_1, \dots, \tilde{\mathbf{V}}_p) dt = 0 \quad (11)$$

on any time step  $\mathcal{T}_n := [t_n, t_{n+1}] \subset \mathcal{T}$  of time step size  $h_n := t_{n+1} - t_n$  based on the *total energy functional*  $\mathcal{H}$ . Since the variation is performed with respect to time derivatives of  $\tilde{\mathbf{U}}_i$  ( $\delta_1$  variations) as well as with respect to time functions  $\tilde{\mathbf{V}}_j$  itself ( $\delta$  or  $\delta_0$  variations), we consider the  $\delta_*$  symbol. We start by summarizing the virtual power  $\delta_* \mathcal{P}_\varphi$  associated with the deformation  $\boldsymbol{\varphi}$ , given by

$$\delta_* \mathcal{P}_\varphi := \delta_* \dot{\mathcal{I}}_\varphi(\dot{\boldsymbol{\varphi}}, \dot{\mathbf{v}}, \dot{\mathbf{p}}) + \delta_* \dot{\Pi}_\varphi^{\text{ext}}(\dot{\boldsymbol{\varphi}}, \dot{\tilde{\mathbf{R}}}) + \delta_* \dot{\Pi}_\varphi^{\text{int}}(\dot{\boldsymbol{\varphi}}, \dot{\tilde{\mathbf{F}}}, \dot{\tilde{\mathbf{C}}}, \dot{\tilde{\mathbf{P}}}, \dot{\tilde{\mathbf{S}}}) \quad (12)$$

The first term of Eq. (12) associated with the inertia of translations of material points  $\mathbf{X} \in \mathcal{B}_0$  is given by

$$\delta_* \dot{\mathcal{I}}_\varphi(\dot{\boldsymbol{\varphi}}, \dot{\mathbf{v}}, \dot{\mathbf{p}}) := \int_{\mathcal{B}_0} \delta_* \dot{\mathbf{v}} \cdot [\rho_0 \mathbf{v} - \mathbf{p}] dV + \int_{\mathcal{B}_0} \delta_* \dot{\mathbf{p}} \cdot [\boldsymbol{\varphi} - \mathbf{v}] dV + \int_{\mathcal{B}_0} \delta_* \dot{\boldsymbol{\varphi}} \cdot \dot{\mathbf{p}} dV \quad (13)$$

Here,  $\mathbf{v}$  and  $\mathbf{p}$  are introduced as independent (mixed) fields. The second term of Eq. (12) introduces volume loads  $\mathbf{B}$ , traction loads  $\tilde{\mathbf{T}}$  and prescribed boundary displacements  $\tilde{\boldsymbol{\varphi}}$  by using the functional

$$\delta_* \dot{\Pi}_\varphi^{\text{ext}}(\dot{\boldsymbol{\varphi}}, \dot{\tilde{\mathbf{R}}}) := - \int_{\mathcal{B}_0} \delta_* \dot{\boldsymbol{\varphi}} \cdot \mathbf{B} dV - \int_{\partial_T \mathcal{B}_0} \delta_* \dot{\boldsymbol{\varphi}} \cdot \tilde{\mathbf{T}} dA - \int_{\partial_\varphi \mathcal{B}_0} \delta_* \dot{\tilde{\mathbf{R}}} \cdot [\dot{\boldsymbol{\varphi}} - \dot{\tilde{\boldsymbol{\varphi}}}] dA - \int_{\partial_\varphi \mathcal{B}_0} \delta_* \dot{\boldsymbol{\varphi}} \cdot \tilde{\mathbf{R}} dA \quad (14)$$

where the reaction force field on the Dirichlet boundary  $\partial_\varphi \mathcal{B}_0 := \partial \mathcal{B}_0 \setminus \partial_T \mathcal{B}_0$  disjunct with the Neumann boundary  $\partial_T \mathcal{B}_0$  is denoted by  $\tilde{\mathbf{R}}$ . The last term takes the form  $\delta_* \dot{\Pi}_\varphi^{\text{int}}(\dot{\boldsymbol{\varphi}}, \dot{\tilde{\mathbf{F}}}, \dot{\tilde{\mathbf{C}}}, \dot{\tilde{\mathbf{P}}}, \dot{\tilde{\mathbf{S}}}) := \delta_* \mathcal{P}_\varphi^{\text{int}}$  with

$$\begin{aligned} \delta_* \mathcal{P}_\varphi^{\text{int}} := & \int_{\mathcal{B}_0} \delta_* \dot{\tilde{\mathbf{P}}} : [\text{Grad}[\dot{\boldsymbol{\varphi}}] - \dot{\tilde{\mathbf{F}}}] dV + \frac{1}{2} \int_{\mathcal{B}_0} \delta_* \dot{\tilde{\mathbf{S}}} : \left[ \frac{\partial}{\partial t} (\tilde{\mathbf{F}}^t \tilde{\mathbf{F}}) - \dot{\tilde{\mathbf{C}}} \right] dV \\ & + \int_{\mathcal{B}_0} \delta_* \dot{\tilde{\mathbf{C}}} : \left[ \frac{\partial \Psi}{\partial \tilde{\mathbf{C}}} - \frac{1}{2} \tilde{\mathbf{S}} \right] dV + \int_{\mathcal{B}_0} \delta_* \dot{\tilde{\mathbf{F}}} : [\tilde{\mathbf{F}} \tilde{\mathbf{S}} - \tilde{\mathbf{P}}] dV + \int_{\mathcal{B}_0} \dot{\tilde{\mathbf{P}}} : \text{Grad}[\delta_* \dot{\boldsymbol{\varphi}}] dV \end{aligned} \quad (15)$$

where  $\tilde{\mathbf{P}}$  and  $\tilde{\mathbf{S}}$  denote the independent fields of the first and second Piola-Kirchhoff stress tensor, respectively. Since we aim at the consideration of thermal material behaviour of the LCE as well as thermal boundary conditions, we consider the virtual thermal power

$$\delta_* \mathcal{P}_\Theta := \delta_* \dot{\Pi}_\Theta^{\text{ext}}(\dot{\Theta}, \tilde{\Theta}, \tilde{\lambda}, \tilde{h}) + \delta_* \dot{\Pi}_\Theta^{\text{int}}(\dot{\Theta}, \dot{\eta}, \tilde{\Theta}) \quad (16)$$

The functional in the first term of Eq. (16) introduces a Dirichlet boundary  $\partial_\Theta \mathcal{B}_0 \cup \partial_{\dot{\Theta}} \mathcal{B}_0 := \partial \mathcal{B}_0 \setminus \partial_Q \mathcal{B}_0$  disjunct with the Neumann boundary  $\partial_Q \mathcal{B}_0$ . On the Dirichlet boundary  $\partial_\Theta \mathcal{B}_0$ , we prescribe the constant ambient temperature  $\Theta_\infty$ , and on the Dirichlet boundary  $\partial_{\dot{\Theta}} \mathcal{B}_0$ , a time evolution  $\tilde{\Theta}$  of the temperature is prescribed. Here, we have to make a difference, because of using the entropy density field  $\eta$  as mixed field. A prescribed time evolution  $\tilde{\Theta}$  then generates a *boundary entropy*  $\tilde{h}$  on  $\partial_{\dot{\Theta}} \mathcal{B}_0$ . The functional reads

$$\begin{aligned} \delta_* \dot{\Pi}_\Theta^{\text{ext}}(\dot{\Theta}, \tilde{\Theta}, \tilde{\lambda}, \tilde{h}) := & \int_{\mathcal{B}_0} \delta_* \tilde{\Theta} \frac{D^{\text{tot}}}{\Theta} dV + \int_{\mathcal{B}_0} \frac{1}{\Theta} \text{Grad}[\delta_* \tilde{\Theta}] \cdot \mathbf{Q} dV + \int_{\partial_Q \mathcal{B}_0} \delta_* \tilde{\Theta} \frac{\bar{Q}}{\Theta} dA + \int_{\partial_\Theta \mathcal{B}_0} \delta_* \tilde{\Theta} \tilde{\lambda} dA \\ & + \int_{\partial_\Theta \mathcal{B}_0} \delta_* \tilde{\lambda} [\tilde{\Theta} - \Theta_\infty] dA - \int_{\partial_{\dot{\Theta}} \mathcal{B}_0} \delta_* \tilde{h} [\dot{\Theta} - \dot{\tilde{\Theta}}] dA - \int_{\partial_{\dot{\Theta}} \mathcal{B}_0} \delta_* \dot{\Theta} \tilde{h} dA \end{aligned} \quad (17)$$

with the inward heat surface density  $\bar{Q}$  on the Neumann boundary  $\partial_Q \mathcal{B}_0$  and the *boundary heat flux*  $\tilde{\lambda}$  on the Dirichlet boundary  $\partial_\Theta \mathcal{B}_0$ . A thermal volume load is given by the total dissipation

$$D^{\text{tot}} := D^{\text{cdu}} + D_\chi^{\text{int}} = -\frac{1}{\Theta} \text{Grad}[\Theta] \cdot \mathbf{Q} + 2 \dot{\boldsymbol{\alpha}} \cdot \boldsymbol{\Sigma}_\chi \quad \text{with} \quad \mathbf{Q} := -k_0 \det[\tilde{\mathbf{F}}] \tilde{\mathbf{C}}^{-1} \text{Grad}[\Theta] \quad (18)$$

by assuming Fourier's law of isotropic heat conduction in its Lagrangian description. The second term of Eq. (16) introduces the specific heat capacity  $c$  and the linear thermal expansion coefficient  $\beta$  of the LCE by means of the functional

$$\delta_* \dot{\Pi}_\Theta^{\text{int}}(\dot{\Theta}, \dot{\eta}, \tilde{\Theta}) := \int_{\mathcal{B}_0} \delta_* \dot{\Theta} \left( \frac{\partial \Psi}{\partial \Theta} + \eta \right) dV + \int_{\mathcal{B}_0} \delta_* \dot{\eta} (\Theta - \tilde{\Theta}) dV - \int_{\mathcal{B}_0} \delta_* \tilde{\Theta} \dot{\eta} dV \quad (19)$$

We refer to the mixed field  $\tilde{\Theta}$  as *assumed temperature*. Now, we present the virtual power associated with  $\boldsymbol{\chi}$ . We begin by defining the micro inertia of the mesogens by the *virtual orientational kinetic power*

$$\delta_* \dot{\mathcal{I}}_\chi(\dot{\boldsymbol{\chi}}, \dot{\mathbf{v}}_\chi, \dot{\mathbf{p}}_\chi) := \int_{\mathcal{B}_0} \delta_* \dot{\mathbf{v}}_\chi \cdot (\mathbf{A}_\chi \mathbf{v}_\chi - \mathbf{p}_\chi) dV + \int_{\mathcal{B}_0} \delta_* \dot{\mathbf{p}}_\chi \cdot [\dot{\boldsymbol{\chi}} - \mathbf{v}_\chi] dV + \int_{\mathcal{B}_0} \delta_* \dot{\boldsymbol{\chi}} \cdot \dot{\mathbf{p}}_\chi dV \quad (20)$$

Then, we introduce volume loads  $\mathbf{B}_\chi$  and a Neumann boundary load  $\bar{\mathbf{W}}$  on the boundary  $\partial_W \mathcal{B}_0$  acting on the orientation (see Fig. 1) with the *virtual orientational external power*

$$\begin{aligned} \delta_* \dot{\Pi}_\chi^{\text{ext}}(\dot{\boldsymbol{\alpha}}, \dot{\boldsymbol{\chi}}, \tilde{\mathbf{Z}}, \tilde{\boldsymbol{\tau}}_n, \tilde{\mathbf{v}}) := & - \int_{\mathcal{B}_0} \delta_* \dot{\boldsymbol{\chi}} \cdot \mathbf{B}_\chi dV - \int_{\partial_W \mathcal{B}_0} \delta_* \dot{\boldsymbol{\chi}} \cdot \bar{\mathbf{W}} dA - \int_{\partial_\chi \mathcal{B}_0} \delta_* \tilde{\mathbf{Z}} \cdot [\dot{\boldsymbol{\chi}} - \dot{\boldsymbol{\chi}}] dA - \int_{\partial_\chi \mathcal{B}_0} \delta_* \dot{\boldsymbol{\chi}} \cdot \tilde{\mathbf{Z}} dA \\ & - \int_{\partial_\chi \mathcal{B}_0} 2 \delta_* \tilde{\boldsymbol{\tau}}_n \cdot \tilde{\mathbf{v}} dA - \int_{\partial_\chi \mathcal{B}_0} 2 \delta_* \tilde{\mathbf{v}} \cdot \tilde{\boldsymbol{\tau}}_n dA + \int_{\mathcal{B}_0} 2 \delta_* \dot{\boldsymbol{\alpha}} \cdot \boldsymbol{\Sigma}_\chi dV \end{aligned} \quad (21)$$

For the sake of completeness, we also introduce a prescribed orientation  $\tilde{\boldsymbol{\chi}}$  on the disjunct Dirichlet boundary  $\partial_\chi \mathcal{B}_0 := \partial \mathcal{B}_0 \setminus \partial_W \mathcal{B}_0$ . The last term denotes the *virtual reorientation dissipation*. Finally, the

functional form  $\delta_* \dot{\Pi}_\chi^{\text{int}}(\dot{\boldsymbol{\alpha}}, \dot{\boldsymbol{\chi}}, \dot{\tilde{\mathbf{F}}}, \dot{\tilde{\mathbf{F}}}_\chi, \dot{\tilde{\mathbf{G}}}, \dot{\tilde{\mathbf{G}}}_\chi, \dot{\tilde{\mathbf{K}}}, \dot{\tilde{\mathbf{K}}}_\chi, \dot{\tilde{\boldsymbol{\tau}}}_n, \dot{\tilde{\mathbf{P}}}, \dot{\tilde{\mathbf{P}}}_K, \dot{\tilde{\mathbf{S}}}, \dot{\tilde{\mathbf{S}}}_K) := \delta_* \mathcal{P}_\chi^{\text{int}}$  of the *virtual orientational internal power* is defined by

$$\begin{aligned}
 \delta_* \mathcal{P}_\chi^{\text{int}} := & \int_{\mathcal{B}_0} \delta_* \dot{\tilde{\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{\boldsymbol{\tau}}_n \cdot [\dot{\boldsymbol{\chi}} + \boldsymbol{\varepsilon} \cdot \dot{\boldsymbol{\alpha}} \cdot \boldsymbol{\chi}] dV + \int_{\mathcal{B}_0} \delta_* \dot{\tilde{\mathbf{P}}}_\chi : [\dot{\boldsymbol{\chi}} \otimes \mathbf{n}_0 - \dot{\tilde{\mathbf{F}}}_\chi] dV \\
 & + \int_{\mathcal{B}_0} \delta_* \dot{\tilde{\mathbf{P}}}_K : [\text{Grad}[\dot{\boldsymbol{\chi}}] - \dot{\tilde{\mathbf{G}}}_\chi] dV + \int_{\mathcal{B}_0} \delta_* \dot{\tilde{\mathbf{S}}}_\chi : \left[ \frac{\partial}{\partial t} (\tilde{\mathbf{F}}^t \tilde{\mathbf{F}}_\chi) - \dot{\tilde{\mathbf{C}}}_\chi \right] dV \\
 & + \int_{\mathcal{B}_0} \delta_* \dot{\tilde{\mathbf{S}}}_K : \left[ \frac{\partial}{\partial t} (\tilde{\mathbf{F}}^t \tilde{\mathbf{G}}_\chi) - \dot{\tilde{\mathbf{K}}}_\chi \right] dV + \int_{\mathcal{B}_0} \delta_* \dot{\tilde{\mathbf{C}}}_\chi : \left[ \frac{\partial \Psi}{\partial \tilde{\mathbf{C}}_\chi} - \tilde{\mathbf{S}}_\chi \right] dV + \int_{\mathcal{B}_0} \delta_* \dot{\tilde{\mathbf{K}}}_\chi : \left[ \frac{\partial \Psi}{\partial \tilde{\mathbf{K}}_\chi} - \tilde{\mathbf{S}}_K \right] dV \\
 & + \int_{\mathcal{B}_0} \delta_* \dot{\tilde{\mathbf{F}}}_\chi : [\tilde{\mathbf{F}} \tilde{\mathbf{S}}_\chi - \tilde{\mathbf{P}}_\chi] dV + \int_{\mathcal{B}_0} \delta_* \dot{\tilde{\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{\boldsymbol{\chi}} \otimes \mathbf{n}_0] dV \\
 & + \int_{\mathcal{B}_0} \tilde{\mathbf{P}}_K : \text{Grad}[\delta_* \dot{\boldsymbol{\chi}}] dV + \int_{\mathcal{B}_0} \left[ \frac{1}{2} \boldsymbol{\varepsilon} : \boldsymbol{\tau}_\chi - \tilde{\boldsymbol{\tau}}_n \cdot \boldsymbol{\varepsilon} \cdot \boldsymbol{\chi} \right] \cdot 2 \delta_* \dot{\boldsymbol{\alpha}} dV + \int_{\mathcal{B}_0} 2 \tilde{\boldsymbol{\tau}}_n \cdot \delta_* \dot{\boldsymbol{\chi}} dV \quad (22)
 \end{aligned}$$

We introduce the *distorsion stress tensor*  $\tilde{\mathbf{S}}_K$  energy-conjugated to  $\tilde{\mathbf{K}}_\chi$ . Further, weakly defined stress tensors are  $\mathbf{P}_\chi := \mathbf{F} \mathbf{S}_\chi$  and  $\mathbf{P}_K := \mathbf{F} \mathbf{S}_K$ , which we refer to as *Piola orientational stress* and *Piola distorsion stress*, respectively. We call the Lagrange multiplier  $2 \boldsymbol{\tau}_n$  the *rotation stress vector*. The weak forms arise from the application of the variational principle in Eq. (11) to the virtual power functional

$$\delta_* \dot{\mathcal{H}} := \delta_* \mathcal{P}_\phi + \delta_* \mathcal{P}_\Theta + \delta_* \dot{\mathcal{I}}_\chi(\dot{\boldsymbol{\chi}}, \dot{\mathbf{v}}_\chi, \dot{\mathbf{p}}_\chi) + \delta_* \dot{\Pi}_\chi^{\text{ext}}(\dot{\boldsymbol{\alpha}}, \dot{\boldsymbol{\chi}}, \dot{\tilde{\mathbf{Z}}}, \dot{\tilde{\boldsymbol{\tau}}}_n, \dot{\tilde{\mathbf{v}}}) + \delta_* \mathcal{P}_\chi^{\text{int}} \quad (23)$$

We obtain four globally weak forms coupled in the deformation  $\boldsymbol{\phi}$ , the temperature  $\Theta$ , the orientation  $\boldsymbol{\chi}$  and the rotation stress vector  $2 \boldsymbol{\tau}_n$ . We solve these weak forms within a monolithic solution strategy. The deformation  $\boldsymbol{\phi}$  is determined by the *weak balance of linear momentum*, given by

$$\int_{\mathcal{T}_n} \int_{\mathcal{B}_0} \delta_* \dot{\boldsymbol{\phi}} \cdot [\dot{\mathbf{p}} - \mathbf{B}] dV dt - \int_{\mathcal{T}_n} \int_{\partial_T \mathcal{B}_0} \delta_* \dot{\boldsymbol{\phi}} \cdot \tilde{\mathbf{T}} dA dt + \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} \tilde{\mathbf{P}} : \text{Grad}[\delta_* \dot{\boldsymbol{\phi}}] dV dt = \int_{\mathcal{T}_n} \int_{\partial_\phi \mathcal{B}_0} \delta_* \dot{\boldsymbol{\phi}} \cdot \tilde{\mathbf{R}} dA dt \quad (24)$$

The temperature  $\Theta$  follows from the *weak balance of thermal momentum*, which can be written as

$$\int_{\mathcal{T}_n} \int_{\mathcal{B}_0} \delta_* \dot{\Theta} \left[ \dot{\eta} - \frac{D^{\text{tot}}}{\Theta} \right] dV dt - \int_{\mathcal{T}_n} \int_{\partial_Q \mathcal{B}_0} \delta_* \dot{\Theta} \frac{\tilde{\mathbf{Q}}}{\Theta} dA dt - \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} \text{Grad}[\delta_* \dot{\Theta}] \cdot \frac{\tilde{\mathbf{Q}}}{\Theta} dV dt = \int_{\mathcal{T}_n} \int_{\partial_\Theta \mathcal{B}_0} \delta_* \dot{\Theta} \tilde{\lambda} dA dt \quad (25)$$

The rotation stress  $2 \boldsymbol{\tau}_n$  is associated with the *weak balance of orientational momentum*, defined by

$$\begin{aligned}
 & \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} \delta_* \dot{\boldsymbol{\chi}} \cdot [\dot{\mathbf{p}}_\chi + 2 \tilde{\boldsymbol{\tau}}_n - \mathbf{B}_\chi] dV dt - \int_{\mathcal{T}_n} \int_{\partial_w \mathcal{B}_0} \tilde{\mathbf{W}} \cdot \delta_* \dot{\boldsymbol{\chi}} dA dt \\
 & + \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} \tilde{\mathbf{P}}_K : \text{Grad}[\delta_* \dot{\boldsymbol{\chi}}] dV dt + \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} \tilde{\mathbf{P}}_\chi : [\delta_* \dot{\boldsymbol{\chi}} \otimes \mathbf{n}_0] dV dt = \int_{\mathcal{T}_n} \int_{\partial_\chi \mathcal{B}_0} \tilde{\mathbf{Z}} \cdot \delta_* \dot{\boldsymbol{\chi}} dA dt \quad (26)
 \end{aligned}$$

The orientation  $\boldsymbol{\chi}$  is determined by the *weak balance of orientation rate*, which takes the form

$$\int_{\mathcal{T}_n} \int_{\mathcal{B}_0} 2 \delta_* \tilde{\boldsymbol{\tau}}_n \cdot [\dot{\boldsymbol{\chi}} + \boldsymbol{\varepsilon} \cdot \dot{\boldsymbol{\alpha}} \cdot \boldsymbol{\chi}] dV dt = \int_{\mathcal{T}_n} \int_{\partial_\chi \mathcal{B}_0} 2 \delta_* \tilde{\boldsymbol{\tau}}_n \cdot \mathbf{v} dA dt \quad (27)$$

The vector field  $\mathbf{v}$  represents a reaction due to a prescribed orientation on the boundary  $\partial_\chi \mathcal{B}_0$ . We refer to this vector field as *reaction velocity field*. The time evolution in Eq. (9) is solved on the element level with an elementwise space approximation and a consistent linearisation as the viscoelasticity in [3].

#### 4 BALANCE LAWS

This weak formulation satisfies different balance laws associated with the time functions defined in Tab. 1 in consequence of symmetry properties of  $\boldsymbol{\varphi}$ ,  $\Theta$ ,  $\boldsymbol{\chi}$  and  $2\tilde{\boldsymbol{\tau}}_n$  with respect to Euclidean transformations. Therefore, by choosing specific variations as test functions, we obtain different balance laws.

**Table 1:** Energy and momentum functions of the non-isothermal 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 $C^{\text{ori}}(t) := \int_{\mathcal{B}_0} [ \boldsymbol{\chi} ^2 - 1] \, dV$	Thermal energy $\Pi^{\text{the}}(t) := \int_{\mathcal{B}_0} \Theta \eta \, dV$
Entropy $S(t) := \int_{\mathcal{B}_0} \eta \, dV$	Total energy $\mathcal{H} := \mathcal{T} + \mathcal{T}_\chi + \Pi^{\text{int}} + \Pi^{\text{the}} + \Pi^{\text{ext}}$	Lyapunov function $\mathcal{F} := \mathcal{H} - \Theta_\infty S$

First, the *balance law of linear momentum* describes a symmetry with respect to virtual translations along any vector  $\mathbf{c} \in \mathbb{R}^{n_{\text{dim}}}$ . This balance law is obtained by choosing the test function  $\delta_* \boldsymbol{\varphi} = \mathbf{c}$ , leading to

$$\mathbf{L}(t_{n+1}) - \mathbf{L}(t_n) = \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} \mathbf{B} \, dV \, dt + \int_{\mathcal{T}_n} \int_{\partial_T \mathcal{B}_0} \bar{\mathbf{T}} \, dA \, dt + \int_{\mathcal{T}_n} \int_{\partial_\varphi \mathcal{B}_0} \tilde{\mathbf{R}} \, dA \, dt \quad (28)$$

Then, we obtain a *balance law of orientational momentum* by choosing the test function  $\delta_* \boldsymbol{\chi} = \mathbf{c}$ , where  $\mathbf{c} \in \mathbb{R}^{n_{\text{dim}}}$  denotes any constant orientation. We arrive at

$$\mathbf{L}_\chi(t_{n+1}) - \mathbf{L}_\chi(t_n) = \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} [\mathbf{B}_\chi - 2\tilde{\boldsymbol{\tau}}_n - \tilde{\mathbf{P}}_\chi \mathbf{n}_0] \, dV \, dt + \int_{\mathcal{T}_n} \int_{\partial_\chi \mathcal{B}_0} \bar{\mathbf{W}} \, dA \, dt + \int_{\mathcal{T}_n} \int_{\partial_\chi \mathcal{B}_0} \tilde{\mathbf{Z}} \, dA \, dt \quad (29)$$

A further symmetry property is associated with a virtual rotation around a constant axial vector  $\mathbf{c} \in \mathbb{R}^{n_{\text{dim}}}$ , introduced by the test function  $\delta_* \boldsymbol{\varphi} = \mathbf{c} \times \boldsymbol{\varphi}$ . Here, we apply the definition  $\mathbf{t}_1 \times \mathbf{t}_2 := \boldsymbol{\varepsilon} : [\mathbf{t}_1 \otimes \mathbf{t}_2]$  of the cross product of two vectors  $\mathbf{t}_1$  and  $\mathbf{t}_2$ . This *balance law of angular momentum* is given by

$$\begin{aligned} \mathbf{J}(t_{n+1}) - \mathbf{J}(t_n) &= \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} \boldsymbol{\varphi} \times \mathbf{B} \, dV \, dt + \int_{\mathcal{T}_n} \int_{\partial_T \mathcal{B}_0} \boldsymbol{\varphi} \times \bar{\mathbf{T}} \, dA \, dt + \int_{\mathcal{T}_n} \int_{\partial_\varphi \mathcal{B}_0} \boldsymbol{\varphi} \times \tilde{\mathbf{R}} \, dA \, dt \\ &+ \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} [\tilde{\mathbf{F}}_\chi \tilde{\mathcal{S}}_\chi^t + \tilde{\mathbf{G}}_\chi \tilde{\mathcal{S}}_K^t] \times \tilde{\mathbf{F}} \, dV \, dt \end{aligned} \quad (30)$$

by using the notation of a cross product  $\mathbf{T}_1 \times \mathbf{T}_2 := \boldsymbol{\varepsilon} : [\mathbf{T}_1 \cdot \mathbf{T}_2^t]$  of second-order tensors  $\mathbf{T}_1$  and  $\mathbf{T}_2$ . Without introducing an orientation  $\boldsymbol{\chi}$ , the last term in Eq. (30) vanishes. But, bearing in mind the rotation of the orientation vector  $\mathbf{n}_i$  during reorientations, we obtain distributed couples. Analogous to the angular momentum balance law, the test function  $\delta_* \boldsymbol{\chi} = \mathbf{c} \times \boldsymbol{\chi}$  leads to a balance law associated with a virtual

rotation of the orientation vector  $\mathbf{n}_t$  around any direction  $\mathbf{c} \in \mathbb{R}^{n_{\text{dim}}}$ . This *balance law of moment of orientational momentum* reads

$$\begin{aligned} \mathbf{J}_\chi(t_{n+1}) - \mathbf{J}_\chi(t_n) &= \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} \boldsymbol{\chi} \times \mathbf{B}_\chi \, dV \, dt + \int_{\mathcal{T}_n} \int_{\partial_W \mathcal{B}_0} \boldsymbol{\chi} \times \bar{\mathbf{W}} \, dA \, dt + \int_{\mathcal{T}_n} \int_{\partial_\chi \mathcal{B}_0} \boldsymbol{\chi} \times \tilde{\mathbf{Z}} \, dA \, dt \\ &\quad - \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} [\tilde{\mathbf{F}}_\chi \tilde{\mathbf{S}}_\chi^t + \tilde{\mathbf{G}}_\chi \tilde{\mathbf{S}}_K^t] \times \tilde{\mathbf{F}} \, dV \, dt - \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} \boldsymbol{\chi} \times 2\tilde{\boldsymbol{\tau}}_n \, dV \, dt \end{aligned} \quad (31)$$

Distributed couples are eliminated by adding Eqs. (30) and (31), with expt of the couples  $\boldsymbol{\chi} \times 2\tilde{\boldsymbol{\tau}}_n$ . A *balance law of thermal momentum* arises by employing the test function  $\delta_* \tilde{\Theta} = c \in \mathbb{R}$ , which reads

$$\mathcal{S}(t_{n+1}) - \mathcal{S}(t_n) = \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} \frac{D^{\text{tot}}}{\Theta} \, dV \, dt + \int_{\mathcal{T}_n} \int_{\partial_Q \mathcal{B}_0} \frac{\bar{Q}}{\Theta} \, dA \, dt + \int_{\mathcal{T}_n} \int_{\partial_\Theta \mathcal{B}_0} \tilde{\lambda} \, dA \, dt \quad (32)$$

Second, we obtain energy balance laws as symmetry with respect to virtual translations along the time axis. Choosing  $\delta_* \dot{\boldsymbol{\phi}} = \dot{\boldsymbol{\phi}}$ , we obtain the *balance law of kinetic energy*

$$\begin{aligned} \mathcal{T}(t_{n+1}) - \mathcal{T}(t_n) &= \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} \mathbf{B} \cdot \dot{\boldsymbol{\phi}} \, dV \, dt + \int_{\mathcal{T}_n} \int_{\partial_T \mathcal{B}_0} \tilde{\mathbf{T}} \cdot \dot{\boldsymbol{\phi}} \, dA \, dt + \int_{\mathcal{T}_n} \int_{\partial_\phi \mathcal{B}_0} \tilde{\mathbf{R}} \cdot \dot{\boldsymbol{\phi}} \, dA \, dt \\ &\quad - \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} [\tilde{\mathbf{S}} : \dot{\tilde{\mathbf{F}}} \tilde{\mathbf{F}} + \tilde{\mathbf{S}}_\chi : \dot{\tilde{\mathbf{F}}} \tilde{\mathbf{F}}_\chi + \tilde{\mathbf{S}}_K : \dot{\tilde{\mathbf{F}}} \tilde{\mathbf{G}}_\chi] \, dV \, dt \end{aligned} \quad (33)$$

Since we also assume a micro inertia of the mesogens, we also obtain a *balance law of orientational kinetic energy* by inserting the test function  $\delta_* \dot{\boldsymbol{\chi}} = \dot{\boldsymbol{\chi}}$ . This leads to the relation

$$\begin{aligned} \mathcal{T}_\chi(t_{n+1}) - \mathcal{T}_\chi(t_n) &= \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} \mathbf{B}_\chi \cdot \dot{\boldsymbol{\chi}} \, dV \, dt + \int_{\mathcal{T}_n} \int_{\partial_\phi \mathcal{B}_0} \bar{\mathbf{W}} \cdot \dot{\boldsymbol{\chi}} \, dA \, dt + \int_{\mathcal{T}_n} \int_{\partial_\chi \mathcal{B}_0} \tilde{\mathbf{Z}} \cdot \dot{\boldsymbol{\chi}} \, dA \, dt \\ &\quad - \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} [\tilde{\mathbf{S}}_\chi : \dot{\tilde{\mathbf{F}}}^t (\tilde{\mathbf{F}}_\chi + \boldsymbol{\varepsilon} \cdot \boldsymbol{\alpha} \cdot \tilde{\mathbf{F}}_\chi) + \tilde{\mathbf{S}}_K : \dot{\tilde{\mathbf{F}}}^t \tilde{\mathbf{G}}_\chi + D_\chi^{\text{int}}] \, dV \, dt \end{aligned} \quad (34)$$

by taking into account the *variational form* of Eq. (9). The *potential energy balance law* follows from the time derivative of the total potential energy  $\Pi := \Pi^{\text{int}} + \Pi^{\text{ext}}$  with the *external potential energy*

$$\Pi^{\text{ext}}(t) := - \int_{\mathcal{B}_0} \mathbf{B} \cdot \dot{\boldsymbol{\phi}} \, dV \, dt - \int_{\mathcal{B}_0} \mathbf{B}_\chi \cdot \dot{\boldsymbol{\chi}} \, dV \, dt \quad (35)$$

with respect to dead loads. The time derivative  $\dot{\Pi}$  then leads to the balance law

$$\begin{aligned} \Pi(t_{n+1}) - \Pi(t_n) &= \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} [\tilde{\mathbf{S}}_\chi : \frac{\partial}{\partial t} (\tilde{\mathbf{F}}^t \tilde{\mathbf{F}}_\chi) + \tilde{\mathbf{S}}_K : \frac{\partial}{\partial t} (\tilde{\mathbf{F}}^t \tilde{\mathbf{G}}_\chi) + \tilde{\mathbf{S}}_\chi : \tilde{\mathbf{F}}^t (\boldsymbol{\varepsilon} \cdot \boldsymbol{\alpha} \cdot \tilde{\mathbf{F}}_\chi)] \, dV \, dt \\ &\quad + \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} \left[ \tilde{\mathbf{S}} : \dot{\tilde{\mathbf{F}}} \tilde{\mathbf{F}} + \frac{\partial \Psi}{\partial \Theta} \dot{\Theta} - \mathbf{B} \cdot \dot{\boldsymbol{\phi}} - \mathbf{B}_\chi \cdot \dot{\boldsymbol{\chi}} \right] \, dV \, dt \end{aligned} \quad (36)$$

We obtain a further balance law by inserting the test function  $\delta_* \tilde{\Theta} = \Theta$ . This balance law reads

$$\begin{aligned} \Pi^{\text{the}}(t_{n+1}) - \Pi^{\text{the}}(t_n) &= \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} \left[ - \frac{\partial \Psi}{\partial \Theta} \dot{\Theta} + D_\chi^{\text{int}} \right] \, dV \, dt + \int_{\mathcal{T}_n} \int_{\partial_\Theta \mathcal{B}_0} \dot{\Theta} \tilde{h} \, dA \, dt \\ &\quad + \int_{\mathcal{T}_n} \int_{\partial_\Theta \mathcal{B}_0} \Theta \tilde{\lambda} \, dA \, dt + \int_{\mathcal{T}_n} \int_{\partial_Q \mathcal{B}_0} \bar{Q} \, dA \, dt \end{aligned} \quad (37)$$



Accordingly, adding Eq. (33), Eq. (34), Eq. (36) and Eq. (37), we obtain the *total energy balance law*, which coincides with the first law of thermodynamics depending on non-conservative loads only. Additionally, the balance law of thermal momentum leads to a *Lyapunov function balance law*, given by

$$\begin{aligned} \mathcal{F}(t_{n+1}) - \mathcal{F}(t_n) &= \int_{\mathcal{T}_n} \int_{\partial_T \mathcal{B}_0} \bar{\mathbf{T}} \cdot \boldsymbol{\phi} \, dA \, dt + \int_{\mathcal{T}_n} \int_{\partial_\varphi \mathcal{B}_0} \bar{\mathbf{R}} \cdot \boldsymbol{\phi} \, dA \, dt + \int_{\mathcal{T}_n} \int_{\partial_\varphi \mathcal{B}_0} \bar{\mathbf{W}} \cdot \boldsymbol{\chi} \, dA \, dt + \int_{\mathcal{T}_n} \int_{\partial_\varphi \mathcal{B}_0} \bar{\mathbf{Z}} \cdot \boldsymbol{\chi} \, dA \, dt \\ &\quad - \int_{\mathcal{T}_n} \int_{\partial_T \mathcal{B}_0} \frac{\Theta_\infty}{\Theta} D^{\text{tot}} \, dV \, dt + \int_{\mathcal{T}_n} \int_{\partial_\Theta \mathcal{B}_0} \Theta \tilde{h} \, dA \, dt + \int_{\mathcal{T}_n} \int_{\partial_Q \mathcal{B}_0} \frac{\Theta - \Theta_\infty}{\Theta} \bar{Q} \, dA \, dt \end{aligned} \quad (38)$$

The last balance law is the *conservation law of reorientation* pertaining to the function  $C^{\text{ori}}$ . Choosing the test function  $\delta_* \tilde{\boldsymbol{\tau}}_n = \boldsymbol{\chi}$ , we arrive at the conservation

$$C^{\text{ori}}(t_{n+1}) - C^{\text{ori}}(t_n) = \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} 2\boldsymbol{\chi} \cdot \dot{\boldsymbol{\chi}} \, dV \, dt \equiv \int_{\mathcal{T}_n} \int_{\mathcal{B}_0} 2\dot{\boldsymbol{\alpha}}_t \cdot [\boldsymbol{\chi} \times \boldsymbol{\chi}] \, dV \, dt \equiv 0 \quad (39)$$

of the length of the orientation vectors  $\|\mathbf{n}_t\| = \|\mathbf{n}_0\| \equiv 1$  on each time step  $\mathcal{T}_n$ .

## 5 SPACE-TIME DISCRETIZATION

Analogous to [3], we introduce in Eq. (23) time approximation polynomials with respect to the normalized time  $\alpha(t) := (t - t_n)/h_n \in [0, 1]$  associated with  $\mathcal{T}_n$ . As mentioned above, we distinguish between time rate variables  $\phi^n \in \{\boldsymbol{\varphi}^n, \mathbf{v}^n, \mathbf{p}^n, \Theta^n, \eta^n, \tilde{\mathbf{F}}^n, \tilde{\mathbf{C}}^n, \boldsymbol{\chi}^n, \mathbf{v}_\chi^n, \mathbf{p}_\chi^n, \boldsymbol{\alpha}^n, \tilde{\mathbf{F}}_\chi^n, \tilde{\mathbf{G}}_\chi^n, \tilde{\mathbf{C}}_\chi^n, \tilde{\mathbf{K}}_\chi^n\}$  and the remainder mixed fields. A time rate variable field  $\phi^n$  on the  $n$ -th time step  $\mathcal{T}_n$  is approximated by  $k$ -order Lagrange polynomials  $M_I(\alpha)$ ,  $I = 1, \dots, k+1$ . Then, we approximate the remainder mixed fields and variations  $\tilde{\phi}^n$  on the  $n$ -th time step by  $k-1$  order Lagrange polynomials  $\tilde{M}_J(\alpha)$ ,  $J = 1, \dots, k$ . We temporally discretize the time integrals by a  $k$ -point Gaussian quadrature rule. In Eq. (23), we apply a *globally continuous* space discretization with hexahedral elements, based on local shape functions  $N_a(\boldsymbol{\zeta})$ ,  $a = 1, \dots, n_{\text{node}}$ , defined on the domain  $\mathcal{B}_\square := [-1, 1] \times [-1, 1] \times [-1, 1]$ , and the associated quadrature rules to the mixed fields  $\Phi_1 \in \{\boldsymbol{\varphi}, \mathbf{v}, \mathbf{p}, \bar{\mathbf{R}}, \Theta, \eta, \tilde{\Theta}, \tilde{h}, \tilde{\lambda}, \boldsymbol{\chi}, \mathbf{v}_\chi, \mathbf{p}_\chi, \tilde{\boldsymbol{\tau}}_n, \tilde{\mathbf{Z}}, \tilde{\mathbf{v}}\}$  and the corresponding variations  $\Phi_2 \in \{\delta_* \boldsymbol{\phi}, \delta_* \mathbf{v}, \delta_* \mathbf{p}, \delta_* \bar{\mathbf{R}}, \delta_* \Theta, \delta_* \eta, \delta_* \tilde{\Theta}, \delta_* \tilde{h}, \delta_* \tilde{\lambda}, \delta_* \boldsymbol{\chi}, \delta_* \mathbf{v}_\chi, \delta_* \mathbf{p}_\chi, \delta_* \tilde{\boldsymbol{\tau}}_n, \delta_* \tilde{\mathbf{Z}}, \delta_* \tilde{\mathbf{v}}\}$ . The remainder fields  $\hat{\Phi}$  on the  $e$ -th finite element are *globally discontinuously* approximated in space by local shape functions  $\hat{N}_b(\boldsymbol{\zeta})$ ,  $b = 1, \dots, \hat{n}_{\text{node}}$ , *well-defined* on the domain  $\mathcal{B}_\square$ . Note that the local shape functions  $\hat{N}_b(\boldsymbol{\zeta})$ ,  $b = 1, \dots, \hat{n}_{\text{node}}$ , also fulfill a completeness condition. Hence, we apply the approximations

$$\phi_\alpha^n := \sum_{I=1}^{k+1} M_I(\alpha) \phi_I^n \quad \tilde{\phi}_\alpha^n := \sum_{J=1}^k \tilde{M}_J(\alpha) \tilde{\phi}_J^n \quad \Phi_\zeta^e := \sum_{a=1}^{n_{\text{node}}} N_a(\boldsymbol{\zeta}) \Phi_a^e \quad \hat{\Phi}_\zeta^e := \sum_{b=1}^{\hat{n}_{\text{node}}} \hat{N}_b(\boldsymbol{\zeta}) \hat{\Phi}_b^e \quad (40)$$

Motivated by Reference [8], we apply for  $\boldsymbol{\alpha}$  and  $\delta_* \boldsymbol{\alpha}$  local shape functions  $\tilde{N}_c(\boldsymbol{\zeta})$ ,  $c = 1, \dots, \tilde{n}_{\text{node}}$ , which are generally different from  $N_a(\boldsymbol{\zeta})$  and  $\hat{N}_b(\boldsymbol{\zeta})$ . In order to satisfy the property in Eq. (36) also in a discrete sense, we extend the stress approximations (cp. [3]). Further, we implemented the dyadic product  $\boldsymbol{\chi} \otimes \mathbf{n}_0$  in a special way, such that a special  $\bar{\mathbf{B}}$ -operator has arisen. We report about these details in a next paper.

## 6 NUMERICAL EXAMPLE

The reorientation of the orientation vectors (mesogens) directly affects the motion. This is obvious from the balance laws. Whereas the linear momentum balance law is not influenced by the reorientation, the angular momentum balance law is affected by the distributed couples. As the dissipative reorientation

process is simulated non-isothermally, we obtain a conserved total energy  $\mathcal{H}$  and a decreasing Lyapunov function  $\mathcal{F}$  without external loads due to the increasing entropy  $\mathcal{S}$ . An isothermal simulation leads to a decreasing total energy  $\mathcal{H}$  due to the reorientation dissipation. In order to demonstrate this dynamical behaviour, we initiate a free rotation of a thin LCE film ( $0.3 \times 12.5 \times 75$  [mm]). The rotation around the center of mass is initiated with an initial angular velocity  $\omega = 32$  [1/s] around the  $z$ -axis. We compare an isothermal and a non-isothermal simulation as well as the motion with and without reorientation. In Fig. 2, we compare the isothermal motion without (left) and with (right) reorientation. Without a reorientation, the film steadily rotates anti-clockwise in the  $x - y$ -plane and the mechanical momenta and total energy are conserved. However, the couples of reorientation leads to an unsteady right-left-rotation with large deformations, and the dissipation  $D_{\chi}^{\text{int}}$  leads to a decreasing total energy. In the non-isothermal motion in Fig. 3, the total energy  $\mathcal{H}$  is now conserved and the Lyapunov function  $\mathcal{F}$  is decreasing.

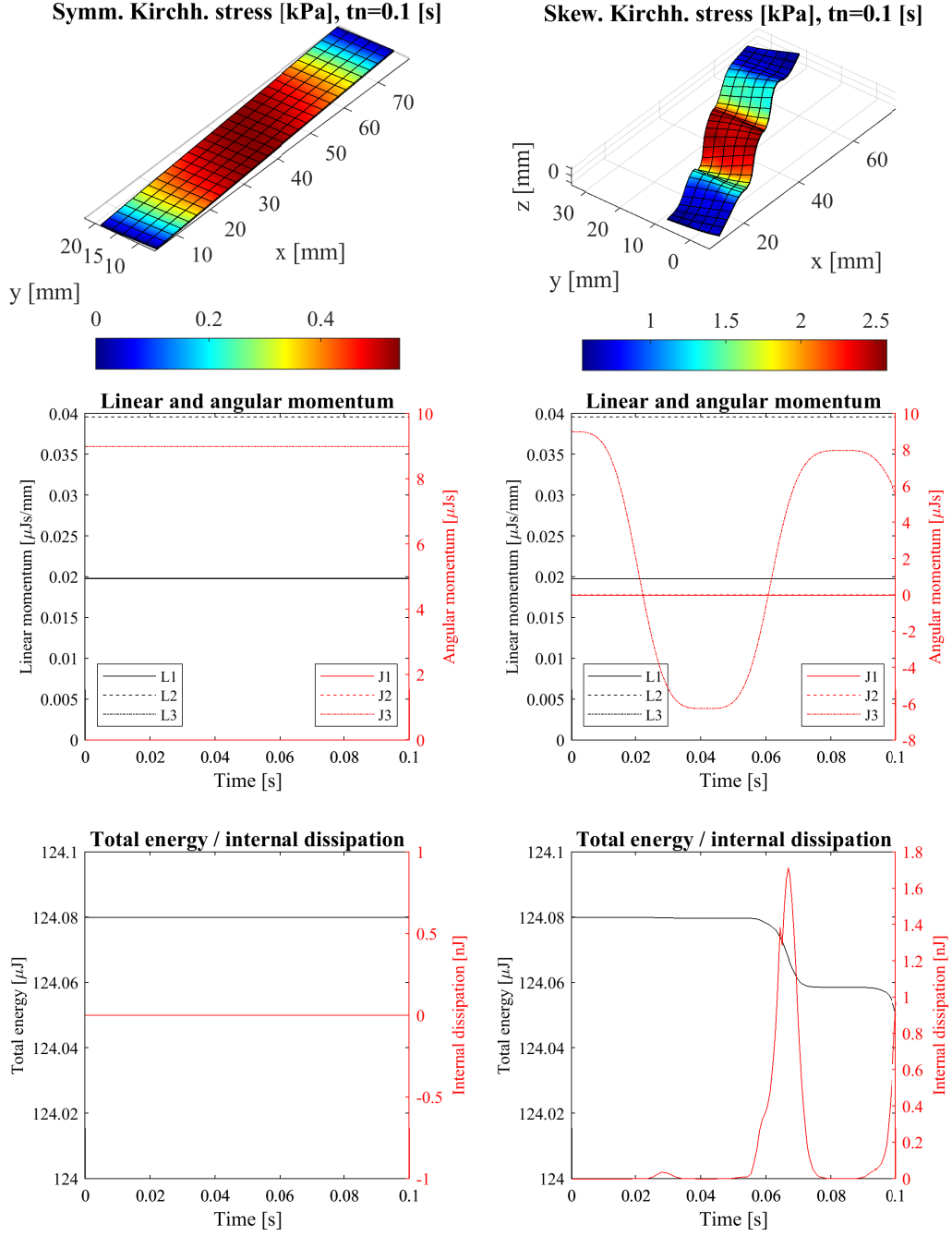
## 7 CONCLUSIONS

According to the non-isothermal formulation of the reorientation of the mesogens with a variational principle the first law of thermodynamics is satisfied analogous to thermo-viscoelasticity. The next step is to include the temperature dependence of the reorientation of the LCE film (see e.g. Reference [1]).

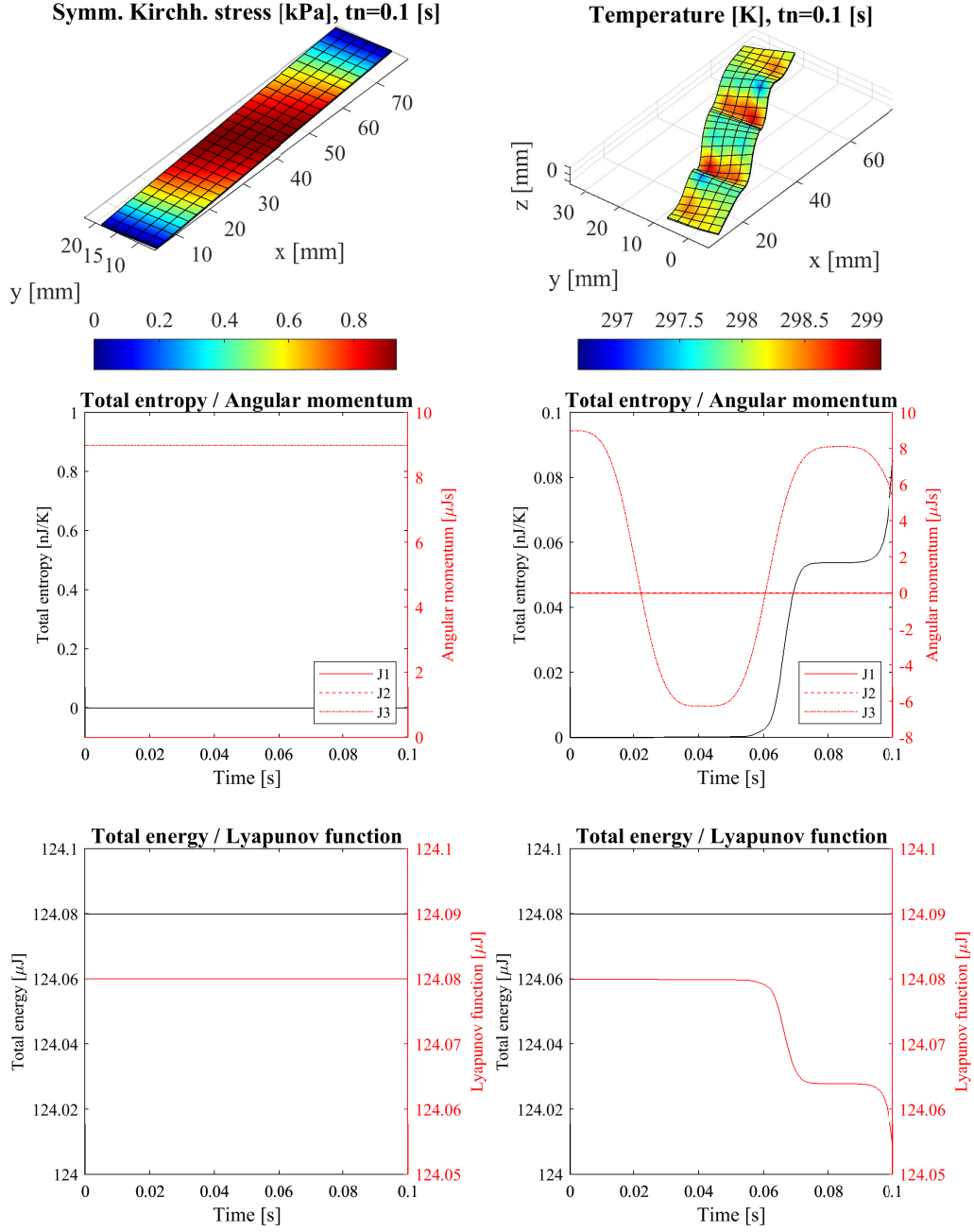
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**Figure 2:** Comparison of *isothermal* time evolutions without (left) and with (right) reorientation. As in [3],  $N_a$  belongs to a 20-node serendipity hexahedral element (H20) and  $\hat{N}_b$  to a 12-node prismatic element (P12). Motivated by [8],  $\tilde{N}_c$  belongs to a 8-node Lagrangian hexahedral element (H8). Colours in the left top plot indicate the Kirchhoff stress  $\boldsymbol{\tau} = \tilde{\mathbf{P}}\mathbf{F}^t$ , where in the right, finite elements are coloured by the skew-symmetric part of  $\boldsymbol{\tau}_\chi$ . The LCE film is defined by polyconvex free energy functions with  $\rho_0 = 0.00176$  [g/mm<sup>3</sup>],  $V_\chi = 1$  [kPa · s], Young's modulus  $E \approx 0.914$  [MPa], Poisson's ratio  $\nu \approx 0.493$ . Further, the initial orientation  $\mathbf{n}_0 = \mathbf{e}_y$  is used.



**Figure 3:** Comparison of *non-isothermal* time evolutions without (left) and with (right) reorientation. The shape functions are chosen as in Fig. 2. Colours in the left top plot indicate the Kirchhoff stress, where in the right, finite elements are coloured by the current temperature  $\Theta$ . The LCE film is defined by the mechanical parameters in Fig. 2, and additionally with the linear thermal expansion coefficient  $\beta = 10^{-3}$  [1/K], specific heat capacity  $302$  [J/(K m<sup>3</sup>)]  $(1 + 0.56$  [1/K]  $(\Theta - \Theta_\infty))$  and thermal conductivity  $k_0 = 0.4 \cdot 10^{-3}$  [W/(mm K)] ( $\Theta_\infty = 298.15$  [K]).