Analysis and Numerical Approximation of Energy-Variational Solutions to the Ericksen–Leslie Equations

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Abstract

We define the concept of energy-variational solutions for the Ericksen–Leslie equations in three spatial dimensions. This solution concept is finer than dissipative solutions and satisfies the weak-strong uniqueness property. For a certain choice of the regularity weight, the existence of energy-variational solutions implies the existence of measure-valued solutions and for a different choice, we construct an energy-variational solution with the help of an implementable, structure-inheriting space-time discretization. Computational studies are performed in order to provide some evidence of the applicability of the proposed algorithm.

1 Introduction

Liquid crystals comprise the structural properties of crystals within a fluid. The fluid flow of the nematic phase of liquid crystals can be described by the Ericksen–Leslie system. In this model, the material behaves like a liquid, *i.e.,* no positional order is present, but the molecules exhibit a long-range self-alignment along a direction (see Fig. 1). In this way, liquid crystals sustain anisotropic dynamics such as the polarization of light or the transfer of heat, but at the same time offer the physical flexibility of a fluid, which makes these materials interesting for engineering and sciences [2]. Ericksen [3] and Leslie [4] derived the Ericksen–Leslie equations during their development of an instationary theory of liquid crystals in the 1960s.

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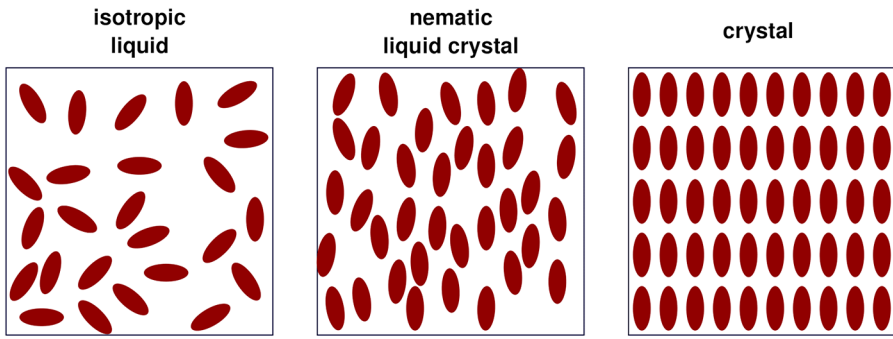
Fig. 1 Alignment of the rod-like molecules in an isotropic liquid, the nematic phase of a liquid crystal, and a solid. [1, Fig. 1.1]

Let $\boldsymbol{v} : \overline{\Omega} \times [0, T] \to \mathbb{R}^3$ denote the velocity of the fluid, $\boldsymbol{p} : \overline{\Omega} \times [0, T] \to \mathbb{R}$ its pressure and $\boldsymbol{d} : \overline{\Omega} \times [0, T] \to \mathbb{R}^3$ the director. We consider the system governed by the equations

$$\partial_t \boldsymbol{v} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{v} + \nabla \boldsymbol{p} + \nabla \cdot \left((\nabla \boldsymbol{d})^T \nabla \boldsymbol{d}\right) - \nabla \cdot \boldsymbol{T}^L = 0, \tag{1a}$$

$$\nabla \cdot \boldsymbol{v} = 0, \tag{1b}$$

$$\partial_t \boldsymbol{d} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{d} - (\nabla \boldsymbol{v})_{skw}\boldsymbol{d} + (I - \boldsymbol{d} \otimes \boldsymbol{d})\left(\lambda(\nabla \boldsymbol{v})_{sym}\boldsymbol{d} - \Delta \boldsymbol{d}\right) = 0, \tag{1c}$$

$$|\boldsymbol{d}| = 1, \tag{1d}$$

where we employ the initial conditions

$$\boldsymbol{v}(0) = \boldsymbol{v}_0, \quad \boldsymbol{d}(0) = \boldsymbol{d}_0 \text{ with } |\boldsymbol{d}_0| = 1 \text{ in } \Omega$$

and boundary conditions

$$\boldsymbol{v} = 0, \quad \boldsymbol{d} = \boldsymbol{d}_\Gamma \text{ with } |\boldsymbol{d}_\Gamma| = 1 \text{ on } \partial\Omega.$$

The Leslie stress tensor $\boldsymbol{T}^L$ is defined by

$$\boldsymbol{T}^L := \boldsymbol{T}^D + \lambda[\boldsymbol{d} \otimes [\boldsymbol{d}]_x^T[\boldsymbol{d}]_x \cdot \Delta \boldsymbol{d}]_{sym} + [\boldsymbol{d} \otimes \Delta \boldsymbol{d}]_{skw},$$

where $\boldsymbol{T}^D$ collects the dissipative terms of the Leslie stress tensor, *i.e.*

$$\boldsymbol{T}^D := (\mu_1 + \lambda^2)(\boldsymbol{d} \cdot (\nabla \boldsymbol{v})_{sym}\boldsymbol{d})(\boldsymbol{d} \otimes \boldsymbol{d}) + \mu_4(\nabla \boldsymbol{v})_{sym}$$
$$+ (\mu_5 + \mu_6 - \lambda^2)(\boldsymbol{d} \otimes (\nabla \boldsymbol{v})_{sym}\boldsymbol{d})_{sym}$$

with $\mu_4 > 0$, $\mu_5 + \mu_6 - \lambda^2 \geq 0$, $\mu_1 + \lambda^2 \geq 0$ in order to ensure the dissipative character of our model.

So far, a vast majority of the mathematical work on the Ericksen–Leslie model considers a simplified system with a relaxed unit-norm constraint that is only enforced approximately by adding a Ginzburg–Landau penalization term $\boldsymbol{F}_\epsilon(\boldsymbol{d}) = \frac{1}{4\epsilon}(|\boldsymbol{d}|^2 - 1)^2$ to the free energy potential $\frac{1}{2}|\nabla \boldsymbol{d}|^2$. With a simplified Leslie-stress tensor, the momentum and director equa-

tion (1a)–(1d) are replaced by

$$\partial_t \boldsymbol{v} - \frac{1}{Re}\Delta \boldsymbol{v} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{v} + \nabla \boldsymbol{p} + \gamma \nabla \cdot \big((\nabla \boldsymbol{d})^T \nabla \boldsymbol{d}\big) = 0, \quad \nabla \cdot \boldsymbol{v} = 0,$$

$$\partial_t \boldsymbol{d} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{d} - \Delta \boldsymbol{d} + \boldsymbol{f}_\varepsilon(\boldsymbol{d}) = 0, \tag{2}$$

respectively, where $\boldsymbol{f}_\varepsilon(\boldsymbol{d}) = \nabla_{\boldsymbol{d}} \boldsymbol{F}_\varepsilon(\boldsymbol{d})$. In the first analysis of this system [5], the authors were able to prove the existence of weak solutions to (2). A rather general model including the full Leslie stress tensor is considered by [6], where again a Ginzburg–Landau penalization approach is introduced to replace the unit-norm constraint of the director. In this setting, the authors prove that weak solutions exist and a blow-up criterion for local strong solutions. In [7] the existence of weak solutions is generalized to a larger class of free energy functions. An overview of the analytical results regarding the Ericksen–Leslie equations and their connection to other models for liquid crystals can be found in [8]. In two spatial dimensions, for the limiting system of (2), where $\boldsymbol{f}_\varepsilon(\boldsymbol{d})$ is replaced by $-|\nabla \boldsymbol{d}|^2 \boldsymbol{d}$, it is known that a unique weak solution exists that is smooth except for finitely many points in time [9].

For a general model of the Ericksen–Leslie equations equipped with the naturally arising anisotropic Oseen–Frank energy, the concept of dissipative solutions is applied in [10], which are shown to be the local average of measure-valued solutions [11] and inherit their weak-strong uniqueness [12]. In comparison to measure-valued solutions, dissipative solutions have the advantage that they have fewer degrees of freedom and can be approximated by numerical schemes. Nevertheless, they form only a subset of measure-valued solutions and are thus not as precise. In the work at hand, we introduce energy-variational solutions (*cf.* [13]), which have one degree of freedom more than dissipative solutions and can be argued to be as fine as measure-valued solutions, but as we will show, they can also be approximated by numerical schemes and have additional advantages. This solution concept is useful where one might either not be able to derive weak solutions for physically relevant models or where weak solutions admit unphysical behaviour, like unphysical non-uniqueness [14]. The solution concept was first introduced in [15]. We will prove that this concept is finer than the so-called dissipative solutions introduced by Lions [16] for the Euler equations and also applied to the Ericksen–Leslie equations by one of the authors [10]. Additionally, in certain scenarios, this concept is finer than the concept of measure-valued solutions. Energy-variational solutions do not only fulfill the standard weak-strong uniqueness property of generalized solution concepts (*cf.* [12]), but they also fulfill the semi-flow property such that prolongations and restrictions of solutions on larger, and smaller time intervals, respectively, are energy-variational solutions again. In [15] it was also argued that energy-variational solutions are amenable to different selection criteria. The set of energy-variational solutions can be seen as a convex, weakly*-closed superset of weak solutions but a subset of dissipative solutions and for a special choice of the regularity weight also a subset of measure-valued solutions. This may allow us to introduce techniques from optimization theory in order to select the physically relevant solution maximizing the dissipation at every point-in-time [15].

In this work, we define the concept of energy-variational solutions for the Ericksen–Leslie equations in three spatial dimensions. This definition has some freedom since it depends on the choice of a certain regularity weight $\mathscr{K}$. For one choice of such a regularity weight, we prove the equivalence to a certain class of measure-valued solutions, and for another choice, we construct an energy-variational solution with the help of an implementable, structure-inheriting space-time discretization based on the finite element method.

Concerning the numerical approximation of the Ericksen–Leslie equations, a first study for the simplified system (2) equipped with the Ginzburg–Landau approximation is conducted in [17]. They combined an implicit Euler scheme in time with Hermite-type finite elements for the director and $Q2$-$Q1$-Taylor–Hood elements for the velocity and pressure. In their subsequent work [18], the authors replace the demanding Hermite finite elements for the director with piecewise quadratic functions. Even a relaxation from C^1 finite elements to C^0 finite elements is realized in [19]. A different approach is proposed in [20], where the Ginzburg–Landau approximation of the unit-norm constraint is interpreted as a saddle-point structure. For the simplified and penalized Ericksen–Leslie system also decoupling techniques and mixed methods are examined in [21, 22]. In [23] two numerical schemes for the simplified model are proposed. The first one uses the Ginzburg–Landau approximation for the unit-norm constraint and the second proposed scheme does not depend on a regularization parameter and fulfills the unit-norm constraint in the limit. However, both schemes do not fulfill the unit-norm constraint at the discrete level exactly. We, therefore, use an approach from [24] by implementing a midpoint rule at the finite element level which solves the sphere constraint exactly at every node of the mesh. But we have to refine this approach by introducing a special projection (see Remark 2.5), which will allow us to identify the limit as an energy-variational solution. The proposed scheme is the first numerical scheme implementing the main properties of the continuous system including the algebraic norm restriction at every node of the mesh such that the approximate solutions converge to an energy-variational solution fulfilling the physically relevant semi-flow property. We think that the concept of energy-variational solutions is a strong tool for identifying the limits of solutions to numerical schemes and can also serve as such in other related models.

After providing the considered system and an overview of the existing literature, we introduce the necessary notation in Sect. 2, we provide the definitions and the main results in Sect. 2.1. The weak-strong uniqueness proof and the relation to measure-valued solutions in considered in Sect. 2.2, whereas the preliminaries are provided in the following subsections on auxiliary lemmata 2.3, finite elements 2.4, and interpolation 2.5. The discrete system is introduced and analysed in Sect. 3, we provide the necessary *a priori* estimates 3.1, extract converging subsequences 3.2, and prove convergence to the director equations 3.3 and the energy-variational inequality 3.4. Finally, some computational studies are presented in Sect. 4 in order to show some evidence of the applicability of the proposed algorithm.

2 Preliminaries, Main Results and Continuous System

We denote the space of smooth solenoidal functions with compact support by $\mathscr{C}_{c,\sigma}^\infty(\Omega; \mathbb{R}^3)$. By $L_\sigma^p(\Omega)$, $H_{0,\sigma}^1(\Omega)$, and $W_{0,\sigma}^{1,p}(\Omega)$, we denote the closure of $\mathscr{C}_{c,\sigma}^\infty(\Omega; \mathbb{R}^3)$ with respect to the norm of $L^p(\Omega)$, $H^1(\Omega)$, and $W^{1,p}(\Omega)$, respectively. By tr we denote the usual trace operator on Sobolev spaces. By $H^1(\Omega; \mathbb{S}^2)$, we denote the functions $\boldsymbol{d} \in H^1(\Omega)$ such that $|\boldsymbol{d}| = 1$ a.e. in Ω. The $L^2(\Omega)$ inner product is thereby denoted by $(.,.)$. The Dual space of a Banach space V is denoted by V^*, where the dual pairing is denoted as $\langle \cdot, \cdot \rangle$. In order to define the cross product, we use the Levi–Civita symbol. The cross product of two vectors $x, y \in \mathbb{R}^3$ is then defined as $(x \times y)_i = \sum_{j,k} \epsilon_{i,j,k} x_j y_k$, the cross product of a vector $x \in \mathbb{R}^3$ with a matrix $A \in \mathbb{R}^{d \times d}$ as $(x \times A)_{i,j} = \sum_{l,m} \epsilon_{i,l,m} x_l A_{m,j}$. We further will make use of the matrix notation of the cross product for three dimensions, *i.e.* $([x]_\times)_{ik} = \sum_j \epsilon_{i,j,k} x_j$. We also introduce the discrete derivative $\boldsymbol{d}_t$ as $\boldsymbol{d}_t f^j := \frac{f^j - f^{j-1}}{k}$ for a constant time-step size $k > 0$ and for a sequence in a normed space $(f_j)_{j=1,\dots,n}$, where we set $\boldsymbol{d}_t f^0 = 0$. Usually,

functions in the continuous setting are denoted by bold letters in contrast to the discrete functions.

By $\mathbb{R}^{d \times d}$ we denote d-dimensional quadratic matrices, by $\mathbb{R}^{d \times d}_{\text{sym}}$ the symmetric subset, and by $\mathbb{R}^{d \times d}_{\text{sym},+}$ the symmetric positive semi-definite matrices. The symmetric and skew-symmetric part of a matrix $A \in \mathbb{R}^{d \times d}$ are denoted by $(A)_{\text{sym}}$ and $(A)_{\text{skw}}$, respectively. The positive and negative semi-definite part of a matrix $A \in \mathbb{R}^{d \times d}$ are denoted by $(A)_+$ and $(A)_-$, respectively. We equip the last set with the usual spectral norm $|A|_2 = \max_{i \in \{1,\dots,d\}} \lambda_i$, where λ_i are the nonnegative eigenvalues of the matrix $A \in \mathbb{R}^{d \times d}_{\text{sym},+}$. The dual norm of the spectral norm with respect to the Frobenius product ($A : B := \sum_{i,j=1}^{d} A_{ji} B_{ij}$ for $A, B \in \mathbb{R}^{d \times d}$) is given by $|A|_2' = \sum_{i=1}^{d} \lambda_i = A : I = \text{Tr}(A)$ for a matrix $A \in \mathbb{R}^{d \times d}_{\text{sym},+}$. By Tr we denote the trace of a matrix. The Radon measures taking values in $\mathbb{R}^{d \times d}_{\text{sym}}$ are denoted by $\mathscr{M}(\overline{\Omega}; \mathbb{R}^{d \times d}_{\text{sym}})$, which may be interpreted as the dual space of the continuous functions, *i.e.*, $\mathscr{M}(\overline{\Omega}; \mathbb{R}^{d \times d}_{\text{sym}}) = (\mathscr{C}(\overline{\Omega}; \mathbb{R}^{d \times d}_{\text{sym}}))^*$. Note that an element $\mu \in \mathscr{M}(\overline{\Omega}; \mathbb{M}^{d \times d}_{\text{sym},+})$ is a Radon measure taking values in the symmetric matrices such that for any $\boldsymbol{\xi} \in \mathbb{R}^d$ the measure $\boldsymbol{\xi} \otimes \boldsymbol{\xi} : \mu$ is nonnegative. By I, we denote the identity matrix in $\mathbb{R}^{d \times d}$.

For a given Banach space $\mathbb{X}$, the space $\mathscr{C}_w([0,T]; \mathbb{X})$ denotes the functions on $[0,T]$ taking values in $\mathbb{X}$ that are continuous with respect to the weak topology of $\mathbb{X}$. The space $L^\infty_{w*}([0,T]; \mathbb{X}^*)$ is the space of all functions on $[0,T]$ taking values in $\mathbb{X}^*$ that are Bochner measurable with respect to $\mathbb{X}^*$ equipped with the weak-* topology and essentially bounded. The total variation of a function $E : [0,T] \to \mathbb{R}$ is given by

$$|E|_{\text{TV}([0,T])} = \sup_{0=t_0 < \cdots < t_n = T} \sum_{k=1}^{n} |E(t_{k-1}) - E(t_k)|,$$

where the supremum is taken over all finite partitions of the interval $[0,T]$. We denote the space of all bounded functions of bounded variations on $[0,T]$ by $\text{BV}([0,T])$. Note that the total variation of a monotone decreasing nonnegative function E only depends on the initial value, *i.e.*,

$$|E|_{\text{TV}([0,T])} = \sup_{0=t_0 < \cdots < t_n = T} \sum_{k=1}^{N} |E(t_{k-1}) - E(t_k)| \le E(0) - E(T) \le E(0).$$

2.1 Main Results

We define the total energy as

$$\mathscr{E}(\boldsymbol{v}, \boldsymbol{d}) := \frac{1}{2} \|\boldsymbol{v}\|^2_{L^2(\Omega)} + \frac{1}{2} \|\nabla \boldsymbol{d}\|^2_{L^2(\Omega)}. \tag{3}$$

The main new idea when defining energy-variational solutions is to introduce an auxiliary variable E as an upper bound of the total energy $\mathscr{E}(\boldsymbol{v}, \boldsymbol{d})$ and add the difference of these two variables to a variational inequality of the energy-dissipation mechanism to close this formulation with respect to the appropriate weak topologies. The difference between the variable E and the energy $\mathscr{E}(\boldsymbol{v}, \boldsymbol{d})$ can be interpreted as a measure of the difference between weak and strong convergence of the approximate solutions. The associated error term represents this difference in the limit of vanishing discretization parameters.

Definition 2.1 (Energy-variational solutions) We call $(\boldsymbol{v}, \boldsymbol{d}, E)$ an energy-variational solution, if

$$\boldsymbol{v} \in \mathscr{C}_w([0, T]; L^2_\sigma(\Omega)) \cap L^2(0, T; H^1_{0,\sigma}(\Omega)), \quad E \in \mathrm{BV}([0, T]),$$

$$\boldsymbol{d} \in \mathscr{C}_w([0, T]; H^1(\Omega; \mathbb{S}^2)) \cap H^1(0, T; L^{3/2}(\Omega; \mathbb{R}^3)) \text{ such that} \quad (4)$$

$$\boldsymbol{d} \times \Delta \boldsymbol{d} \in L^2(0, T; L^2(\Omega; \mathbb{R}^3)),$$

and $E \geq \mathscr{E}(\boldsymbol{v}, \boldsymbol{d})$ on $[0, T]$ as well as $|\boldsymbol{d}| = 1$ a.e. in $\Omega \times (0, T)$. The term $\boldsymbol{d} \times \Delta \boldsymbol{d}$ has to be understood as the weak divergence of $\boldsymbol{d} \times \nabla \boldsymbol{d}$. The solution fulfills the energy-variational inequality

$$\left[E - \int_\Omega \boldsymbol{v} \cdot \tilde{\boldsymbol{v}} \mathrm{d}x \right]\Big|_{s-}^t + \int_s^t \int_\Omega \boldsymbol{v} \cdot \partial_t \tilde{\boldsymbol{v}} - (\boldsymbol{v} \cdot \nabla)\boldsymbol{v} \cdot \tilde{\boldsymbol{v}} \mathrm{d}x\mathrm{d}\tau + \int_s^t \langle \boldsymbol{T}^E(\boldsymbol{d}), \tilde{\boldsymbol{v}} \rangle \mathrm{d}\tau$$

$$+ \int_s^t \int_\Omega \left((\mu_1 + \lambda^2)(\boldsymbol{d} \cdot (\nabla\boldsymbol{v})_{sym}\boldsymbol{d})(\boldsymbol{d} \otimes \boldsymbol{d}) + \mu_4(\nabla\boldsymbol{v})_{sym} \right) : (\nabla\boldsymbol{v} - \nabla\tilde{\boldsymbol{v}})\mathrm{d}x\mathrm{d}\tau$$

$$+ \int_s^t \int_\Omega (\mu_5 + \mu_6 - \lambda^2)(\boldsymbol{d} \otimes (\nabla\boldsymbol{v})_{sym}\boldsymbol{d})_{sym} : (\nabla\boldsymbol{v} - \nabla\tilde{\boldsymbol{v}}) + |\boldsymbol{d} \times \Delta\boldsymbol{d}|^2 \mathrm{d}x\mathrm{d}\tau$$

$$+ \int_s^t \int_\Omega \left(\lambda[\boldsymbol{d} \otimes [\boldsymbol{d}]_x^T[\boldsymbol{d}]_x \cdot \Delta\boldsymbol{d}]_{sym} + [\boldsymbol{d} \otimes \Delta\boldsymbol{d}]_{skw} \right) : \nabla\tilde{\boldsymbol{v}}\mathrm{d}x\mathrm{d}\tau$$

$$+ \int_s^t \mathscr{K}(\tilde{\boldsymbol{v}}) \left[\mathscr{E}(\boldsymbol{v}, \boldsymbol{d}) - E \right] \mathrm{d}\tau \leq 0, \quad (5)$$

for all $s, t \in (0, T)$ and for all $\tilde{\boldsymbol{v}} \in \mathscr{C}^1([0, T]; (H^1_{0,\sigma}(\Omega))^*) \cap L^2(0, T; H^1_{0,\sigma}(\Omega))$ such that $\mathscr{K}(\tilde{\boldsymbol{v}}) \in L^1(0, T)$. The initial values are fulfilled in a weak sense $\boldsymbol{v}(0) = \boldsymbol{v}_0$, $\boldsymbol{d}(0) = \boldsymbol{d}_0$ and $\boldsymbol{d}$ fulfills the inhomogeneous Dirichlet boundary conditions in the sense of the trace $\mathrm{tr}(\boldsymbol{d}(t)) = \mathrm{tr}(\boldsymbol{d}_\Gamma)$ for a.e. $t \in (0, T)$. Additionally, it holds

$$\partial_t \boldsymbol{d} + (\boldsymbol{v} \cdot \nabla)\boldsymbol{d} - (\nabla\boldsymbol{v})_{skw}\boldsymbol{d} + (I - \boldsymbol{d} \otimes \boldsymbol{d})\left(\lambda(\nabla\boldsymbol{v})_{sym}\boldsymbol{d} - \Delta\boldsymbol{d} \right) = 0 \quad (6)$$

a.e. in $\Omega \times (0, T)$. In this work, we choose $\mathscr{K}_1(\tilde{\boldsymbol{v}}) = \frac{1}{2}\|\tilde{\boldsymbol{v}}\|^2_{L^\infty(\Omega)}$ and $\mathscr{K}_2(\tilde{\boldsymbol{v}}) = 2\|(\nabla\tilde{\boldsymbol{v}})_{sym,-}\|_{\mathscr{C}(\overline{\Omega})}$, where c_L is given in (23), with the associated Ericksen stresses being defined as

$$\langle \boldsymbol{T}^E_1(\boldsymbol{d}), \tilde{\boldsymbol{v}} \rangle = \int_\Omega (\boldsymbol{d} \times (\tilde{\boldsymbol{v}} \cdot \nabla)\boldsymbol{d}) \cdot (\boldsymbol{d} \times \Delta\boldsymbol{d})\mathrm{d}x \text{ or } \langle \boldsymbol{T}^E_2(\boldsymbol{d}), \tilde{\boldsymbol{v}} \rangle = -\int_\Omega (\nabla\boldsymbol{d}^T\nabla\boldsymbol{d}) : \nabla\tilde{\boldsymbol{v}}\mathrm{d}x,$$

respectively.

Remark (Ericksen stress) The main obstacle when passing to the limit in an approximation of the Ericksen–Leslie equations is often the so-called Ericksen stress, which can be seen as a kind of Korteweg stress coupling the elastic deformations of the director field to the evolution of the velocity field. This term is the main reason that we have to consider a generalized solution framework different from usual weak solutions. Via Lemma 2.6 we

observe that both formulations T_1^E and T_2^E are formally equivalent via the reformulation

$$- \int_\Omega (\tilde{\boldsymbol{v}} \cdot \nabla) \boldsymbol{d} \cdot [\boldsymbol{d}]_x^T [\boldsymbol{d}]_x \Delta \boldsymbol{d} \, \mathrm{d}x = - \int_\Omega (\tilde{\boldsymbol{v}} \cdot \nabla) \boldsymbol{d} \cdot (\Delta \boldsymbol{d} + |\nabla \boldsymbol{d}|^2 \boldsymbol{d}) \mathrm{d}x$$

$$= \int_\Omega (\nabla \boldsymbol{d}^T \nabla \boldsymbol{d}) : \nabla \tilde{\boldsymbol{v}} \mathrm{d}x + \frac{1}{2} \int_\Omega (\tilde{\boldsymbol{v}} \cdot \nabla) |\nabla \boldsymbol{d}|^2 - |\nabla \boldsymbol{d}|^2 (\tilde{\boldsymbol{v}} \cdot \nabla) |\boldsymbol{d}|^2 \mathrm{d}x \,,$$

where the second term on the right-hand side vanishes formally due to the fact that $\tilde{\boldsymbol{v}} \in H_{0,\sigma}^1(\Omega)$ and $|\boldsymbol{d}| = 1$. Thus, in the case of a regular solution with $\boldsymbol{d} \in L^2(0, T; H^2(\Omega; \mathbb{S}^2))$ and $E = \mathscr{E}(\boldsymbol{v}, \boldsymbol{d})$ a.e. in $(0, T)$ both solution concepts coincide with usual weak solutions.

Remark (Strong continuity of the initial value) From the monotony of $t \mapsto E(t)$ and the weak continuity of $t \mapsto (\boldsymbol{v}(t), \boldsymbol{d}(t))$, we infer by the lower semi-continuity of the energy functional and the inequality $E(t) \geq \mathscr{E}(\boldsymbol{v}(t), \boldsymbol{d}(t))$ for all $t \in [0, T]$ that for any sequence $t \searrow 0$ it holds

$$\mathscr{E}(\boldsymbol{v}_0, \boldsymbol{d}_0) = E(0) \geq \lim_{t \searrow 0} E(t) \geq \liminf_{t \searrow 0} \mathscr{E}(\boldsymbol{v}(t), \boldsymbol{d}(t)) \geq \mathscr{E}(\boldsymbol{v}_0, \boldsymbol{d}_0) \,.$$

This implies that all inequalities are in-fact equations such that we infer from the uniform convexity of $L^2(\Omega)$ that

$$\left. \begin{cases} (\boldsymbol{v}(t), \boldsymbol{d}(t)) \rightharpoonup & (\boldsymbol{v}_0, \boldsymbol{d}_0) \text{ as } t \searrow 0 \text{ in } L_\sigma^2(\Omega) \times L^2(\Omega; \mathbb{R}^3) \\ \mathscr{E}(\boldsymbol{v}(t), \boldsymbol{d}(t)) \longrightarrow & \mathscr{E}(\boldsymbol{v}_0, \boldsymbol{d}_0) \text{ as } t \searrow 0 \text{ in } \mathbb{R} \end{cases} \right\} \Longrightarrow$$

$$(\boldsymbol{v}(t), \boldsymbol{d}(t)) \longrightarrow (\boldsymbol{v}_0, \boldsymbol{d}_0) \text{ as } t \searrow 0 \text{ in } L_\sigma^2(\Omega) \times L^2(\Omega; \mathbb{R}^3) \,.$$

Remark (Properties of generalized solutions) Energy-variational solutions fulfill several properties, which are desirable for generalized solution concepts. That generalized solutions coincide with classical solutions, if the latter exists, is the so-called weak-strong uniqueness property and is covered by Theorem 2.5.

Furthermore, energy-variational solutions fulfill the so-called semi-flow property such that restrictions and concatenations of solutions are solutions again, which is an important property of a reasonable solution concept (*cf.* [13]).

Remark (Different definition) We could also identify $E(t) = E^1(t) + \frac{1}{2} \|\boldsymbol{v}(t)\|_{L^2(\Omega)}^2$ for a.e. $t \in (0, T)$ such that $E^1(t) \geq \frac{1}{2} \|\nabla \boldsymbol{d}(t)\|_{L^2(\Omega)}^2$ for a.e. $t \in (0, T)$ in the inequality (5). This can be done due to the strong convergence of $\boldsymbol{v}$ a.e. in $\Omega \times (0, T)$. We would also replace $\mathscr{E}(\boldsymbol{v}, \boldsymbol{d}) - E = \frac{1}{2} \|\nabla \boldsymbol{d}\|_{L^2(\Omega)}^2 - E^1$. The disadvantage would be that the adapted inequality (5) is only fulfilled for a.e. $s \in (0, T)$ and all $t \in (s, T]$.

Theorem 2.2 *Let $\Omega \subset \mathbb{R}^3$ be a bounded convex polyhedral domain. Let $(\boldsymbol{v}_0, \boldsymbol{d}_0) \in H_{0,\sigma}^1(\Omega) \times H^2(\Omega; \mathbb{R}^3)$, with $|\boldsymbol{d}_0| = 1$ a.e. in Ω and $\boldsymbol{d}_\Gamma = \mathrm{tr}(\boldsymbol{d}_0)$ a.e. on $\partial\Omega$. Then there exists an energy-variational solution in the sense of Definition 2.1 with $\mathscr{K}(\tilde{\boldsymbol{v}}) = \frac{1}{2} \|\tilde{\boldsymbol{v}}\|_{L^\infty(\Omega)}^2$ such that $E(0) = \mathscr{E}(\boldsymbol{v}_0, \boldsymbol{d}_0)$.*

Remark (Choice of boundary conditions) Note that the boundary condition $\mathrm{tr}(\boldsymbol{d}) = \mathrm{tr}(\boldsymbol{d}_0)$ is a usual compatibility condition for parabolic problems. The same choice of boundary conditions for a model of the Ericksen–Leslie–equations was considered in [5–7, 25]. Other

choices however are most certainly possible. For instance, homogeneous Neumann boundary conditions for the director would be feasible, i.e. $\nabla \boldsymbol{d} \cdot \boldsymbol{n} = 0$ as considered in [6, 26]. This alternative choice would change the following analysis only at some choices of spaces, since an energy-dissipation mechanism can nevertheless be inferred, see also [6, Remark 1.1]. Another natural choice would be a free-slip condition or orthogonality condition for the director, i.e. $\boldsymbol{d} \cdot \boldsymbol{n} = 0$ on $\partial \Omega$. Such a choice favours alignment of the director at the boundary along the direction with the smallest principal curvature [27]. Incorporating this boundary condition into our framework would require additional technical adaptations, but should be possible in general.

We are going to prove the theorem by the convergence of a fully discrete, unconditionally solvable scheme in the following sections. The proposed scheme in Sect. 3 is a fully implementable numerical scheme for the Ericksen–Leslie system that fulfills the norm restriction $|\boldsymbol{d}| = 1$ for every approximate solution in every node of the mesh. We even infer that the norm of the approximate solutions converges to 1 with the order 1 (*cf.* Proposition 3.4).

Energy-variational solutions can be seen as a generalized solution concept, which generalizes the well-known weak solutions, but is finer than the usual concept of so-called measure-valued solutions [11].

Definition 2.3 We call the tuple $(\boldsymbol{v}, \boldsymbol{d}, \boldsymbol{m})$ a measure-valued solution to the Ericksen–Leslie equations (1a)–(1d), if $\boldsymbol{v} \in \mathscr{C}_w([0, T]; L^2_\sigma(\Omega)) \cap L^2(0, T; H^1_{0,\sigma}(\Omega))$, $\boldsymbol{d} \in \mathscr{C}_w([0, T]; H^1(\Omega; \mathbb{S}^2))$, as well as $\boldsymbol{m} \in L^\infty_{w*}(0, T; \mathscr{M}(\overline{\Omega}; \mathbb{R}^{3 \times 3}_{\mathrm{sym},+}))$, and if (6) is fulfilled with the appropriate initial and boundary conditions as well as the measure-valued formulation of the Navier–Stokes equation

$$\int_0^T \left[\int_\Omega \boldsymbol{T}_L : (\nabla \tilde{\boldsymbol{v}})_{\mathrm{sym}} - (\boldsymbol{v} \otimes \boldsymbol{v} + \nabla \boldsymbol{d}^T \nabla \boldsymbol{d}) : \nabla \tilde{\boldsymbol{v}} \right. \tag{7}$$
$$\left. - \boldsymbol{v} \cdot \partial_t \tilde{\boldsymbol{v}} \mathrm{d}x - 2 \int_{\overline{\Omega}} (\nabla \tilde{\boldsymbol{v}})_{\mathrm{sym}} : \mathrm{d}\boldsymbol{m}(x) \right] \mathrm{d}s = 0$$

for all $\tilde{\boldsymbol{v}} \in \mathscr{C}^\infty_c(\Omega \times (0, T))$, the initial condition $\boldsymbol{v}(0) = \boldsymbol{v}_0$ is attained in a weak sense, and the energy-inequality

$$\frac{1}{2} \left(\|\boldsymbol{v}\|^2_{L^2(\Omega)} + \|\nabla \boldsymbol{d}\|^2_{L^2(\Omega)} + \int_{\overline{\Omega}} I : \mathrm{d}\boldsymbol{m}(x) \right) \Big|_0^t \tag{8}$$
$$+ \int_0^t \int_\Omega \boldsymbol{T}^D : (\nabla \boldsymbol{v})_{\mathrm{sym}} + |\boldsymbol{d} \times \Delta \boldsymbol{d}|^2 \mathrm{d}x \mathrm{d}s \leq 0$$

for a.e. $t \in (0, T)$.

Theorem 2.4 *Let $(\boldsymbol{v}, \boldsymbol{d}, E)$ be an energy-variational solution with $\mathscr{K}(\tilde{\boldsymbol{v}}) = 2\|(\nabla \tilde{\boldsymbol{v}})_{sym,-}\|_{\mathscr{C}(\overline{\Omega})}$ in the sense of Definition 2.1 such that $E(0) = \mathscr{E}(\boldsymbol{v}_0, \boldsymbol{d}_0)$. Then there exists a measure-valued solution $(\boldsymbol{v}, \boldsymbol{d}, \boldsymbol{m})$ in the sense of Definition 2.3 with*

$$\frac{1}{2} \langle \boldsymbol{m}, I \rangle = \frac{1}{2} \int_{\overline{\Omega}} I : d\boldsymbol{m} = \frac{1}{2} \int_{\overline{\Omega}} d \mathrm{Tr}(\boldsymbol{m}) \leq E - \mathscr{E}(\boldsymbol{v}, \boldsymbol{d}) \quad a.e. \text{ in } (0, T). \tag{9}$$

Theorem 2.5 *Let $(\boldsymbol{v}, \boldsymbol{d}, E)$ be an energy-variational solution in the sense of Definition* 2.1 *with $E(0) = \mathscr{E}(\boldsymbol{v}_0, \boldsymbol{d}_0)$, $\boldsymbol{d}_\Gamma = \mathrm{tr}(\boldsymbol{d}_0)$ and let $(\tilde{\boldsymbol{v}}, \tilde{\boldsymbol{d}})$ fulfill*

$$\tilde{\boldsymbol{v}} \in L^2(0, T; H_{0,\sigma}^1(\Omega) \cap L^\infty(\Omega) \cap W^{1,3}(\Omega)) \cap L^1(0, T; \mathscr{C}^1(\overline{\Omega}))$$
$$\cap H^1(0, T; (H_{0,\sigma}^1(\Omega))^*) \tag{10a}$$

$$\tilde{\boldsymbol{d}} \in L^1(0, T; W^{2,\infty}(\Omega)) \cap L^2(0, T; W^{3,3}(\Omega)) \cap H^1(0, T; H^1(\Omega)) \tag{10b}$$

such that $\mathscr{K}(\tilde{\boldsymbol{v}}) \in L^1(0, T)$, $|\tilde{\boldsymbol{d}}| = 1$ everywhere in $\overline{\Omega} \times [0, T]$ as well as $\mathrm{tr}(\tilde{\boldsymbol{d}}) = \boldsymbol{d}_0$. Then the relative energy inequality

$$\frac{1}{2}\left[\|\boldsymbol{v}(t) - \tilde{\boldsymbol{v}}(t)\|_{L^2(\Omega)}^2 + \|\nabla\boldsymbol{d}(t) - \nabla\tilde{\boldsymbol{d}}(t)\|_{L^2(\Omega)}^2 \right]$$

$$+ \frac{1}{2}\int_0^t \int_\Omega (\mu_1 + \lambda^2)(\boldsymbol{d} \cdot (\nabla\boldsymbol{v} - \nabla\tilde{\boldsymbol{v}})_{sym}\boldsymbol{d})^2 + \mu_4|(\nabla\boldsymbol{v} - \nabla\tilde{\boldsymbol{v}})_{sym}|^2 \mathrm{d}x e^{\int_s^t \mathscr{Q}(\tilde{\boldsymbol{v}},\tilde{\boldsymbol{d}})d\tau}\mathrm{d}s$$

$$+ \frac{1}{2}\int_0^t \int_\Omega (\mu_5 + \mu_6 - \lambda^2)|(\nabla\boldsymbol{v} - \nabla\tilde{\boldsymbol{v}})_{sym}\boldsymbol{d}|^2 + |\boldsymbol{d} \times \Delta(\boldsymbol{d} - \tilde{\boldsymbol{d}})|^2 \mathrm{d}x e^{\int_s^t \mathscr{Q}(\tilde{\boldsymbol{v}},\tilde{\boldsymbol{d}})d\tau}\mathrm{d}s$$

$$+ \int_0^t \left\langle \partial_t\tilde{\boldsymbol{v}} + (\tilde{\boldsymbol{v}} \cdot \nabla)\tilde{\boldsymbol{v}} + \nabla\cdot(\nabla\tilde{\boldsymbol{d}}^T\nabla\tilde{\boldsymbol{d}}) - \nabla\cdot\tilde{\boldsymbol{T}}^L, \boldsymbol{v} - \tilde{\boldsymbol{v}} \right\rangle e^{\int_s^t \mathscr{Q}(\tilde{\boldsymbol{v}},\tilde{\boldsymbol{d}})d\tau}\mathrm{d}s \tag{11}$$

$$+ \int_0^t \left\langle \nabla\left(\partial_t\tilde{\boldsymbol{d}} + (\tilde{\boldsymbol{v}} \cdot \nabla)\tilde{\boldsymbol{d}} - (\nabla\tilde{\boldsymbol{v}})_{skw}\tilde{\boldsymbol{d}}\right), \nabla(\boldsymbol{d} - \tilde{\boldsymbol{d}}) \right\rangle e^{\int_s^t \mathscr{Q}(\tilde{\boldsymbol{v}},\tilde{\boldsymbol{d}})d\tau}\mathrm{d}s$$

$$+ \int_0^t \left\langle \nabla\left((I - \tilde{\boldsymbol{d}} \otimes \tilde{\boldsymbol{d}})(\lambda(\nabla\tilde{\boldsymbol{v}})_{sym} - \Delta\tilde{\boldsymbol{d}})\right), \nabla(\boldsymbol{d} - \tilde{\boldsymbol{d}}) \right\rangle e^{\int_s^t \mathscr{Q}(\tilde{\boldsymbol{v}},\tilde{\boldsymbol{d}})d\tau}\mathrm{d}s$$

$$\leq \frac{1}{2}\left[\|\boldsymbol{v}_0 - \tilde{\boldsymbol{v}}(0)\|_{L^2(\Omega)}^2 + \|\nabla\boldsymbol{d}_0 - \nabla\tilde{\boldsymbol{d}}(0)\|_{L^2(\Omega)}^2 \right] e^{\int_0^t \mathscr{Q}(\tilde{\boldsymbol{v}},\tilde{\boldsymbol{d}})ds},$$

holds for a.e. $t \in (0, T)$, where

$$\mathscr{Q}(\tilde{\boldsymbol{v}}, \tilde{\boldsymbol{d}}) := \|\tilde{\boldsymbol{v}}\|_{L^\infty(\Omega)}^2 + \|\nabla\tilde{\boldsymbol{v}}\|_{L^\infty(\Omega)} + \|\Delta\tilde{\boldsymbol{d}}\|_{L^3(\Omega)}^2 + \|\nabla\tilde{\boldsymbol{v}}\|_{L^3(\Omega)}^2$$
$$+ \|\Delta\tilde{\boldsymbol{d}}\|_{L^\infty(\Omega)} + \|\Delta\tilde{\boldsymbol{d}}\|_{W^{1,3}(\Omega)}^2 + \mathscr{K}(\tilde{\boldsymbol{v}}).$$

Additionally, if $(\tilde{\boldsymbol{v}}, \tilde{\boldsymbol{d}})$ is a classical solution to the Ericksen–Leslie system on $(0, T^*)$, then both solutions coincide on this time-interval, i.e.,

$$\boldsymbol{v} \equiv \tilde{\boldsymbol{v}} \qquad \boldsymbol{d} \equiv \tilde{\boldsymbol{d}} \quad \text{a.e. on } (0, T^*).$$

Remark (Dissipative solutions) Theorem 2.5 does not only show the weak-strong uniqueness of energy-variational solutions, but it also shows that every energy-variational solution is a dissipative solution. A dissipative solution is defined via the relative-energy inequality (11), *i.e.,* $(\boldsymbol{v}, \boldsymbol{d})$ is called a dissipative solution, if it fulfills the relative energy-inequality (11) for all functions $(\tilde{\boldsymbol{v}}, \tilde{\boldsymbol{d}})$ fulfilling the regularity properties (10a)–(10b). The concept of energy-variational solutions is thus strictly finer than the concept of dissipative solutions.

2.2 Proofs for the Continuous System

Proof of Theorem 2.4 Let $(\boldsymbol{v}, \boldsymbol{d}, E)$ be an energy-variational solution according to Definition 2.1 with $\mathscr{K}(\tilde{\boldsymbol{v}}) = 2\|\nabla\tilde{\boldsymbol{v}}\|_{\mathscr{C}(\overline{\Omega})}$. Then, we may choose $\tilde{\boldsymbol{v}} = 0$ in order to infer

$$E\Big|_0^t + \int_0^t \int_\Omega (\mu_1 + \lambda^2)(\boldsymbol{d} \cdot (\nabla\boldsymbol{v})_{\text{sym}}\boldsymbol{d})^2 + \mu_4 |(\nabla\boldsymbol{v})_{\text{sym}}|^2 \mathrm{d}x\mathrm{d}\tau$$
$$+ \int_0^t \int_\Omega (\mu_5 + \mu_6 - \lambda^2)|(\nabla\boldsymbol{v})_{\text{sym}}\boldsymbol{d}|^2 + |\boldsymbol{d} \times \Delta\boldsymbol{d}|^2 \mathrm{d}x\mathrm{d}\tau \leq 0. \qquad (12)$$

Furthermore, we may choose $\tilde{\boldsymbol{v}} = \alpha\tilde{\boldsymbol{u}}$ with $\alpha \geq 0$ and multiply the energy-variational inequality (5) by $1/\alpha$. In the limit $\alpha \to \infty$, we find

$$-\int_\Omega \boldsymbol{v} \cdot \tilde{\boldsymbol{u}}\mathrm{d}x\Big|_0^t + \int_0^t \int_\Omega \boldsymbol{v} \cdot \partial_t \tilde{\boldsymbol{u}} + \left[\boldsymbol{v} \otimes \boldsymbol{v} + \nabla\boldsymbol{d}^T\nabla\boldsymbol{d} - \boldsymbol{T}_L\right] : \nabla\tilde{\boldsymbol{u}}\mathrm{d}x\mathrm{d}s$$
$$+ \int_0^t 2\|(\nabla\tilde{\boldsymbol{u}})_{\text{sym},-}\|_{\mathscr{C}(\overline{\Omega};\mathbb{R}^{3\times3})}\left[\mathscr{E}(\boldsymbol{v}, \boldsymbol{d}) - E\right]\mathrm{d}s \leq 0$$

for all $\tilde{\boldsymbol{u}} \in \mathscr{C}^1([0, T]) \otimes \mathscr{C}_0^1(\Omega)$. By the definition of the weak time derivative, we infer that

$$-\int_0^T \langle\partial_t \boldsymbol{v}, \tilde{\boldsymbol{u}}\rangle\mathrm{d}t = -\int_\Omega \boldsymbol{v} \cdot \tilde{\boldsymbol{u}}\mathrm{d}x\Big|_0^T + \int_0^T \int_\Omega \boldsymbol{v} \cdot \partial_t \tilde{\boldsymbol{u}}\mathrm{d}x\mathrm{d}t$$
$$\leq \left(\|\boldsymbol{v}\|_{L^\infty(0,T;L^2(\Omega))}^2 + \|\nabla\boldsymbol{d}\|_{L^\infty(0,T;L^2(\Omega))}^2\right)\|\nabla\tilde{\boldsymbol{u}}\|_{L^1(0,T;\mathscr{C}(\overline{\Omega}))}$$
$$+ 2\|\nabla\tilde{\boldsymbol{u}}\|_{L^1(0,T;\mathscr{C}(\overline{\Omega}))}\|E - \mathscr{E}(\boldsymbol{v}, \boldsymbol{d})\|_{L^\infty(0,T)} + \|\boldsymbol{T}_L\|_{L^2(0,T;L^2(\Omega))}\|\nabla\tilde{\boldsymbol{u}}\|_{L^2(0,T;L^2(\Omega))}.$$

First this is only well defined for $\tilde{\boldsymbol{u}} \in \mathscr{C}^1([0, T]) \otimes \mathscr{C}_0^1(\Omega)$. Since this is a linear subspace of the Banach space $L^1(0, T; \mathscr{C}_0^1(\Omega)) \cap L^2(0, T; H^1(\Omega))$, we infer from the Hahn–Banach theorem [28, Thm. 1.1] the existence of an element

$$\partial_t \boldsymbol{v} \in \left(L^1(0, T; \mathscr{C}_0^1(\Omega)) \cap L^2(0, T; H^1(\Omega))\right)^*$$
$$= L_{w^*}^\infty(0, T; (\mathscr{C}_0^1(\Omega))^*) + L^2(0, T; W^{-1,2}(\Omega)).$$

This allows us to write the linear form

$$\langle\boldsymbol{l}(t), \tilde{\boldsymbol{u}}(t)\rangle_{L_{w^*}^\infty(0,T;(\mathscr{C}_0^1(\Omega))^*),L^1(0,T;\mathscr{C}_0^1(\Omega))} :=$$
$$-\int_0^T \langle\partial_t \boldsymbol{v}(t), \tilde{\boldsymbol{u}}(t)\rangle\mathrm{d}t + \int_0^T \int_\Omega \left[\boldsymbol{v}(t) \otimes \boldsymbol{v}(t) + \nabla\boldsymbol{d}^T(t)\nabla\boldsymbol{d}(t) - \boldsymbol{T}_L(t)\right] : \nabla\tilde{\boldsymbol{u}}(t)\mathrm{d}x\mathrm{d}t$$
$$\leq 2\int_0^T \|(\nabla\tilde{\boldsymbol{u}}(t))_{\text{sym},-}\|_{L^1(0,T;\mathscr{C}(\overline{\Omega};\mathbb{R}^{3\times3}))}\left[E(t) - \mathscr{E}(\boldsymbol{v}(t), \boldsymbol{d}(t))\right]\mathrm{d}t \qquad (13)$$

for a.e. $t \in (0, T)$. This implies that the linear form $\boldsymbol{l} \in L_{w^*}^\infty(0, T; (\mathscr{C}_0^1(\Omega))^*)$ can be identified via considering the gradient operator

$$\nabla : L^1(0, T; \mathscr{C}_0^1(\Omega)) \to L^1(0, T; \mathscr{C}(\overline{\Omega}; \mathbb{R}^{3\times3})),$$

we set $G = \nabla(L^1(0, T; \mathscr{C}_0^1(\Omega)))$ the range of the gradient, the set of all gradient fields equipped with the norm of $L^1(0, T; \mathscr{C}(\overline{\Omega}; \mathbb{R}^{3\times 3}))$. Note that this mapping is injective due to the prescribed Dirichlet boundary conditions. We may set $S = \nabla^{-1} : G \to L^1(0, T; \mathscr{C}_0^1(\Omega))$ such that for $h \in G$ the functional $h \mapsto \langle l, Sh \rangle$ is a continuous linear functional on G. By the Hahn–Banach theorem [28, Thm. 1.1], this linear functional can be extended to a continuous linear functional Φ on $(L^1(0, T; \mathscr{C}(\overline{\Omega}; \mathbb{R}^{3\times 3})))^* = L_w^\infty(0, T; \mathscr{M}(\overline{\Omega}; \mathbb{R}^{3\times 3}))$ with

$$\langle \Phi(t); A \rangle \leq 2\|(A)_{\text{sym},-}\|_{\mathscr{C}(\overline{\Omega}; \mathbb{R}^{3\times 3})}[E(t) - \mathscr{E}(v(t), d(t))] \tag{14}$$

for all $A \in \mathscr{C}(\overline{\Omega}; \mathbb{R}^{3\times 3})$ a.e. in $(0, T)$, where the estimate follows from (13) and Hahn–Banach's theorem written in its point-wise a.e.-form. By the Riesz representation theorem, we know that there exists a measure $m \in L_{w^*}^\infty(0, T; \mathscr{M}(\overline{\Omega}; \mathbb{R}^{3\times 3}))$ such that

$$\langle l(t), \tilde{u}(t) \rangle_{L_w^\infty(0,T;(\mathscr{C}_0^1(\Omega))^*), L^1(0,T;\mathscr{C}_0^1(\Omega))} = \langle \Phi(t), \nabla\tilde{u}(t) \rangle_{L_w^\infty(0,T;(\mathscr{C}(\overline{\Omega}))^*), L^1(0,T;\mathscr{C}(\overline{\Omega}))}$$

$$= -\int_0^T \int_{\overline{\Omega}} \nabla\tilde{u}(t) : \mathrm{d}m_t \mathrm{d}t,$$

which implies the formulation (7) by the definition of l in (13). From the estimate (14), we infer that the measure m vanishes for all continuous functions with values in the skew-symmetric matrices, such that $m \in L_w^\infty(0, T; \mathscr{M}(\overline{\Omega}; \mathbb{R}_{\text{sym}}^{3\times 3}))$. Additionally, (14) allows to insert $A = \xi \otimes \xi\phi$ for any $\xi \in \mathbb{R}^3$ and $\phi \in \mathscr{C}(\overline{\Omega}; [0, \infty))$ such that $\int_{\overline{\Omega}} \phi\xi \otimes \xi : \mathrm{d}m_t \geq 0$ for all $\phi \in \mathscr{C}(\overline{\Omega}; [0, \infty))$, which is the definition of a positive definite measure $m \in L_w^\infty(0, T; \mathscr{M}(\overline{\Omega}; \mathbb{R}_{\text{sym},+}^{3\times 3}))$. From the estimate in (14), we additionally infer by choosing $\Phi(t) = \phi(t)I$ for $\phi \in \mathscr{C}_0^1([0, T])$ with $\phi \geq 0$ a.e. in $(0, T)$ that

$$\int_0^T \phi(t) \int_{\overline{\Omega}} I : \mathrm{d}m(x)\mathrm{d}t = \int_0^T \phi(t) \int_{\overline{\Omega}} \mathrm{Tr}(m)(x)\mathrm{d}t \leq 2\int_0^T \phi(t)[E(t) - \mathscr{E}(v(t), d(t))]\mathrm{d}t.$$

This implies that $\langle m, I \rangle \leq 2[E - \mathscr{E}(v, d)]$ for a.e. $t \in (0, T)$, which in turn implies together with (12) the inequality (8).

Note that we use the usual spectral-norm for symmetric matrices $|A|_2 = \max_{i\in\{1,2,3\}} |\lambda_i|$, where λ_i denote the eigenvalues of the matrix $A \in \mathbb{R}_{\text{sym}}^{3\times 3}$. The dual-norm with respect to the Frobenius product : is given by $|A|_2' = \sum_{i=1}^3 |\lambda_i|$ for $A \in \mathbb{R}^{3\times 3}$. For a positive definite matrix, all eigenvalues are non-negative, such that we may write $|A|_2' = \sum_{i=1}^3 \lambda_i = \mathrm{Tr}(A) = A : I$. This implies that we may identify the norm $|A|_2' = I : A$. $\qquad\square$

Proof of Theorem 2.5 We observe that (6) tested with $\Delta\tilde{d}$ and integrated-in-time gives

$$\int_0^t \int_\Omega \left(\partial_t d + (v \cdot \nabla)d - (\nabla v)_{\text{skw}}d + (I - d \otimes d)(\lambda(\nabla v)_{\text{sym}}d - \Delta d)\right)\Delta\tilde{d}\mathrm{d}x\mathrm{d}s = 0. \tag{15}$$

Additionally, the equation (1a) for the strong solution tested with $\tilde{v} - v$ and (1c) for the strong solution tested with $\Delta(d - \tilde{d})$ implies

$$0 = \frac{1}{2}\|\tilde{v}\|_{L^2(\Omega)}^2\Big|_0^t$$

$$- \int_0^t \int_\Omega \partial_t\tilde{v} \cdot v + (\tilde{v} \cdot \nabla)\tilde{v} \cdot v - \nabla\tilde{d}^T\nabla\tilde{d} : \nabla v + \mu_4(\nabla\tilde{v})_{\text{sym}} : (\nabla v - \nabla\tilde{v})\mathrm{d}x\mathrm{d}s$$

$$- \int_0^t \int_\Omega (\mu_1 + \lambda^2)(\tilde{\boldsymbol{d}} \cdot (\nabla \tilde{\boldsymbol{v}})_{\text{sym}} \tilde{\boldsymbol{d}})(\tilde{\boldsymbol{d}} \otimes \tilde{\boldsymbol{d}}) : (\nabla \boldsymbol{v} - \nabla \tilde{\boldsymbol{v}}) \mathrm{d}x \mathrm{d}s$$

$$- \int_0^t \int_\Omega (\mu_5 + \mu_6 - \lambda^2)(\tilde{\boldsymbol{d}} \otimes (\nabla \tilde{\boldsymbol{v}})_{\text{sym}} \tilde{\boldsymbol{d}}) : (\nabla \boldsymbol{v} - \nabla \tilde{\boldsymbol{v}}) \mathrm{d}x \mathrm{d}s$$

$$- \int_0^t \int_\Omega \lambda \left((\nabla \boldsymbol{v})_{\text{sym}} \tilde{\boldsymbol{d}} \cdot (I - \tilde{\boldsymbol{d}} \otimes \tilde{\boldsymbol{d}}) \Delta \tilde{\boldsymbol{d}} + \nabla \left((I - \tilde{\boldsymbol{d}} \otimes \tilde{\boldsymbol{d}})(\nabla \tilde{\boldsymbol{v}})_{\text{sym}} \tilde{\boldsymbol{d}} \right) : \nabla \boldsymbol{d} \right) \mathrm{d}x \mathrm{d}s$$

$$+ \frac{1}{2} \|\nabla \tilde{\boldsymbol{d}}\|_{L^2(\Omega)}^2 \Big|_0^t - \int_0^t \int_\Omega \nabla \left((I - \tilde{\boldsymbol{d}} \otimes \tilde{\boldsymbol{d}}) \Delta \tilde{\boldsymbol{d}} \right) : (\nabla \boldsymbol{d} - \nabla \tilde{\boldsymbol{d}}) \mathrm{d}x \mathrm{d}t$$

$$- \int_0^t \int_\Omega \partial_t \nabla \tilde{\boldsymbol{d}} : \nabla \boldsymbol{d} + \nabla \left((\tilde{\boldsymbol{v}} \cdot \nabla) \tilde{\boldsymbol{d}} \right) : \nabla \boldsymbol{d} - (\nabla \boldsymbol{v})_{\text{skw}} \tilde{\boldsymbol{d}} \cdot \Delta \tilde{\boldsymbol{d}} - \nabla \left((\nabla \tilde{\boldsymbol{v}})_{\text{skw}} \tilde{\boldsymbol{d}} \right) : \nabla \boldsymbol{d} \mathrm{d}x \mathrm{d}s$$

$$+ \int_0^t \left\langle \partial_t \tilde{\boldsymbol{v}} + (\tilde{\boldsymbol{v}} \cdot \nabla) \tilde{\boldsymbol{v}} + \nabla \cdot (\nabla \tilde{\boldsymbol{d}}^T \nabla \tilde{\boldsymbol{d}}) - \nabla \cdot \tilde{\boldsymbol{T}}^L, \boldsymbol{v} - \tilde{\boldsymbol{v}} \right\rangle \mathrm{d}s$$

$$+ \int_0^t \left\langle \nabla \left(\partial_t \tilde{\boldsymbol{d}} + (\tilde{\boldsymbol{v}} \cdot \nabla) \tilde{\boldsymbol{d}} - (\nabla \tilde{\boldsymbol{v}})_{\text{skw}} \tilde{\boldsymbol{d}} + (I - \tilde{\boldsymbol{d}} \otimes \tilde{\boldsymbol{d}})(\lambda(\nabla \tilde{\boldsymbol{v}})_{\text{sym}} \tilde{\boldsymbol{d}} - \Delta \tilde{\boldsymbol{d}}) \right), \nabla(\boldsymbol{d} - \tilde{\boldsymbol{d}}) \right\rangle \mathrm{d}s \,.$$

$$(16)$$

We observe that

$$- \int_0^t \int_\Omega \partial_t \nabla \tilde{\boldsymbol{d}} : \nabla \boldsymbol{d} - \partial_t \boldsymbol{d} \cdot \Delta \tilde{\boldsymbol{d}} \mathrm{d}x \mathrm{d}s = \int_\Omega \nabla \boldsymbol{d} : \nabla \tilde{\boldsymbol{d}} \mathrm{d}x \Big|_0^t \,.$$

Adding up (5), (15), and (16) implies

$$[E - \mathscr{E}(\boldsymbol{v}, \boldsymbol{d})] \Big|_{0-}^t + \frac{1}{2} \left[\|\boldsymbol{v} - \tilde{\boldsymbol{v}}\|_{L^2(\Omega)}^2 + \|\nabla \boldsymbol{d} - \nabla \tilde{\boldsymbol{d}}\|_{L^2(\Omega)}^2 \right] \Big|_0^t$$

$$+ \int_0^t \int_\Omega (\mu_1 + \lambda^2)(\boldsymbol{d} \cdot (\nabla \boldsymbol{v} - \nabla \tilde{\boldsymbol{v}})_{sym} \boldsymbol{d})^2 + \mu_4 |(\nabla \boldsymbol{v} - \nabla \tilde{\boldsymbol{v}})_{sym}|^2 \mathrm{d}x \mathrm{d}s$$

$$+ \int_0^t \int_\Omega (\mu_5 + \mu_6 - \lambda^2)|(\nabla \boldsymbol{v} - \nabla \tilde{\boldsymbol{v}})_{sym} \boldsymbol{d}|^2 + |\boldsymbol{d} \times \Delta(\boldsymbol{d} - \tilde{\boldsymbol{d}})|^2 \mathrm{d}x \mathrm{d}s$$

$$+ \int_0^t \left\langle \partial_t \tilde{\boldsymbol{v}} + (\tilde{\boldsymbol{v}} \cdot \nabla) \tilde{\boldsymbol{v}} + \nabla \cdot (\nabla \tilde{\boldsymbol{d}}^T \nabla \tilde{\boldsymbol{d}}) - \nabla \cdot \tilde{\boldsymbol{T}}^L, \boldsymbol{v} - \tilde{\boldsymbol{v}} \right\rangle \mathrm{d}s$$

$$+ \int_0^t \left\langle \nabla \left(\partial_t \tilde{\boldsymbol{d}} + (\tilde{\boldsymbol{v}} \cdot \nabla) \tilde{\boldsymbol{d}} - (\nabla \tilde{\boldsymbol{v}})_{\text{skw}} \tilde{\boldsymbol{d}} + (I - \tilde{\boldsymbol{d}} \otimes \tilde{\boldsymbol{d}})(\lambda(\nabla \tilde{\boldsymbol{v}})_{\text{sym}} - \Delta \tilde{\boldsymbol{d}}) \right), \nabla(\boldsymbol{d} - \tilde{\boldsymbol{d}}) \right\rangle \mathrm{d}s$$

$$\leq \int_0^t \int_\Omega (\boldsymbol{v} \cdot \nabla) \boldsymbol{v} \cdot \tilde{\boldsymbol{v}} + (\tilde{\boldsymbol{v}} \cdot \nabla) \tilde{\boldsymbol{v}} \cdot \boldsymbol{v} \mathrm{d}x \mathrm{d}s$$

$$+ \int_0^t \int_\Omega \boldsymbol{T}^E(\boldsymbol{d}) : \nabla \tilde{\boldsymbol{v}} - \nabla \tilde{\boldsymbol{d}}^T \nabla \tilde{\boldsymbol{d}} : \nabla \boldsymbol{v} - (\boldsymbol{v} \cdot \nabla) \boldsymbol{d} \cdot \Delta \tilde{\boldsymbol{d}} + \nabla \left((\tilde{\boldsymbol{v}} \cdot \nabla) \tilde{\boldsymbol{d}} \right) : \nabla \boldsymbol{d} \mathrm{d}x \mathrm{d}s$$

$$- \int_0^t \int_\Omega (\mu_1 + \lambda^2) \left(\boldsymbol{d} \cdot (\nabla \tilde{\boldsymbol{v}})_{\text{sym}} \boldsymbol{d}(\boldsymbol{d} \otimes \boldsymbol{d}) - \tilde{\boldsymbol{d}} \cdot (\nabla \tilde{\boldsymbol{v}})_{\text{sym} \tilde{\boldsymbol{d}}}(\tilde{\boldsymbol{d}} \otimes \tilde{\boldsymbol{d}}) \right) : (\nabla \boldsymbol{v} - \nabla \tilde{\boldsymbol{v}})_{\text{sym}} \mathrm{d}x \mathrm{d}s$$

$$- \int_0^t \int_\Omega (\mu_5 + \mu_6 - \lambda^2) \left((\nabla \tilde{\boldsymbol{v}})_{\text{sym}}(\boldsymbol{d} \otimes \boldsymbol{d} - \tilde{\boldsymbol{d}} \otimes \tilde{\boldsymbol{d}}) : (\nabla \boldsymbol{v} - \nabla \tilde{\boldsymbol{v}})_{\text{sym}} \right) \mathrm{d}x \mathrm{d}s$$

$$- \int_0^t \int_\Omega \nabla \left[\left(\boldsymbol{d} \otimes \boldsymbol{d} - \tilde{\boldsymbol{d}} \otimes \tilde{\boldsymbol{d}} \right) \Delta \tilde{\boldsymbol{d}} \right] : \left(\nabla \boldsymbol{d} - \nabla \tilde{\boldsymbol{d}} \right) \mathrm{d}x \mathrm{d}s$$

$$- \lambda \int_0^t \int_\Omega \left((I - \boldsymbol{d} \otimes \boldsymbol{d})(\nabla \boldsymbol{v})_{\mathrm{sym}} \boldsymbol{d} - (I - \tilde{\boldsymbol{d}} \otimes \tilde{\boldsymbol{d}})(\nabla \boldsymbol{v})_{\mathrm{sym}} \tilde{\boldsymbol{d}} \right) \cdot \Delta \tilde{\boldsymbol{d}} \mathrm{d}x \mathrm{d}s$$

$$- \lambda \int_0^t \int_\Omega \nabla \boldsymbol{d} : \nabla \left((I - \boldsymbol{d} \otimes \boldsymbol{d})(\nabla \tilde{\boldsymbol{v}})_{\mathrm{sym}} \boldsymbol{d} - (I - \tilde{\boldsymbol{d}} \otimes \tilde{\boldsymbol{d}})(\nabla \tilde{\boldsymbol{v}})_{\mathrm{sym}} \tilde{\boldsymbol{d}} \right) \mathrm{d}x \mathrm{d}s$$

$$+ \int_0^t \int_\Omega \nabla((\nabla \tilde{\boldsymbol{v}})_{\mathrm{skw}}(\boldsymbol{d} - \tilde{\boldsymbol{d}})) : \nabla \boldsymbol{d} + ((\nabla \boldsymbol{v})_{\mathrm{skw}}(\boldsymbol{d} - \tilde{\boldsymbol{d}})) \cdot \Delta \tilde{\boldsymbol{d}} \mathrm{d}x \mathrm{d}s$$

$$+ \int_0^t \mathcal{K}(\tilde{\boldsymbol{v}}) \left[E - \mathcal{E}(\boldsymbol{v}, \boldsymbol{d}) \right] \mathrm{d}s. \tag{17}$$

We recall the identity, which is a special case of the identity (6.7) in [12],

$$0 = \int_\Omega \nabla \tilde{\boldsymbol{v}} : (\nabla \tilde{\boldsymbol{d}}^T \nabla \boldsymbol{d}) + \nabla \tilde{\boldsymbol{v}} : (\nabla \boldsymbol{d}^T \nabla \tilde{\boldsymbol{d}}) + (\tilde{\boldsymbol{v}} \cdot \nabla) \boldsymbol{d} \cdot \Delta \tilde{\boldsymbol{d}} - \nabla \left((\tilde{\boldsymbol{v}} \cdot \nabla) \tilde{\boldsymbol{d}} \right) : \nabla \boldsymbol{d} \mathrm{d}x.$$

This identity helps to transform the second line on the right-hand side of (17) in the case of $\boldsymbol{T}^E = \boldsymbol{T}_2^E$ into

$$- \int_\Omega \nabla \boldsymbol{d}^T \nabla \boldsymbol{d} : \nabla \tilde{\boldsymbol{v}} + \nabla \tilde{\boldsymbol{d}}^T \nabla \tilde{\boldsymbol{d}} : \nabla \boldsymbol{v} + (\boldsymbol{v} \cdot \nabla) \boldsymbol{d} \cdot \Delta \tilde{\boldsymbol{d}} - \nabla \left((\tilde{\boldsymbol{v}} \cdot \nabla) \tilde{\boldsymbol{d}} \right) : \nabla \boldsymbol{d} \mathrm{d}x$$

$$= - \int_\Omega (\nabla \boldsymbol{d} - \nabla \tilde{\boldsymbol{d}})^T (\nabla \boldsymbol{d} - \nabla \tilde{\boldsymbol{d}}) : \nabla \tilde{\boldsymbol{v}} + (\nabla \tilde{\boldsymbol{d}}^T \nabla \tilde{\boldsymbol{d}}) : (\nabla \boldsymbol{v} - \nabla \tilde{\boldsymbol{v}}) + ((\boldsymbol{v} - \tilde{\boldsymbol{v}}) \cdot \nabla) \boldsymbol{d} \cdot \Delta \tilde{\boldsymbol{d}} \mathrm{d}x$$

$$= - \int_\Omega (\nabla \boldsymbol{d} - \nabla \tilde{\boldsymbol{d}})^T (\nabla \boldsymbol{d} - \nabla \tilde{\boldsymbol{d}}) : \nabla \tilde{\boldsymbol{v}} + ((\boldsymbol{v} - \tilde{\boldsymbol{v}}) \cdot \nabla)(\boldsymbol{d} - \tilde{\boldsymbol{d}}) \cdot \Delta \tilde{\boldsymbol{d}} \mathrm{d}x.$$

In the case of $\boldsymbol{T}^E = \boldsymbol{T}_1^E$, we may observe from the unit-norm restriction and additional manipulations that

$$\int_\Omega (\tilde{\boldsymbol{v}} \cdot \nabla) \boldsymbol{d} [\boldsymbol{d}]_x [\boldsymbol{d}]_x \Delta \boldsymbol{d} - \nabla \tilde{\boldsymbol{d}}^T \nabla \tilde{\boldsymbol{d}} : \nabla \boldsymbol{v} - (\boldsymbol{v} \cdot \nabla) \boldsymbol{d} \cdot \Delta \tilde{\boldsymbol{d}} + \nabla \left((\tilde{\boldsymbol{v}} \cdot \nabla) \tilde{\boldsymbol{d}} \right) : \nabla \boldsymbol{d} \mathrm{d}x$$

$$= \int_\Omega (\tilde{\boldsymbol{v}} \cdot \nabla) \boldsymbol{d} [\boldsymbol{d}]_x^T [\boldsymbol{d}]_x \Delta \boldsymbol{d} + \left[[\tilde{\boldsymbol{d}}]_x^T [\tilde{\boldsymbol{d}}]_x \nabla \tilde{\boldsymbol{d}} - [\boldsymbol{d}]_x^T [\boldsymbol{d}]_x \nabla \boldsymbol{d} \right] \cdot (\Delta \tilde{\boldsymbol{d}} \otimes \boldsymbol{v}) \mathrm{d}x$$

$$+ \int_\Omega \nabla \left((\tilde{\boldsymbol{v}} \cdot \nabla) \tilde{\boldsymbol{d}} [\tilde{\boldsymbol{d}}]_x^T [\tilde{\boldsymbol{d}}]_x \right) : \nabla \boldsymbol{d} \mathrm{d}x$$

$$= \int_\Omega (\tilde{\boldsymbol{v}} \cdot \nabla)(\boldsymbol{d} - \tilde{\boldsymbol{d}}) [\boldsymbol{d}]_x^T [\boldsymbol{d}]_x (\Delta \boldsymbol{d} - \Delta \tilde{\boldsymbol{d}}) - ((\boldsymbol{v} - \tilde{\boldsymbol{v}}) \cdot \nabla)(\boldsymbol{d} - \tilde{\boldsymbol{d}}) \cdot [\boldsymbol{d}]_x^T [\boldsymbol{d}]_x \Delta \tilde{\boldsymbol{d}} \mathrm{d}x$$

$$- \int_\Omega \nabla \left[(\tilde{\boldsymbol{v}} \cdot \nabla) \tilde{\boldsymbol{d}} ([\boldsymbol{d}]_x^T [\boldsymbol{d}]_x - [\tilde{\boldsymbol{d}}]_x^T [\tilde{\boldsymbol{d}}]_x) \right] : (\nabla \boldsymbol{d} - \nabla \tilde{\boldsymbol{d}}) \mathrm{d}x$$

$$+ \int_\Omega ((\boldsymbol{v} - \tilde{\boldsymbol{v}}) \cdot \nabla) \tilde{\boldsymbol{d}} \cdot ([\boldsymbol{d}]_x^T [\boldsymbol{d}]_x - [\tilde{\boldsymbol{d}}]_x^T [\tilde{\boldsymbol{d}}]_x) \Delta \tilde{\boldsymbol{d}} \mathrm{d}x.$$

The resulting terms can now be estimated in terms of the relative energy and the relative dissipation, *i.e.,* the terms on the left-hand side. Similar arguments have already been applied in [12] and [29]. We remark, that in the term in the fifth line on the right-hand side of (17),

we have to apply the product rule to infer

$$-\int_\Omega \nabla\left[\left(\boldsymbol{d}\otimes\boldsymbol{d}-\tilde{\boldsymbol{d}}\otimes\tilde{\boldsymbol{d}}\right)\Delta\tilde{\boldsymbol{d}}\right]:\left(\nabla\boldsymbol{d}-\nabla\tilde{\boldsymbol{d}}\right)\mathrm{d}x$$

$$=-\int_\Omega(\nabla\boldsymbol{d}-\nabla\tilde{\boldsymbol{d}}):\nabla\left(\boldsymbol{d}\otimes\boldsymbol{d}-\tilde{\boldsymbol{d}}\otimes\tilde{\boldsymbol{d}}\right)\cdot\Delta\tilde{\boldsymbol{d}}$$

$$+\left((\nabla\boldsymbol{d}-\nabla\tilde{\boldsymbol{d}})^T\left(\boldsymbol{d}\otimes\boldsymbol{d}-\tilde{\boldsymbol{d}}\otimes\tilde{\boldsymbol{d}}\right)\right):\nabla\Delta\tilde{\boldsymbol{d}}\mathrm{d}x.$$

In order to prove the weak-strong uniqueness result, the terms on the right-hand side of (17) have to be estimated by terms on the left-hand side and Gronwall's inequality is applied in the end. Since most of the estimates are rather standard and done using Hölder's and Young's inequality, we refrain from displaying it in full detail here. The interested reader may consult the article [12] for more details, where these estimates were performed for a more involved system.

Estimating all terms appropriately, we find that there exists a constant $C > 0$ such that

$$[E-\mathscr{E}(\boldsymbol{v},\boldsymbol{d})]\Big|_{0-}^t+\frac{1}{2}\left[\|\boldsymbol{v}-\tilde{\boldsymbol{v}}\|_{L^2(\Omega)}^2+\|\nabla\boldsymbol{d}-\nabla\tilde{\boldsymbol{d}}\|_{L^2(\Omega)}^2\right]\Big|_0^t$$

$$+\frac{1}{2}\int_0^t\int_\Omega(\mu_1+\lambda^2)(\boldsymbol{d}\cdot(\nabla\boldsymbol{v}-\nabla\tilde{\boldsymbol{v}})_{sym}\boldsymbol{d})^2+\mu_4|(\nabla\boldsymbol{v}-\nabla\tilde{\boldsymbol{v}})_{sym}|^2\mathrm{d}x\mathrm{d}s$$

$$+\frac{1}{2}\int_0^t\int_\Omega(\mu_5+\mu_6-\lambda^2)|(\nabla\boldsymbol{v}-\nabla\tilde{\boldsymbol{v}})_{sym}\boldsymbol{d}|^2+|\boldsymbol{d}\times\Delta(\boldsymbol{d}-\tilde{\boldsymbol{d}})|^2\mathrm{d}x\mathrm{d}s$$

$$+\int_0^t\left\langle\partial_t\tilde{\boldsymbol{v}}+(\tilde{\boldsymbol{v}}\cdot\nabla)\tilde{\boldsymbol{v}}+\nabla\cdot(\nabla\tilde{\boldsymbol{d}}^T\nabla\tilde{\boldsymbol{d}})-\nabla\cdot\tilde{\boldsymbol{T}}^L,\boldsymbol{v}-\tilde{\boldsymbol{v}}\right\rangle\mathrm{d}s$$

$$+\int_0^t\left\langle\nabla\left(\partial_t\tilde{\boldsymbol{d}}+(\tilde{\boldsymbol{v}}\cdot\nabla)\tilde{\boldsymbol{d}}-(\nabla\tilde{\boldsymbol{v}})_{\mathrm{skw}}\tilde{\boldsymbol{d}}+(I-\tilde{\boldsymbol{d}}\otimes\tilde{\boldsymbol{d}})(\lambda(\nabla\tilde{\boldsymbol{v}})_{\mathrm{sym}}-\Delta\tilde{\boldsymbol{d}})\right),\nabla(\boldsymbol{d}-\tilde{\boldsymbol{d}})\right\rangle\mathrm{d}s$$

$$\le C\int_0^t\left(\|\tilde{\boldsymbol{v}}\|_{L^\infty(\Omega)}^2+\|\nabla\tilde{\boldsymbol{v}}\|_{L^\infty(\Omega)}+\|\Delta\tilde{\boldsymbol{d}}\|_{L^3(\Omega)}^3\right)\left[\|\boldsymbol{v}-\tilde{\boldsymbol{v}}\|_{L^2(\Omega)}^2+\|\nabla\boldsymbol{d}-\nabla\tilde{\boldsymbol{d}}\|_{L^2(\Omega)}^2\right]\mathrm{d}s$$

$$+C\int_0^t\left(\|\nabla\tilde{\boldsymbol{v}}\|_{L^3(\Omega)}^2+\|\Delta\tilde{\boldsymbol{d}}\|_{L^\infty(\Omega)}+\|\Delta\tilde{\boldsymbol{d}}\|_{W^{1,3}(\Omega)}^2\right)\left[\|\boldsymbol{v}-\tilde{\boldsymbol{v}}\|_{L^2(\Omega)}^2+\|\nabla\boldsymbol{d}-\nabla\tilde{\boldsymbol{d}}\|_{L^2(\Omega)}^2\right]\mathrm{d}s$$

$$+\int_0^t\mathscr{K}(\tilde{\boldsymbol{v}})\left[E-\mathscr{E}(\boldsymbol{v},\boldsymbol{d})\right]\mathrm{d}s. \tag{18}$$

Gronwall's inequality implies the relative energy inequality (11). Choosing $(\tilde{\boldsymbol{v}},\tilde{\boldsymbol{d}})$ to be a solution, implies that the fourth and fifth line of (11) vanish. Since all terms on the left-hand side of (11) are non-negative, if $\boldsymbol{v}_0=\tilde{\boldsymbol{v}}(0)$ and $\boldsymbol{d}_0=\tilde{\boldsymbol{d}}(0)$ the right-hand side of (11) is zero such that $\boldsymbol{v}(t)=\tilde{\boldsymbol{v}}(t)$ and $\boldsymbol{d}(t)=\tilde{\boldsymbol{d}}(t)$ for a.e. $t\in(0,T^*)$, which implies the assertion of Theorem 2.5.   □

Remark (Weak-strong uniqueness extended) It may seem strange that all calculations in the above proof are conducted on the time interval $(0,t)$, when the definition of energy-variational solutions 2.1 is formulated on every interval (s,t) for all $s<t\in(0,T)$. Indeed, the calculations of the above proof can also be carried out for all intervals (s,t) such that we may infer inequality (18) with 0 replaced by s. Thus, the weak-strong uniqueness result can

be sharpened: If there exists an $s \in (0, T)$ such that there exists a solution $(\tilde{v}, \tilde{d})$ fulfilling the regularity assumptions (10a)–(10b) on (s, T) with $v(s) = \tilde{v}(s), d(s) = \tilde{d}(s)$ and additionally $\mathscr{E}(\tilde{v}(s), \tilde{d}(s)) = E(s)$, then it holds

$$v \equiv \tilde{v}, \qquad d \equiv \tilde{d} \qquad \text{on } (s, T).$$

2.3 Auxiliary Lemmata

Lemma 2.6 *Let* $d \in L^\infty(\Omega) \cap H^1(\Omega)$ *with* $d \times \Delta d \in L^2(\Omega)$ *and* $|d(x, t)| = 1$ *a.e. in* $\Omega \times (0, T)$ *such that for the trace* $|\operatorname{tr}(d)| = 1$ *a.e. on* $\partial\Omega$. *Then we can identify the terms* $-d \times (d \times \Delta d) = [d]_x^T [d]_x \Delta d = (I - d \otimes d)\Delta d = \Delta d + |\nabla d|^2 d$ *in* $L^2(\Omega)$, *which implies*

$$\int_\Omega |d \times \Delta d|^2 dx = \int_\Omega |\Delta d + |\nabla d|^2 d|^2 dx.$$

Remark We note that the notation $\Delta d + |\nabla d|^2 d$ is the usual formulation in the Euler–Lagrange equation of harmonic maps into the sphere [30]. The norm of this term appears as a dissipative term in the energy-dissipation mechanism of the system (see (5) below). Formally this implies that the solution to such a system is forced to approximately fulfill the Euler–Lagrange equation of the Dirichlet energy minimized over all functions with values in the sphere, in the large-time limit.

Proof For all $\varphi \in H^1(\Omega; \mathbb{S}^2)$, we find by an integration-by-parts and $\nabla|d|^2 = 0$ a.e. in Ω as well as a.e. on $\partial\Omega$ that

$$\int_\Omega \varphi \cdot (I - d \otimes d) \Delta d \, dx = -\int_\Omega \nabla\varphi : (I - d \otimes d)\nabla d - \varphi \cdot d|\nabla d|^2 - (\nabla d^T \varphi) \cdot (\nabla d^T d) dx$$

$$+ \int_{\partial\Omega} \varphi \cdot (I - d \otimes d)\nabla d \cdot n \, dS$$

$$= -\int_\Omega \nabla\varphi : \nabla d - \varphi \cdot |\nabla d|^2 d \, dx - \frac{1}{2}\int_\Omega \nabla(\varphi \cdot d) \cdot \nabla|d|^2 dx$$

$$+ \int_{\partial\Omega} \varphi \cdot \nabla d \cdot n - \frac{1}{2}\varphi \cdot d n \cdot \nabla|d|^2 dS$$

$$= \int_\Omega \varphi \cdot (\Delta d + |\nabla d|^2 d) dx,$$

which implies the equivalence of the terms in $L^2(\Omega)$. The unit-norm constraint implies $(I - d \otimes d) = (I - d \otimes d)(I - d \otimes d)$ such that we infer the second equality

$$\int_\Omega |d \times \Delta d|^2 dx = \int_\Omega \Delta d \cdot (I - d \otimes d)\Delta d \, dx = \int_\Omega ((I - d \otimes d)\Delta d) \cdot (I - d \otimes d)\Delta d \, dx$$

$$= \int_\Omega |\Delta d + |\nabla d|^2 d|^2 dx.$$

This implies the assertion. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

Lemma 2.7 ([13, Lemma 2.4]) *Let $f \in L^1(0, T)$ and $g \in L^\infty(0, T)$ with $g \geq 0$ a.e. in $(0, T)$. Then the two inequalities*

$$-\int_0^T \phi'(t) g(t) dt + \int_0^T \phi(t) f(t) dt \leq 0$$

for all $\phi \in \mathscr{C}_c^1((0, T))$ with $\phi \geq 0$ for all $t \in (0, T)$ and

$$g(t) - g(s) + \int_s^t f(\tau) d\tau \leq 0 \quad \text{for a.e. } t, s \in (0, T), s \leq t \tag{19}$$

are equivalent.

Moreover, from (19) *we can infer that there exists a function $h \in \mathrm{BV}([0, T])$ such that $h = g$ a.e. in $(0, T)$ and the inequality* (19) *holds for every $s, t \in (0, T)$ with g replaced by h.*

2.4 Finite Element Spaces

For the rest of this paper we presume the following assumptions.

1. The domain $\Omega \subset \mathbb{R}^3$ is a convex polyhedron.
2. The subdivision $\mathscr{T}^h$ of tetrahedra of our domain $\Omega \subset \mathbb{R}^3$ is quasi-uniform (in the sense of [31, 4.4.15]).
3. All $T \in \mathscr{T}^h$ have at least one node that is not on the boundary $\partial\Omega$.
4. Every $T \in \mathscr{T}^h$ is equipped with a Lagrangian finite element.

In order to apply well known results for the numerical approximation of incompressible flows, we choose ($P2$-$P1$) Taylor–Hood elements (*cf.* [32]) for the velocity. By X_h and M_h we denote the finite element spaces for the velocity and pressure,

$$M_h := \{q \in C(\overline{\Omega}) : \int_\Omega q \, dx = 0, \quad q|_K \in \mathbb{P}_1(K) \quad \forall K \in \mathscr{T}_h\},$$

$$X_h := \{v \in C(\overline{\Omega}) : v = 0 \text{ on } \partial\Omega, \quad v|_K \in \mathbb{P}_2(K) \quad \forall K \in \mathscr{T}_h\},$$

where $\mathbb{P}_k(\Omega)$ is the set of polynomials of degree k or less on the domain Ω. For better readability, we denote approximately divergence-free functions in X_h as the space V_h, *i.e.*

$$V_h := \{v \in [X_h]^3, \quad (\nabla \cdot v, q) = 0 \text{ for all } q \in M_h\}. \tag{20}$$

It is a well-known result (*cf.* [33]) that this choice of spaces fulfills the inf-sup condition (sometimes also called *LBB* or *Ladyzhenskaya–Babuska–Brezzi* condition) under our given assumptions (1–4), that is

$$\sup_{v_h \in [X_h]^3 \setminus \{0\}} \frac{(\nabla \cdot v_h, q_h)}{\|\nabla v_h\|_{L^2(\Omega)}} \geq C \|q_h\|_{L^2(\Omega)}$$

for all $q_h \in M_h$ and for some constant $C > 0$. The director and discrete Laplacian are approximated using piecewise linear functions,

$$Z_h := \{v \in C(\overline{\Omega}) : v|_K \in \mathbb{P}_1(K) \quad \forall K \in \mathscr{T}_h\}.$$

The homogeneous Dirichlet boundary conditions can be implied in the space by

$$Y_h := \{v \in C(\overline{\Omega}) : v = 0 \text{ on } \partial\Omega, \quad v|_K \in \mathbb{P}_1(K) \quad \forall K \in \mathscr{T}_h\}.$$

Our final mixed finite element space will be denoted by,

$$U_h := V_h \times [Y_h]^3$$

Lemma 2.8 (Inverse estimate, *cf.* [31, Thm. 4.5.11]) *Under the assumptions* (1–4), *let* $p, q \in [1, \infty]$ *and* $0 \le m \le l \le 1$. *Then there exists a constant* C *independent of* h, *such that*

$$\|v\|_{W^{l,p}(\Omega)} \le C h^{m-l+\min\{0,3/p-3/q\}} \|v\|_{W^{m,q}(\Omega)}$$

holds for all $v \in [Z_h]^3$, V_h.

For the finite element spaces $[Y_h]^3$ and V_h and a function $f \in L^2(\Omega)$ the standard L^2-projection, is denoted by $\mathscr{P}_h : L^2(\Omega)^3 \to [Y_h]^3$ and $\mathscr{Q}_h : L^2_\sigma(\Omega) \to V_h$, respectively.

Lemma 2.9 (Projection operator, *cf.* [34], [35, Lem. 1.131, Prop. 1.134]) *Under the previously given assumptions* (1–4), *the* L^2 *projection onto* $[Y_h]^3$ *is stable in* $L^p(\Omega)$ *for all* $1 \le p \le \infty$ *and* $H^1(\Omega)$, *i.e. we have*

$$\|\mathscr{P}_h(\boldsymbol{u}_1)\|_{L^p(\Omega)} \le C \|\boldsymbol{u}_1\|_{L^p(\Omega)},$$

$$\|\mathscr{P}_h\boldsymbol{u}_2 - \boldsymbol{u}_2\|_{L^2(\Omega)} + h \|\mathscr{P}_h(\boldsymbol{u}_2)\|_{H^1(\Omega)} \le C h \|\boldsymbol{u}_2\|_{H^1(\Omega)}$$

for all $\boldsymbol{u}_1 \in L^2(\Omega) \cap L^p(\Omega)$, $\boldsymbol{u}_2 \in H^1(\Omega)$.

For the projection onto the finite element space for the velocity V_h, $\mathscr{Q}_h$ admits the error and stability estimates

$$\|\mathscr{Q}_h(\boldsymbol{v}) - \boldsymbol{v}\|_{L^2(\Omega)} \le C h \|\nabla \boldsymbol{v}\|_{L^2(\Omega)}$$

$$\|\mathscr{Q}_h\tilde{\boldsymbol{v}} - \tilde{\boldsymbol{v}}\|_{H^1(\Omega)} + h\|\mathscr{Q}_h\tilde{\boldsymbol{v}}\|_{H^2(\Omega)} \le C h\|\tilde{\boldsymbol{v}}\|_{H^2(\Omega)} \tag{21}$$

for all $\boldsymbol{v} \in H^1_{0,\sigma}(\Omega)$ and $\tilde{\boldsymbol{v}} \in H^2(\Omega) \cap H^1_{0,\sigma}(\Omega)$. This follows from [36, Lem. 4.3] and the regularity of the Stokes problem on convex polygons (see [37], see also [38, Proposition 2] or [39, Cor. 1.8]).

2.5 Interpolation and Mass-Lumping

We define the nodal interpolation operator $\mathscr{I}_h : \mathscr{C}(\Omega) \to [Z_h]^3$ by

$$\mathscr{I}_h(f) := \sum_{z \in \mathscr{N}_h} f(z)\phi_z,$$

for all functions $f \in C(\Omega)$, where $\mathscr{N}_h$ is the set of all nodes in our mesh. For continuous functions $y_1, y_2 \in C(\Omega; \mathbb{R}^3)$ we introduce the lumped inner product (*cf.* [40, 41]) and the according norm as

$$(y_1, y_2)_h := \int_\Omega \mathscr{I}_h(y_1 \cdot y_2)\mathrm{d}x = \sum_{z \in \mathscr{N}_h} y_1(z) \cdot y_2(z) \int_\Omega \phi_z \mathrm{d}x, \tag{22}$$

$$\|y_1\|_h^2 := (y_1, y_1)_h.$$

For the interpolation operator we observe the following standard error estimate:

Lemma 2.10 *Under the assumptions (1–4), let $3/2 < p \leq \infty$. Then there exists a constant $C > 0$ independent of h and the function f, such that*

$$\| f - \mathscr{I}_h(f) \|_{W^{k,p}(\Omega)} \leq C h^{2-k} |f|_{W^{2,p}(\Omega)}$$

holds for all $0 \leq k \leq 2$ and $f \in W^{2,p}(\Omega)$.

The above theorem is standard and can for example be found in [31, Thm. 4.4.20]. There exists a generic constant $c_L > 0$ independent of $h > 0$ such that for functions $y_1, y_2 \in [Z_h]^3$ the estimates

$$\| y_1 \|_{L^2(\Omega)} \leq \| y_1 \|_h \leq c_L \| y_1 \|_{L^2(\Omega)} \tag{23}$$

hold.

Lemma 2.11 *Let $\frac{1}{p} + \frac{1}{q} = 1$. There exists a generic constant $C > 0$ independent of $h > 0$ such that*

$$|(y_1, y_2)_h - (y_1, y_2)| \leq C h \| y_1 \|_{L^p(\Omega)} \| \nabla y_2 \|_{L^q(\Omega)}$$
$$|(y_h, g)_h - (y_h, g)| \leq C h \| y_h \|_{L^p(\Omega)} \| g \|_{W^{2,q}(\Omega)}, \tag{24}$$

for all $y_1, y_2, y_h \in [Z_h]^3$, $g \in W^{2,q}(\Omega)$ with $q > 3/2$.

Proof We proceed as in [41] and find for $y_1, y_2 \in Z_h$

$$
\begin{aligned}
|(y_1, y_2)_h - (y_1, y_2)| &\leq \int_\Omega |\mathscr{I}_h(y_1 \cdot y_2) - y_1 \cdot y_2| \, \mathrm{d}x \\
&\leq \sum_{K \in \mathscr{T}^h} \| \mathscr{I}_h(y_1 \cdot y_2) - y_1 \cdot y_2 \|_{L^2(K)} \| 1 \|_{L^2(K)} \\
&\leq C h^2 \sum_{K \in \mathscr{T}^h} \left\| \nabla^2 (y_1 \cdot y_2) \right\|_{L^2(K)} \| 1 \|_{L^2(K)} \\
&\leq C h^2 \sum_{K \in \mathscr{T}^h} \| \nabla y_1 : \nabla y_2 \|_{L^2(K)} \| 1 \|_{L^2(K)} \\
&\leq C h^2 \sum_{K \in \mathscr{T}^h} \| \nabla y_1 \|_{L^p(K)} \| \nabla y_2 \|_{L^q(K)} \\
&\leq C h^2 \| \nabla y_1 \|_{L^p(\Omega)} \| \nabla y_2 \|_{L^q(\Omega)} \\
&\leq C h \| y_1 \|_{L^p(\Omega)} \| \nabla y_2 \|_{L^q(\Omega)}.
\end{aligned}
\tag{25}
$$

The first inequality is a triangle inequality, the second one uses Hölder's inequality, the third bounds the interpolation error by Lemma 2.10. Since $[Z_h]^3$ consists of piecewise affine-linear functions the second derivative of a function in $[Z_h]^3$ vanishes. This together with Hölder's inequality, local and global inverse estimates (*cf.* 2.8) allow to conclude. Note that the choice of exponents in the third step is necessary in order to make sure that we can indeed apply Lemma 2.10.

In case that one function is not a finite element functions, we have to estimate the difference with the interpolated function, *i.e.*,

$$|(\mathscr{I}_h y_h, \mathscr{I}_h g) - (y_h, g)| = |(y_h, \mathscr{I}_h g) - (y_h, g)|$$
$$\leq C \|y_h\|_{L^p(\Omega)} \|(\mathscr{I}_h - I)g\|_{L^q(\Omega)} \leq Ch^2 \|y_h\|_{L^p(\Omega)} \|\nabla^2 g\|_{L^q(\Omega)}, \quad (26)$$

and estimate the last factor on the right-hand side of (25) by

$$\|\nabla \mathscr{I}_h g\|_{L^q(\Omega)} \leq \|\nabla(\mathscr{I}_h - I)g\|_{L^q(\Omega)} + \|\nabla g\|_{L^q(\Omega)}$$
$$\leq Ch \|\nabla^2 g\|_{L^q(\Omega)} + \|\nabla g\|_{L^q(\Omega)} \leq C \|\nabla g\|_{W^{1,q}(\Omega)}. \qquad \square$$

We introduce another interpolation operator $\widetilde{\mathscr{I}}_h : L^1(\Omega; \mathbb{R}^3) \to [Z_h]^3$ by

$$\widetilde{\mathscr{I}}_h(g) := \sum_{z \in \mathscr{N}_h} \frac{\int_\Omega g(x)\phi_z(x)dx}{\int_\Omega \phi_z(x)dx} \phi_z. \qquad (27)$$

We observe the identity

$$(\mathscr{I}_h f, g) = \int_\Omega \sum_{z \in \mathscr{N}_h} f(z)\phi_z(x)g(x)dx$$
$$= \sum_{z \in \mathscr{N}_h} f(z) \int_\Omega \phi_z(x)g(x)dx = (f, \widetilde{\mathscr{I}}_h g)_h. \qquad (28)$$

Lemma 2.12 *Let* $f \in \mathscr{C}(\overline{\Omega})$. *Then it holds*

$$\|f - \widetilde{\mathscr{I}}_h f\|_{\mathscr{C}(\overline{\Omega})} \to 0 \text{ as } h \to 0.$$

Proof Consider any $y \in \overline{\Omega}$. We obtain the pointwise estimate

$$f(y) - \widetilde{\mathscr{I}}_h f(y) = \sum_z f(y)\phi_z(y) - \sum_z \int_\Omega f(x)\phi_z(x)dx\phi_z(y)\frac{1}{\int_\Omega \phi_z(x)dx}$$
$$= \sum_z \phi_z(y)\frac{\int_\Omega [f(y) - f(x)]\phi_z(x)dx}{\int_\Omega \phi_z(x)dx}$$
$$\leq \sum_z \phi_z(y) \max_{x \in supp(\phi_z)} |f(x) - f(y)|$$
$$= \max_{z \in \mathscr{N}_h} \max_{x,s \in supp(\phi_z)} |f(x) - f(s)|,$$

where the last term converges to 0 as $h \to 0$, since f is continuous. Above, we used that $\sum_z \phi_z(y) = 1$ and that support of the shape functions ϕ_z vanishes as $h \to 0$. Since y was arbitrary the assertion follows. $\qquad \square$

Further, we introduce the discrete Laplacian in a slightly different way than usual, since we further equip it with mass lumping. Then the discrete Laplacian $\Delta_h : H^1(\Omega) \to [Y_h]^3$ of

a function $f \in H^1(\Omega)$ is defined via

$$(-\Delta_h f, b)_h = (\nabla f, \nabla b) \quad \text{for all } b \in Y_h. \tag{29}$$

Similarly, we define an adapted projection via $\mathscr{R}_h : L^2(\Omega; \mathbb{R}^3) \to [Z_h]^3$ via

$$(\mathscr{R}_h f, b)_h = (f, b) \quad \text{for all } b \in [Z_h]^3. \tag{30}$$

This choice allows to infer with (23) that

$$\|\mathscr{R}_h f\|_h^2 = (\mathscr{R}_h f, \mathscr{R}_h f)_h = (f, \mathscr{R}_h f) \le \|f\|_{L^2(\Omega)} \|\mathscr{R}_h f\|_{L^2(\Omega)} \le \|f\|_{L^2(\Omega)} \|\mathscr{R}_h f\|_h , \tag{31}$$

which implies together with (23) that $\|\mathscr{R}_h f\|_{L^2(\Omega)} \le \|\mathscr{R}_h f\|_h \le \|f\|_{L^2(\Omega)}$.

Remark (Adapted discretization of convection term) In comparison to the discretization in [24], we use the above projection $\mathscr{R}_h$ in the definition of the convection term in comparison to the L^2-projection $\mathscr{P}_h$. This change is needed in order to show the convergence to the finer concept of energy-variational solutions. In [24] only the convergence to dissipative solutions was shown, which is a bigger class of solutions. One key ingredient for this improvement are the above norm-equivalences.

3 Discrete System

In order to restrict ourselves to finite element spaces with a zero trace, we decompose the spatial approximation of our director into its interior and its non-homogeneous Dirichlet boundary condition, *i.e.*

$$d^j = d_\circ^j + \mathscr{I}_h \boldsymbol{d}_0, \tag{32}$$

with $\text{tr}(d_\circ^j) = 0$ and $\boldsymbol{d}_0 \in H^2(\Omega)$.

Scheme 33 *Let $(v^0, d^0) = (\mathscr{Q}_h v_0, \mathscr{I}_h d_0)$. For $1 \le j \le J$ and $(v^{j-1}, d_\circ^{j-1}) \in U_h$, we want to find $(v^j, d_\circ^j) \in U_h$, such that*

$$(\boldsymbol{d}_t v^j, a) + ((v^{j-1} \cdot \nabla) v^j, a) + \frac{1}{2}([\nabla \cdot v^{j-1}] v^j, a)$$
$$- ([\mathscr{R}_h \nabla d^{j-1}]^T [d^{j-1/2} \times (d^{j-1/2} \times \Delta_h d^{j-1/2})], a)_h + (T_L^j, \nabla a) = 0, \tag{33a}$$

$$(\boldsymbol{d}_t d^j, c)_h + (d^{j-1/2} \times [\mathscr{R}_h \nabla d^{j-1} v^j], d^{j-1/2} \times c)_h$$
$$+ \lambda (d^{j-1/2} \times [(\nabla v^j)_{sym} d^{j-1/2}], d^{j-1/2} \times c)_h \tag{33b}$$
$$- (d^{j-1/2} \times \Delta_h d^{j-1/2}, d^{j-1/2} \times c)_h - ((\nabla v^j)_{skw} d^{j-1/2}, c)_h = 0,$$

for all $(a, c) \in U_h$. Hereby we discretize the Leslie stress tensor as

$$(T_L^j, \nabla a) := (T_D^j, \nabla a) + \lambda (d^{j-1/2} \times [(\nabla a)_{sym} d^{j-1/2}], d^{j-1/2} \times \Delta_h d^{j-1/2})_h$$
$$+ ((\nabla a)_{skw} \Delta_h d^{j-1/2}, d^{j-1/2})_h, \tag{34}$$

where T_D^j collects the dissipative terms of the discrete Leslie stress tensor again, i.e.

$$(T_D^j, \nabla a) := (\mu_1 + \lambda^2)((d^j \cdot (\nabla v^j)_{sym} d^j), (d^j \cdot (\nabla a)_{sym} d^j))$$
$$+ \mu_4 \left((\nabla v^j)_{sym}, (\nabla a)_{sym} \right) + (\mu_5 + \mu_6 - \lambda^2) \left((\nabla v^j)_{sym} d^j, (\nabla a)_{sym} d^j \right).$$

Remark (Features of the discrete system) The mass lumping is applied on the director equation (33b) to guarantee the unit-norm restriction of d^j at every node. In order to find a discrete energy law, the associated terms in the momentum equation (33a) and the discrete Laplacian are mass-lumped as well. Since the gradient of the director is piecewise constant and therefore not well-defined at the nodes of the mesh, we apply the mass-lumped L^2 projection $\mathscr{R}_h$ in the convection term. Note this is computationally not too expensive, since it only affects the gradient of the past iterate.

Additionally, we note that solving the discrete system amounts to introducing two additional coupled equations, one to calculate the discrete Laplacian (29) and one to assure that the solution v^j fulfills the discrete vanishing divergence condition (20).

3.1 *A Priori* Estimates

The proposed scheme is unconditionally solvable.

Proposition 3.1 (Existence of discrete solutions) *Let $k, h > 0$, $j \in \mathbb{N}$ and $1 \le j \le J = \lfloor T/k \rfloor$. Then there exists a solution $u^j = (v^j, d_\circ^j) \in U_h$ solving Scheme (33a)–(33b).*

Proof We show that the map $\Pi : U_h \to U_h$ implicitly defined by the above scheme (33a)–(33b), whose zero is the next iterate in terms of $u = (v^j, -\Delta_h d^{j-1/2})$, fulfills

$$(\Pi(u), u)_{U_h} \ge 0 \tag{35}$$

for all $\|u\|_{U_h} \ge R_{j-1}$ for some constant $R_{j-1} > 0$. Where the dependency on d^j has to be interpreted via the discrete Greens function $\mathscr{G}_h$ associated with the discrete Laplacian and given by

$$(\nabla \mathscr{G}_h(w), \nabla b) = (w, b)_h \quad \text{for all } b \in Y_h.$$

Noting that this operator is a continuous bijection due to Lax–Milgram, we observe that the associated mapping Π corresponding to our discrete scheme is actually well-defined and continuous. Then the existence of solutions to our discrete scheme (33a)–(33b) follows from a non-linear version of Brouwer's fix-point theorem (*cf.* [42]). In particular, we evaluate

$$(\Pi(v^j, -\Delta_h d^{j-1/2}), (v^j, -\Delta_h d^{j-1/2}))_{U_h}$$
$$= \frac{1}{2} d_t \|v^j\|_{L^2(\Omega)}^2 + \frac{1}{2} d_t \|\nabla d^j\|_{L^2(\Omega)}^2 + \frac{k}{2} \|d_t v^j\|_{L^2(\Omega)}^2$$
$$+ (\mu_1 + \lambda^2) \|d^j \cdot (\nabla v^j)_{sym} d^j\|_{L^2(\Omega)} + \mu_4 \|(\nabla v^j)_{sym}\|_{L^2(\Omega)} \tag{36}$$
$$+ (\mu_5 + \mu_6 - \lambda^2) \|(\nabla v^j)_{sym} d^j\|_{L^2(\Omega)} + \|\mathscr{I}_h(d^{j-1/2} \times \Delta_h d^{j-1/2})\|_h^2,$$

where we used the discrete identities

$$(d_t v^j, v^j) = \frac{1}{2} d_t \|v^j\|_{L^2(\Omega)}^2 + \frac{k}{2} \|d_t v^j\|_{L^2(\Omega)}^2, \quad (-\Delta_h d^{j-1/2}, d_t d^j)_h = \frac{1}{2} d_t \|\nabla d^j\|_{L^2(\Omega)}^2. \tag{37}$$

Equation (36) is indeed positive, if

$$\left\|v^j\right\|^2_{L^2(\Omega)} + \left\|\nabla d^j\right\|^2_{L^2(\Omega)} \geq \left\|v^{j-1}\right\|^2_{L^2(\Omega)} + \left\|\nabla d^{j-1}\right\|^2_{L^2(\Omega)}$$

holds, which only depends on u^{j-1}, k, h. This is implied by choosing an appropriate norm since we have

$$\left\|v^j\right\|^2_{L^2(\Omega)} + \left\|\nabla d^j\right\|^2_{L^2(\Omega)} + \left\|\nabla d^{j-1}\right\|^2_{L^2(\Omega)} \geq \left\|v^j\right\|^2_{L^2(\Omega)} + \frac{2(c_l h)^2}{3}\left\|\Delta_h d^{j-1/2}\right\|^2_{L^2(\Omega)}.$$

Note that the second term stems from a simple calculation obtained by applying the inverse estimate:

$$\left\|\Delta_h d^{j-1/2}\right\|^2_{L^2(\Omega)} \leq c\left\|\Delta_h d^{j-1/2}\right\|^2_h = c(\nabla d^{j-1/2}, \nabla(-\Delta_h d^{j-1/2}))$$
$$\leq (c_l h)^{-1}\left\|\nabla d^{j-1/2}\right\|_{L^2(\Omega)}\left\|\Delta_h d^{j-1/2}\right\|_{L^2(\Omega)}. \qquad \square$$

Proposition 3.2 (Properties of the discrete system) *Let $u^j = (v^j, d_\circ^j) \in U_h$ be a solution of the discrete scheme (33a)–(33b) for all $1 \leq j \leq n$. Then the following energy equality holds,*

$$\frac{1}{2}\left\|v^n\right\|^2_{L^2(\Omega)} + \frac{1}{2}\left\|\nabla d^n\right\|^2_{L^2(\Omega)} + \frac{k^2}{2}\sum_{j=1}^n\left\|d_t v^j\right\|^2_{L^2(\Omega)}$$

$$+ k\sum_{j=1}^n(\mu_1 + \lambda^2)\left\|d^j \cdot (\nabla v^j)_{sym} d^j\right\|^2_{L^2(\Omega)} + k\sum_{j=1}^n\mu_4\left\|(\nabla v^j)_{sym}\right\|^2_{L^2(\Omega)}$$

$$+ k\sum_{j=1}^n(\mu_5 + \mu_6 - \lambda^2)\left\|(\nabla v^j)_{sym}d^j\right\|^2_{L^2(\Omega)} + k\sum_{j=1}^n\left\|\mathscr{I}_h(d^{j-1/2} \times \Delta_h d^{j-1/2})\right\|^2_h$$

$$= \frac{1}{2}\left\|v^0\right\|^2_{L^2(\Omega)} + \frac{1}{2}\left\|\nabla d^0\right\|^2_{L^2(\Omega)} \qquad (38)$$

for all $1 \leq n \leq J$. The algebraic restriction is fulfilled in every node

$$|d^j(z)| = 1 \text{ for all } z \in \mathcal{N}_h, \qquad (39)$$

where $\mathcal{N}_h$ is the set of all nodes of the mesh. Additionally, it holds for some constant $C > 0$ that

$$k\sum_{l=1}^j\left[\left\|d_t d^l\right\|^2_{L^{3/2}(\Omega)} + \left\|d_t v^l\right\|^2_{(H^2(\Omega)\cap H^1_{0,\sigma}(\Omega))^*} + \left\|\nabla v^l\right\|^2_{L^2(\Omega)}\right] \leq C\left(\mathscr{E}(v_0, d_0) + 1\right). \qquad (40)$$

Proof The discrete energy estimate (38) follows simply from iterating (36). In order to show (39), we adapt the approach in [24]. Therefore, the director equation (33b) is tested with $d^{j-1/2}(\hat{z})\phi_{\hat{z}}$, where $\hat{z} \in \mathcal{N}_h$ is a node of the mesh. All terms except for the one including the time-derivative of the director vanish due to the mass lumping and the skew-symmetry. Then, we are left with

$$0 = (d_t d^j, d^{j-1/2}(\hat{z})\phi_{\hat{z}})_h = \sum_{z\in\mathcal{N}_h}d_t d^{j-1/2}(z) \cdot d^{j-1/2}(\hat{z})\phi_{\hat{z}}\int_\Omega\phi_z dx$$

$$= \frac{1}{2k}(|d^j(\hat{z})|^2 - |d^{j-1}(\hat{z})|^2)\int_\Omega\phi_{\hat{z}}dx,$$

which yields the result for all interior nodes $\hat{z}$. At the boundary, the unit-norm constraint is fulfilled by the assumption on d_0, our inhomogeneous Dirichlet boundary condition. Korn's inequality yields the estimate for the last addend in (40).

Since $d_t d^j \in Y_h$, the definition of the L^2-projection yields for a smooth test function $\phi \in \mathscr{C}_c^\infty(\Omega)$ that

$$(d_t d^j, \phi) = (d_t d^j, \mathscr{P}_h(\phi)).$$

Using a duality argument, we are able to estimate the time derivative of the director in a L^p-norm by

$$
\begin{aligned}
\left\| d_t d^j \right\|_{L^{3/2}(\Omega)} &= \sup_{\phi \in L^3(\Omega)} \left| \frac{(d_t d^j, \mathscr{P}_h(\phi))}{\|\phi\|_{L^3(\Omega)}} \right| \\
&\leq \sup_{\phi \in L^3(\Omega)} \left| \frac{(d_t d^j, \mathscr{P}_h(\phi))_h}{\|\phi\|_{L^3(\Omega)}} \right| + \sup_{\phi \in L^3(\Omega)} \left| \frac{(d_t d^j, \mathscr{P}_h(\phi)) - (d_t d^j, \mathscr{P}_h(\phi))_h}{\|\phi\|_{L^3(\Omega)}} \right|. \quad (41)
\end{aligned}
$$

The first term can easily be estimated using our discrete director equation (33b) for $c \in Y_h$:

$$
\begin{aligned}
\left| (d_t d^j, c)_h \right| \leq{}& C \left\| d^{j-1/2} \right\|_{L^\infty(\Omega)}^2 \left\| v^j \right\|_{L^6(\Omega)} \left\| \mathscr{R}_h(\nabla d^{j-1}) \right\|_{L^2(\Omega)} \|c\|_{L^3(\Omega)} \\
&+ C \left\| d^{j-1/2} \times \Delta_h d^{j-1/2} \right\|_h \left\| d^{j-1/2} \right\|_{L^\infty(\Omega)} \|c\|_{L^2(\Omega)} \\
&+ C \left\| d^{j-1/2} \right\|_{L^\infty(\Omega)}^3 \left\| \nabla v^j \right\|_{L^2(\Omega)} \|c\|_{L^2(\Omega)} \\
\leq{}& C \left(\left\| \nabla v^j \right\|_{L^2(\Omega)} + \left\| \mathscr{I}_h \left(d^{j-1/2} \times \Delta_h d^{j-1/2} \right) \right\|_h \right) \|c\|_{L^3(\Omega)}.
\end{aligned}
\quad (42)
$$

Choosing $c = \mathscr{P}_h(\phi)$ for $\phi \in H^1(\Omega)$ and using the embedding $H^1(\Omega) \hookrightarrow L^6(\Omega)$, the stability of the projection, Lemma 2.9, and the *a priori* estimates of Proposition 3.2 allow us to obtain a bound for the right-hand side. The second term in (41) describes the error introduced by the mass-lumping. It must be estimated locally as in (25), *i.e.* by additionally applying the inverse estimate one obtains

$$
\begin{aligned}
\int_\Omega (I - \mathscr{I}_h)(d_t d^j \cdot \mathscr{P}_h(\phi)) \mathrm{d}x &\leq \sum_{K \in \mathscr{T}_h} \int_K (I - \mathscr{I}_h)(d_t d^j \cdot \mathscr{P}_h(\phi)) \mathrm{d}x \\
&\leq C \sum_{K \in \mathscr{T}_h} \left\| d_t d^j \right\|_{L^2(K)} \|\mathscr{P}_h(\phi)\|_{L^3(K)} \|1\|_{L^6(K)} \quad (43) \\
&\leq C h^{1/2} \sum_{K \in \mathscr{T}_h} \left\| d_t d^j \right\|_{L^2(K)} \|\mathscr{P}_h(\phi)\|_{L^3(K)}.
\end{aligned}
$$

For the time derivative of the director $d_t d^j$ in the L^2-norm, we observe a local version of (42) by choosing $c = \sum_{z \in \mathscr{N}_h \cap K} d_t d_j(z) \phi_z$, that is

$$
\begin{aligned}
\left\| d_t d^j \right\|_{L^2(K)}^2 &\leq C \int_K \mathscr{I}_h \left(|d_t d^j|^2 \right) \mathrm{d}x \\
&\leq C \Big(\left\| v^j \right\|_{L^6(K)} \left\| \mathscr{R}_h(\nabla d^{j-1}) \right\|_{L^2(K)} \left\| d_t d^j \right\|_{L^3(K)} \\
&\quad + \left(\int_K \mathscr{I}_h \left[d^{j-1/2} \times \Delta_h d^{j-1/2} \right]^2 \mathrm{d}x + \left\| \nabla v^j \right\|_{L^2(K)} \right) \left\| d_t d^j \right\|_{L^2(K)} \Big).
\end{aligned}
$$

With the inverse estimate, we can also bound the time derivative in the L^3-norm by

$$\left\| \boldsymbol{d}_t d^j \right\|_{L^3(K)} \leq C h^{-1/2} \left\| \boldsymbol{d}_t d^j \right\|_{L^2(K)}.$$

Putting the above together and reinserting it into (43) yields

$$\int_\Omega (I - \mathscr{I}_h)(\boldsymbol{d}_t d^j \cdot \mathscr{P}_h(\boldsymbol{\phi})) \mathrm{d}x$$

$$\leq C \left\| v^j \right\|_{L^6(\Omega)} \left\| \mathscr{R}_h(\nabla d^{j-1}) \right\|_{L^2(\Omega)} \left\| \mathscr{P}_h(\boldsymbol{\phi}) \right\|_{L^3(\Omega)}$$

$$+ C \left(\left\| \nabla v^j \right\|_{L^2(\Omega)} + \left\| d^{j-1/2} \times \Delta_h d^{j-1/2} \right\|_h \right) \left\| \mathscr{P}_h(\boldsymbol{\phi}) \right\|_{L^2(\Omega)}.$$

Multiplying by k and summing up leads to the estimate of $\boldsymbol{d}_t d^j$, due to the *a priori* estimates (38).

For the velocity, we proceed as in [7]: We test the time derivative of the velocity with a smooth solenoidal test function $\boldsymbol{\phi}$ and apply the projection $\mathscr{Q}_h$ such that $\langle \boldsymbol{d}_t v^j, \boldsymbol{\phi} \rangle = (\boldsymbol{d}_t v^j, \mathscr{Q}_h \boldsymbol{\phi})$ and equation (33a) yield

$$\left| \langle \boldsymbol{d}_t v^j, \boldsymbol{\phi} \rangle \right| = |((v^{j-1} \cdot \nabla)v^j, \mathscr{Q}_h(\boldsymbol{\phi})) + \frac{1}{2}([\nabla \cdot v^{j-1}]v^j, \mathscr{Q}_h(\boldsymbol{\phi}))$$

$$- ([\mathscr{R}_h \nabla d^{j-1}]^T [d^{j-1/2} \times (d^{j-1/2} \times \Delta_h d^{j-1/2})], \mathscr{Q}_h(\boldsymbol{\phi}))_h + (T_L^j, \nabla \mathscr{Q}_h(\boldsymbol{\phi}))|.$$

The convective terms can be estimated by a constant using (38) and

$$\left| ((v^{j-1} \cdot \nabla)v^j, \mathscr{Q}_h(\boldsymbol{\phi})) + \frac{1}{2}([\nabla \cdot v^{j-1}]v^j, \mathscr{Q}_h(\boldsymbol{\phi})) \right|$$

$$\leq (\left\| v^{j-1} \right\|_{L^2(\Omega)} \left\| \nabla v^j \right\|_{L^2(\Omega)} + \left\| v^j \right\|_{L^2(\Omega)} \left\| \nabla v^{j-1} \right\|_{L^2(\Omega)}) \left\| \mathscr{Q}_h(\boldsymbol{\phi}) \right\|_{L^\infty(\Omega)}.$$

For the Leslie stress tensor, we infer the estimate

$$\left| (T_L^j : \nabla \mathscr{Q}_h \boldsymbol{\phi}) \right| \leq \left| (T_D^j : \nabla \mathscr{Q}_h \boldsymbol{\phi}) \right| + |(d^{j-1/2}, (\nabla \mathscr{Q}_h \boldsymbol{\phi})_{skw} \Delta_h d^{j-1/2})_h|$$

$$+ \lambda |(d^{j-1/2} \times [(\nabla \mathscr{Q}_h \boldsymbol{\phi})_{sym} d^{j-1/2}], d^{j-1/2} \times \Delta_h d^{j-1/2})_h|$$

$$\leq C \Big[\left\| (\nabla v^j)_{sym} \right\|_{L^2(\Omega)} \left\| (\nabla \mathscr{Q}_h \boldsymbol{\phi})_{sym} \right\|_{L^2(\Omega)}$$

$$+ \left\| \mathscr{I}_h (d^{j-1/2} \times \Delta_h d^{j-1/2}) \right\|_{L^2(\Omega)} \left\| \nabla \mathscr{Q}_h \boldsymbol{\phi} \right\|_{L^2(\Omega)} \Big].$$

Note that we hereby reformulated the term including the skew-symmetric part of the velocity's gradient on the algebraic level, *i.e.*

$$(\Delta_h d^{j-1/2}, (\nabla \mathscr{Q}_h \boldsymbol{\phi})_{skw} d^{j-1/2})_h = (d^{j-1/2} \times \Delta_h d^{j-1/2}, d^{j-1/2} \times [(\nabla \mathscr{Q}_h \boldsymbol{\phi})_{skw}] d^{j-1/2})_h,$$

since $[d]_x^T [d]_x (A)_{skw} d = (I - d \otimes d)(A)_{skw} d = (A)_{skw} d$ holds. The Ericksen stress tensor can be estimated in a similar fashion

$$\left| ([\mathscr{R}_h \nabla d^{j-1}]^T [d^{j-1/2} \times (d^{j-1/2} \times \Delta_h d^{j-1/2})], \mathscr{Q}_h \boldsymbol{\phi})_h \right|$$

$$\leq C \left\| \mathscr{R}_h \nabla d^{j-1} \right\|_{L^2(\Omega)} \left\| \mathscr{I}_h (d^{j-1/2} \times \Delta_h d^{j-1/2}) \right\|_{L^2(\Omega)} \left\| \mathscr{Q}_h(\boldsymbol{\phi}) \right\|_{L^\infty(\Omega)}.$$

Summing over j, using the embedding $H^2(\Omega) \hookrightarrow L^\infty(\Omega)$ and the stability of the projection onto V_h due to (21) yields the assertion. $\square$

Proposition 3.3 *Let $u^j = (v^j, d_o^j) \in U_h$ be a solution to scheme (33a)–(33b). Then the discrete energy-variational inequality*

$$
\begin{aligned}
& d_t E^j + \frac{k}{2} \left\| d_t v^j \right\|_{L^2(\Omega)}^2 \\
& + \left(T_D^j; (\nabla v^j)_{sym} - (\nabla \mathcal{Q}_h \tilde{v})_{sym} \right) + \left\| d^{j-1/2} \times \Delta_h d^{j-1/2} \right\|_h^2 \\
& - (d_t v^j, \mathcal{Q}_h \tilde{v}) - \left((v^{j-1} \cdot \nabla) v^j, \mathcal{Q}_h \tilde{v} \right) - \frac{1}{2} \left((\nabla \cdot v^{j-1}) v^j, \mathcal{Q}_h \tilde{v} \right) \\
& - \left([\mathcal{R}_h \nabla d^{j-1}]^T [d^{j-1/2} \times (d^{j-1/2} \times \Delta_h d^{j-1/2})], \mathcal{Q}_h \tilde{v} \right)_h \\
& - \lambda (d^{j-1/2} \times [(\nabla \mathcal{Q}_h \tilde{v})_{sym} d^{j-1/2}], d^{j-1/2} \times \Delta_h d^{j-1/2})_h \\
& + ((\nabla \mathcal{Q}_h \tilde{v})_{skw} \Delta_h d^{j-1/2}, d^{j-1/2})_h \\
& + \mathcal{K}(\mathcal{Q}_h \tilde{v}) \left(\frac{1}{2} \|v^{j-1}\|_{L^2(\Omega)}^2 + \frac{1}{2} \|\nabla d^{j-1}\|_{L^2(\Omega)}^2 - E^{j-1} \right) = 0
\end{aligned}
\tag{44}
$$

with the energy E^j and the regularity weight $\mathcal{K}$ given by

$$
E^j := \frac{1}{2} \left\| v^j \right\|_{L^2(\Omega)}^2 + \frac{1}{2} \left\| \nabla d^j \right\|_{L^2(\Omega)}^2 \qquad \mathcal{K}(\tilde{v}) := \frac{1}{2} \|\tilde{v}\|_{L^\infty(\Omega)}^2
$$

holds for all $\tilde{v} \in H^1(0, T; (H^1_{0,\sigma}(\Omega))^*) \cap L^2(0, T; H^1_{0,\sigma}(\Omega)) \cap \mathscr{C}(\overline{\Omega} \times [0, T])$.

Proof Adding (33a) tested with $-\mathcal{Q}_h \tilde{v}^j$ to (38), we find the variational-energy inequality

$$
\begin{aligned}
& \frac{1}{2k} \|v^j\|_{L^2(\Omega)}^2 + \frac{1}{2k} \|\nabla d^j\|_{L^2(\Omega)}^2 + \frac{k}{2} \left\| d_t v^j \right\|_{L^2(\Omega)}^2 \\
& + \left(T_D^j; (\nabla v^j)_{\text{sym}} - (\nabla \mathcal{Q}_h \tilde{v})_{\text{sym}} \right) + \left\| d^{j-1/2} \times \Delta_h d^{j-1/2} \right\|_h^2 \\
& - (d_t v^j, \mathcal{Q}_h \tilde{v}) - \left((v^{j-1} \cdot \nabla) v^j, \mathcal{Q}_h \tilde{v} \right) - \frac{1}{2} \left((\nabla \cdot v^{j-1}) v^j, \mathcal{Q}_h \tilde{v} \right) \\
& - \left([\mathcal{R}_h \nabla d^{j-1}]^T [d^{j-1/2} \times (d^{j-1/2} \times \Delta_h d^{j-1/2})], \mathcal{Q}_h \tilde{v} \right)_h \\
& - \lambda (d^{j-1/2} \times [(\nabla \mathcal{Q}_h \tilde{v})_{sym} d^{j-1/2}], d^{j-1/2} \times \Delta_h d^{j-1/2})_h \\
& + ((\nabla \mathcal{Q}_h \tilde{v})_{skw} \Delta_h d^{j-1/2}, d^{j-1/2})_h = \frac{1}{2k} \left\| v^{j-1} \right\|_{L^2(\Omega)}^2 + \frac{1}{2k} \left\| \nabla d^{j-1} \right\|_{L^2(\Omega)}^2 .
\end{aligned}
$$

By defining the variable E^j and adding $\mathcal{K}(\mathcal{Q}_h \tilde{v})\left(\frac{1}{2}\|v^{j-1}\|_{L^2(\Omega)}^2 + \frac{1}{2}\|\nabla d^{j-1}\|_{L^2(\Omega)}^2 - E^{j-1}\right) = 0$ implies (44). $\square$

3.2 Converging Subsequences

Let $\{u^j\}_{j=0,\dots,J}$ be a sequence of measurable functions in space. We define their constant and linear interpolates in time as follows,

$$
\overline{u}_h^k(t) := u^j, \qquad\qquad \underline{\overline{u}}_h^k(t) := \frac{1}{2}(\overline{u}_h^k(t) + \underline{u}_h^k(t)),
$$

$$\underline{u}_h^k(t) := u^{j-1}, \qquad\qquad u_h^k(t) := \frac{u^j - u^{j-1}}{k}(t - jk) + u^j,$$

for $(j-1)k < t \le jk$. This yields the standard relation between the continuous and discrete time derivative, $\partial_t u_h^k(t) = \frac{u^j - u^{j-1}}{k} = d_t u^j$. Analogously we define the interpolates for a smooth test function $\tilde{u} \in C([0,T]; \mathbb{Y})$ for $(j-1)k < t \le jk$ by,

$$\overline{\tilde{u}}^k(t) := \tilde{u}(jk), \quad \underline{\tilde{u}}^k(t) := \tilde{u}((j-1)k), \quad \hat{\tilde{u}}^k(t) := \frac{\tilde{u}(jk) - \tilde{u}((j-1)k)}{k}(t - jk) + \tilde{u}(jk).$$

The *a priori* estimates (38) allow us to extract converging subsequences which we do not relabel and $(\boldsymbol{v}, \boldsymbol{d}, E)$ fulfilling (4) such that

$$\overline{v}_h^k, \underline{v}_h^k, v_h^k \overset{*}{\rightharpoonup} \boldsymbol{v} \text{ in } L^\infty(0,T; L_\sigma^2(\Omega)),$$

$$\overline{v}_h^k, \underline{v}_h^k, v_h^k \rightharpoonup \boldsymbol{v} \text{ in } L^2(0,T; H_0^1(\Omega)),$$

$$\partial_t v_k^h \rightharpoonup \partial_t \boldsymbol{v} \text{ in } L^2(0,T; (H^2(\Omega) \cap H_{0,\sigma}^1(\Omega))^*), \tag{45}$$

$$\overline{d}_h^k, \underline{d}_h^k, d_h^k \overset{*}{\rightharpoonup} \boldsymbol{d} \text{ in } L^\infty(0,T; L^\infty(\Omega)) \cap L^\infty(0,T; H^1(\Omega)),$$

$$\partial_t d_k^h \rightharpoonup \partial_t \boldsymbol{d} \text{ in } L^2(0,T; L^{3/2}(\Omega)),$$

$$\overline{d}_h^k \cdot (\nabla \overline{v}_h^k)_{sym} \overline{d}_h^k \rightharpoonup \boldsymbol{d} \cdot (\nabla \boldsymbol{v})_{sym} \boldsymbol{d} \text{ in } L^2(0,T; L^2(\Omega)),$$

$$(\nabla \overline{v}_h^k)_{sym} \overline{d}_h^k \rightharpoonup (\nabla \boldsymbol{v})_{sym} \boldsymbol{d} \text{ in } L^2(0,T; L^2(\Omega)),$$

$$\mathscr{I}_h(\overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_k^h) \rightharpoonup \boldsymbol{d} \times \Delta \boldsymbol{d} \text{ in } L^2(0,T; L^2(\Omega)), \tag{46}$$

$$\underline{E}_h^k(t) \rightarrow E(t) \text{ for all } t \in [0,T],$$

where the last convergence follows from Helly's selection theorem (*cf.* [28, Ex. 8.3]). We can refine the convergence for the director by using the following compact embeddings, referred to as Aubin–Lions–Simon Lemma [43],

$$\{\boldsymbol{d} \in L^2(0,T; H^1(\Omega)) : \partial_t \boldsymbol{d} \in L^2(0,T; L^{3/2}(\Omega))\} \overset{c}{\hookrightarrow} L^2(0,T; L^2(\Omega)),$$

$$\{\boldsymbol{d} \in L^\infty(0,T; H^1(\Omega)) : \partial_t \boldsymbol{d} \in L^2(0,T; L^{3/2}(\Omega))\} \overset{c}{\hookrightarrow} C^0(0,T; L^2(\Omega)), \tag{47}$$

which yields strong convergence for the director

$$d_k^h \rightarrow \boldsymbol{d} \text{ in } L^2(0,T; L^2(\Omega)).$$

A standard interpolation inequality (*cf.* [44, p. 192 ff.]) and the uniform bound in $L^\infty(0,T; L^\infty(\Omega))$ yields strong convergence,

$$d_k^h \rightarrow \boldsymbol{d} \text{ in } L^p(0,T; L^p(\Omega)) \text{ for all } p \in [1, \infty). \tag{48}$$

For the term $\boldsymbol{d} \times \Delta \boldsymbol{d}$, note that due to the above convergences and (24), we have

$$\int_0^T (\mathscr{I}_h(\overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_k^h), \phi) \mathrm{d}t$$

$$= \int_0^T (\mathscr{I}_h(\overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_k^h), \phi) - (\overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_k^h, \phi)_h \mathrm{d}t + \int_0^T (\overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_k^h, \phi)_h \mathrm{d}t$$

$$\leq Ch \left\| \mathscr{I}_h(\overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_k^h) \right\|_{L^2(0,T;L^2(\Omega))} \|\nabla \phi\|_{L^2(0,T;H^1(\Omega))} - \int_0^T (\nabla \overline{\underline{d}}_k^h, \nabla \phi \times \overline{\underline{d}}_h^k) \mathrm{d}t$$

for $\phi \in C_c^\infty([0, T] \times \Omega; \mathbb{R}^3)$. Now note that the first term vanishes as $h \to 0$ and the last term converges to

$$-\int_0^T (\nabla \boldsymbol{d}, \nabla \phi \times \boldsymbol{d}) \mathrm{d}t = -\int_0^T (\boldsymbol{d} \times \nabla \boldsymbol{d}, \nabla \phi) \mathrm{d}t = \int_0^T (\boldsymbol{d} \times \Delta \boldsymbol{d}, \phi) \mathrm{d}t$$

where the last equality, $\nabla \cdot (\boldsymbol{d} \times \nabla \boldsymbol{d}) = \boldsymbol{d} \times \Delta \boldsymbol{d}$, has to be understood in the distributional sense. The fact that all interpolates in (45) converge against the same limit can be confirmed as in [45]. Consider exemplary for the velocity,

$$\left\| v_h^k - \underline{v}_h^k \right\|_{L^2(0,T;L^2(\Omega))}^2 \leq \sum_{j=1}^J \left\| v^j - v^{j-1} \right\|_{L^2(\Omega)}^2 \int_{j(k-1)}^{jk} \left(\frac{t - jk}{k} \right)^2 \mathrm{d}t$$

$$\leq k \sum_{j=1}^J \frac{k^2}{3} \left\| \boldsymbol{d}_t v^j \right\|_{L^2(\Omega)}^2,$$

which vanishes for $k \to 0$, since the term on the right-hand side is bounded by our energy estimate (38). In order to deduce that the velocity is solenoidal, we use standard arguments (e.g. as in [46]). We test the divergence of the velocity with a test function $\boldsymbol{\phi} \in C_c^\infty(\Omega \times (0, T])$ with $\int_\Omega \boldsymbol{\phi} \mathrm{d}x = 0$ and use our discrete divergence-zero condition to obtain

$$\int_0^T (\nabla \cdot \boldsymbol{v}(s), \boldsymbol{\phi}) \mathrm{d}s = \int_0^T (\nabla \cdot (\boldsymbol{v}(s) - v_k^h(s)), \boldsymbol{\phi}) + (\nabla \cdot v_k^h(s), \boldsymbol{\phi} - \Pi_h \boldsymbol{\phi}) \mathrm{d}s,$$

where Π_h is the L^2-projection onto M_h. The first term vanishes due to the weak convergence of the velocity in (45). The second summand vanishes for $h \to 0$ simply due to the uniform boundedness v_k^h and a standard approximation property of the space M_h (see e.g. [31, Lemma 12.4.3]), by

$$\int_0^T (\nabla \cdot v_k^h, \boldsymbol{\phi} - \Pi_h(\boldsymbol{\phi})) \mathrm{d}s \leq \left\| v_k^h \right\|_{L^2(0,T;H_0^1(\Omega))} \|\boldsymbol{\phi} - \Pi_h \boldsymbol{\phi}\|_{L^2(0,T;L^2(\Omega))}$$

$$\leq Ch^2 \left\| \nabla^2 \boldsymbol{\phi} \right\|_{L^2(0,T;L^2(\Omega))}.$$

The convergence for our non-homogeneous Dirichlet boundary conditions of the director follows from the trace theorem (*cf.* [47, Thm. 6.3.10]) and the interpolation error estimate

(2.10),

$$\begin{aligned}
\left\|\mathrm{tr}(\boldsymbol{d}_0) - \mathrm{tr}(d_k^h(t))\right\|_{L^2(\partial\Omega)} &= \left\|\mathrm{tr}(\boldsymbol{d}_0) - \mathrm{tr}(\mathscr{I}_h\boldsymbol{d}_0) - \mathrm{tr}(d_{k,\circ}^h(t))\right\|_{L^2(\partial\Omega)} \\
&= \left\|\mathrm{tr}((I - \mathscr{I}_h)\boldsymbol{d}_0)\right\|_{L^2(\partial\Omega)} \\
&\leq C \left\|(I - \mathscr{I}_h)\boldsymbol{d}_0\right\|_{H^1(\Omega)} \leq Ch \left\|\boldsymbol{d}_0\right\|_{H^2(\Omega)},
\end{aligned} \tag{49}$$

for every $t \in [0, T]$. Analogously, we observe for the initial condition of the director

$$\left\|d_k^h(0) - \boldsymbol{d}_0\right\|_{H^1(\Omega)} = \left\|\mathscr{I}_h(\boldsymbol{d}_0) - \boldsymbol{d}_0\right\|_{H^1(\Omega)} \leq Ch \left\|\boldsymbol{d}_0\right\|_{H^2(\Omega)}. \tag{50}$$

For the initial condition of the velocity, we can derive an analogous estimate – however in the L^2 norm instead – by making use of (21), since we approximated the initial condition with the respective projection operator, $v^0 = \mathscr{Q}_h(\boldsymbol{v}_0)$.

3.3 Unit-Norm Restriction and Convergence for the Director Equations

From (39), we can infer that the unit-norm restriction $|d| = 1$ holds at every node $z \in \mathscr{N}_h$. In the limit as $h \to 0$, this restriction will be fulfilled almost everywhere on Ω, since $\mathscr{I}_h(|d^j|^2 - 1) = 0$ holds. By subsequently applying the interpolation error bound (*cf.* Lemma 2.10) and the inverse estimate (*cf.* Lemma 2.8), one obtains

$$\begin{aligned}
\left\||d^j|^2 - 1\right\|_{L^2(\Omega)} &= \left\|(I - \mathscr{I}_h)(|d^j|^2 - 1)\right\|_{L^2(\Omega)} \\
&= \sqrt{\sum_{K \in \mathscr{T}_h} \left\|(I - \mathscr{I}_h)(|d^j|^2 - 1)\right\|_{L^2(K)}^2} \\
&\leq Ch^2 \sqrt{\sum_{K \in \mathscr{T}_h} \left\|\nabla^2 |d^j|^2\right\|_{L^2(K)}^2} \\
&\leq Ch \left\|\nabla |d^j|^2\right\|_{L^2(\Omega)} \\
&\leq Ch \left\|\nabla d^j\right\|_{L^2(\Omega)} \left\|d^j\right\|_{L^\infty(\Omega)},
\end{aligned}$$

where the right-hand side is bounded uniformly due to our *a priori* energy estimate (38). This gives us the result of Proposition 3.4.

Proposition 3.4 *Let d_h^k be the approximate solution in the sense of the discrete scheme* (33a)–(33b) *that converges to a limit as in* (45). *Then the norm of d_h^k converges to 1 in a linear order, i.e.*

$$\left\||d_h^k(t)|^2 - 1\right\|_{L^2(\Omega)} \in \mathscr{O}(h).$$

In order to prove the convergence of the approximate solution to (33b) to a solution of (6), we consider equation (33b) tested with the projection $\mathscr{P}_h\boldsymbol{c}$ of a smooth test function $\boldsymbol{c} \in C_c^\infty(\Omega \times (0, T))$ and observe, for instance by Lemma 2.11 that

$$\begin{aligned}
\int_0^T (\boldsymbol{d}_t d_h^k, \mathscr{P}_h\boldsymbol{c})_h - (\boldsymbol{d}_t d_h^k, \mathscr{P}_h\boldsymbol{c})\mathrm{d}t &\leq Ch \left\|\boldsymbol{d}_t d_h^k\right\|_{L^2(0,T;L^2(\Omega))} \left\|\mathscr{P}_h\boldsymbol{c}\right\|_{L^2(0,T;H^1(\Omega))} \\
&\leq Ch^{1/2} \left\|\boldsymbol{d}_t d_h^k\right\|_{L^2(0,T;L^{3/2}(\Omega))} \left\|\mathscr{P}_h\boldsymbol{c}\right\|_{L^2(0,T;H^1(\Omega))}.
\end{aligned}$$

This term vanishes as $h \to 0$ since the last factor is bounded for smooth $\boldsymbol{c}$ due to 2.9. For the convection term, we infer due to the definition 30 that

$$\left(\overline{\underline{d}}_h^k \times [\mathscr{R}_h \nabla \underline{d}_h^k \overline{v}_h^k], \overline{\underline{d}}_h^k \times \mathscr{P}_h \boldsymbol{c}\right)_h$$

$$= -\left(\mathscr{R}_h \nabla \underline{d}_h^k, \mathscr{I}_h \left[\overline{\underline{d}}_h^k \times \left(\overline{\underline{d}}_h^k \times \mathscr{P}_h \boldsymbol{c}\right) \otimes \overline{v}_h^k\right]\right)_h$$

$$= -\left(\nabla \underline{d}_h^k, \left[\overline{\underline{d}}_h^k \times \left(\overline{\underline{d}}_h^k \times \mathscr{P}_h \boldsymbol{c}\right) \otimes \overline{v}_h^k\right]\right) - \left(\nabla \underline{d}_h^k, (\mathscr{I}_h - I) \left[\overline{\underline{d}}_h^k \times \left(\overline{\underline{d}}_h^k \times \mathscr{P}_h \boldsymbol{c}\right) \otimes \overline{v}_h^k\right]\right).$$

For the last term, we infer

$$\left|\left(\nabla \underline{d}_h^k, (\mathscr{I}_h - I) \left[\overline{\underline{d}}_h^k \times \left(\overline{\underline{d}}_h^k \times \mathscr{P}_h \boldsymbol{c}\right) \otimes \overline{v}_h^k\right]\right)\right|$$

$$\leq \left\|\nabla \underline{d}_h^k\right\|_{L^2(\Omega)} \left\|(\mathscr{I}_h - I) \left[\overline{\underline{d}}_h^k \times \left(\overline{\underline{d}}_h^k \times \mathscr{P}_h \boldsymbol{c}\right) \otimes \overline{v}_h^k\right]\right\|_{L^2(\Omega)}$$

such that we find

$$\left\|(\mathscr{I}_h - I) \left[\overline{\underline{d}}_h^k \times \left(\overline{\underline{d}}_h^k \times \mathscr{P}_h \boldsymbol{c}\right) \otimes \overline{v}_h^k\right]\right\|_{L^2(\Omega)}^2$$

$$\leq Ch^4 \sum_{K \in \mathscr{T}_h} \left\|\nabla^2 \left[\overline{\underline{d}}_h^k \times \left(\overline{\underline{d}}_h^k \times \mathscr{P}_h \boldsymbol{c}\right) \otimes \overline{v}_h^k\right]\right\|_{L^2(K)}^2$$

$$\leq Ch^4 \sum_{K \in \mathscr{T}_h} \left(\left\|\nabla \overline{\underline{d}}_h^k \times \left(\nabla \overline{\underline{d}}_h^k \times \mathscr{P}_h \boldsymbol{c}\right) \otimes \overline{v}_h^k + \nabla \overline{\underline{d}}_h^k \times \left(\overline{\underline{d}}_h^k \times \nabla \mathscr{P}_h \boldsymbol{c}\right) \otimes \overline{v}_h^k\right\|_{L^2(K)}\right)^2$$

$$+ Ch^4 \sum_{K \in \mathscr{T}_h} \left(\left\|\nabla \overline{\underline{d}}_h^k \times \left(\overline{\underline{d}}_h^k \times \mathscr{P}_h \boldsymbol{c}\right) \otimes \nabla \overline{v}_h^k + \overline{\underline{d}}_h^k \times \left(\nabla \overline{\underline{d}}_h^k \times \nabla \mathscr{P}_h \boldsymbol{c}\right) \otimes \overline{v}_h^k\right\|_{L^2(K)}\right)^2$$

$$+ Ch^4 \sum_{K \in \mathscr{T}_h} \left(\left\|\overline{\underline{d}}_h^k \times \left(\nabla \overline{\underline{d}}_h^k \times \mathscr{P}_h \boldsymbol{c}\right) \otimes \nabla \overline{v}_h^k + \overline{\underline{d}}_h^k \times \left(\overline{\underline{d}}_h^k \times \nabla \mathscr{P}_h \boldsymbol{c}\right) \otimes \nabla \overline{v}_h^k\right\|_{L^2(K)}\right)^2$$

$$+ Ch^4 \sum_{K \in \mathscr{T}_h} \left\|\overline{\underline{d}}_h^k \times \left(\overline{\underline{d}}_h^k \times \mathscr{P}_h \boldsymbol{c}\right) \otimes \nabla^2 \overline{v}_h^k\right\|_{L^2(K)}^2$$

$$\leq C \left[h \left\|\nabla \overline{\underline{d}}_h^k\right\|_{L^2(\Omega)}^2 \left\|\overline{v}_h^k\right\|_{L^6(\Omega)}^2 + h^2 \left\|\overline{\underline{d}}_h^k\right\|_{L^\infty(\Omega)}^2 \left\|\nabla \overline{v}_h^k\right\|_{L^2(\Omega)}^2\right] \left\|\overline{\underline{d}}_h^k\right\|_{L^\infty(\Omega)}^2 \left\|\mathscr{P}_h \boldsymbol{c}\right\|_{L^\infty(\Omega)}^2.$$

The first inequality is due to Lemma 2.10, in the second inequality, we calculate the derivative, where we used that the second derivative of $P1$ finite elements vanishes on every tetrahedron. In order to infer the last inequality, we use Hölder's inequality and inverse estimates.

In order to pass from the mass-lumped inner product to the standard $L^2(\Omega)$ inner product, other occurring terms have to be estimated in the same fashion, but locally. Regarding the second term, we observe for example

$$\int_\Omega (I - \mathscr{I}_h)(\overline{\underline{d}}_h^k \times [(\nabla \overline{v}_h^k)_{\mathrm{sym}} \overline{\underline{d}}_h^k] \cdot \overline{\underline{d}}_h^k \times \mathscr{P}_h \boldsymbol{c}) \mathrm{d}x$$

$$\leq Ch^2 \sum_{K \in \mathscr{T}_h} \left\|\nabla^2 (\overline{\underline{d}}_h^k \times [(\nabla \overline{v}_h^k)_{\mathrm{sym}} \overline{\underline{d}}_h^k] \cdot \overline{\underline{d}}_h^k \times \mathscr{P}_h \boldsymbol{c})\right\|_{L^2(K)} \|1\|_{L^2(K)}$$

$$\leq Ch^{2+3/2} \sum_{K \in \mathscr{T}_h} \sum_{i,j=1}^{3} \left\| \partial_{x_i} \overline{\underline{d}}_h^k \times [\partial_{x_j} (\nabla \overline{v}_h^k)_{\mathrm{sym}} \overline{\underline{d}}_h^k] \cdot (\overline{\underline{d}}_h^k \times \mathscr{P}_h c) \right\|_{L^2(K)}$$

$$+ Ch^{2+3/2} \sum_{K \in \mathscr{T}_h} \sum_{i,j=1}^{3} \left\| \partial_{x_i} \overline{\underline{d}}_h^k \times [(\nabla \overline{v}_h^k)_{\mathrm{sym}} \partial_{x_j} \overline{\underline{d}}_h^k] \cdot (\overline{\underline{d}}_h^k \times \mathscr{P}_h c) \right\|_{L^2(K)}$$

$$+ Ch^{2+3/2} \sum_{K \in \mathscr{T}_h} \sum_{i,j=1}^{3} \left\| \partial_{x_i} \overline{\underline{d}}_h^k \times [(\nabla \overline{v}_h^k)_{\mathrm{sym}} \overline{\underline{d}}_h^k] \cdot \partial_{x_j} (\overline{\underline{d}}_h^k \times \mathscr{P}_h c) \right\|_{L^2(K)}$$

$$+ Ch^{2+3/2} \sum_{K \in \mathscr{T}_h} \sum_{i,j=1}^{3} \left\| \overline{\underline{d}}_h^k \times [\partial_{x_i} (\nabla \overline{v}_h^k)_{\mathrm{sym}} \partial_{x_j} \overline{\underline{d}}_h^k] \cdot (\overline{\underline{d}}_h^k \times \mathscr{P}_h c) \right\|_{L^2(K)}$$

$$+ Ch^{2+3/2} \sum_{K \in \mathscr{T}_h} \sum_{i,j=1}^{3} \left\| \overline{\underline{d}}_h^k \times [\partial_{x_i} (\nabla \overline{v}_h^k)_{\mathrm{sym}} \overline{\underline{d}}_h^k] \cdot \partial_{x_j} (\overline{\underline{d}}_h^k \times \mathscr{P}_h c) \right\|_{L^2(K)}$$

$$+ Ch^{2+3/2} \sum_{K \in \mathscr{T}_h} \sum_{i,j=1}^{3} \left\| \overline{\underline{d}}_h^k \times [(\nabla \overline{v}_h^k)_{\mathrm{sym}} \partial_{x_i} \overline{\underline{d}}_h^k] \cdot \partial_{x_j} (\overline{\underline{d}}_h^k \times \mathscr{P}_h c) \right\|_{L^2(K)}$$

$$+ Ch^{2+3/2} \sum_{K \in \mathscr{T}_h} \sum_{i,j=1}^{3} \left\| \overline{\underline{d}}_h^k \times [(\nabla \overline{v}_h^k)_{\mathrm{sym}} \overline{\underline{d}}_h^k] \cdot \partial_{x_i x_j}^2 (\overline{\underline{d}}_h^k \times \mathscr{P}_h c) \right\|_{L^2(K)},$$

where we used that the second derivatives of the Lagrangian finite element functions vanish on the set K. Using Hölder's inequality and inverse estimates for all appearing terms, we infer

$$\int_\Omega (I - \mathscr{I}_h)(\overline{\underline{d}}_h^k \times [(\nabla \overline{v}_h^k)_{\mathrm{sym}} \overline{\underline{d}}_h^k] \cdot \overline{\underline{d}}_h^k \times \mathscr{P}_h c) \mathrm{d}x$$

$$\leq Ch \left\| (\nabla \overline{v}_h^k)_{\mathrm{sym}} \right\|_{L^2(\Omega)} \left\| \overline{\underline{d}}_h^k \right\|_{L^\infty(\Omega)}^2 \left\| \nabla \overline{\underline{d}}_h^k \right\|_{L^2(\Omega)} \| \mathscr{P}_h c \|_{L^\infty(\Omega)}$$

$$+ Ch \left\| (\nabla \overline{v}_h^k)_{\mathrm{sym}} \right\|_{L^2(\Omega)} \left\| \overline{\underline{d}}_h^k \right\|_{L^\infty(\Omega)}^3 \| \nabla \mathscr{P}_h c \|_{L^2(\Omega)}.$$

The right-hand side is bounded due to the H^1-stability of the L^2 projection (*cf.* Lemma 2.9). The estimates for the difference of the mass-lumped and $L^2(\Omega)$ inner product for the other terms follow analogously. Thus, it remains to pass to the limit in (33b) with $L^2(\Omega)$ inner products instead of the lumped-inner products. Note that by standard approximation arguments $\mathscr{P}_h c \to c$ in $L^3(\Omega \times (0, T))$ for $c \in \mathscr{C}_c^\infty(\Omega \times (0, T))$, *cf.* Lemma 2.9, the weak convergences of (45) and (46) allow us to pass to the limit in all occurring terms, and we infer

$$\int_0^T \int_\Omega \partial_t d \cdot c - (\nabla v)_{\mathrm{skw}} d \cdot c + (d \times (\nabla d v + \lambda (\nabla v)_{\mathrm{sym}} d - \Delta d)) \cdot (d \times c) \mathrm{d}x \mathrm{d}t = 0$$

for all $c \in L^2(0, T; L^3(\Omega))$ by density arguments. The regularity of d suffices to infer $2d \cdot (\nabla d v) = (v \cdot \nabla)|d|^2$ such that $(d \times \nabla d v) \cdot (d \times c) = (v \cdot \nabla) d \cdot c$. Since the relation holds for all $c \in L^2(0, T; L^3(\Omega))$ it also holds a.e. in $\Omega \times (0, T)$, which is nothing else than (6).

3.4 Convergence to the Energy-Variational Formulation

Multiplying the discrete energy-variational formulation (44) by ϕ^j for a $\phi \in C_c^\infty(0,T)$ applying an discrete integration as well as a discrete integration-by-parts, we find

$$
\begin{aligned}
&-\int_0^T (\partial_t \hat{\phi}^k)\underline{E}^k \mathrm{d}t + \int_0^T \overline{\phi}^k \frac{1}{2} \left\| \partial_t \hat{v}_h^k \right\|_{L^2(\Omega)}^2 \mathrm{d}t \\
&+ \int_0^T \overline{\phi}^k \left[\left(\overline{T_{Dh}}^k ; (\nabla \overline{v}_h^k)_{\mathrm{sym}} - (\nabla \mathscr{Q}_h \overline{\tilde{v}}^k)_{\mathrm{sym}} \right) + \left\| \overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_h^k \right\|_h^2 \right] \mathrm{d}t \\
&+ \int_0^T \left[\left(\underline{v}_h^k, \partial_t \mathscr{Q}_h \overline{\tilde{v}}^k \overline{\phi}^k + \mathscr{Q}_h \tilde{\underline{v}} \partial_t \overline{\phi}^k \right) - \overline{\phi}^k \left((\underline{v}_h^k \cdot \nabla) \overline{v}_h^k, \mathscr{Q}_h \overline{\tilde{v}}^k \right) \right] \mathrm{d}t \\
&- \int_0^T \overline{\phi}^k \left[\frac{1}{2} \left((\nabla \cdot \underline{v}_h^k) \overline{v}_h^k, \mathscr{Q}_h \overline{\tilde{v}}^k \right) + \left([\mathscr{R}_h \nabla \underline{d}^k]^T [\overline{\underline{d}}_h^k \times (\overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_h^k)], \mathscr{Q}_h \overline{\tilde{v}}^k \right)_h \right] \mathrm{d}t \\
&- \int_0^T \overline{\phi}^k \left[\lambda (\overline{\underline{d}}_h^k \times [(\nabla \mathscr{Q}_h \overline{\tilde{v}}^k)_{sym} \overline{\underline{d}}_h^k], \overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_h^k)_h - ((\nabla \mathscr{Q}_h \overline{\tilde{v}}^k)_{skw} \Delta_h \overline{\underline{d}}_h^k, \overline{\underline{d}}_h^k)_h \right] \mathrm{d}t \\
&+ \int_0^T \overline{\phi}^k \mathscr{K}(\mathscr{Q}_h \overline{\tilde{v}}^k) \left(\frac{1}{2} \| \underline{v}_h^k \|_{L^2(\Omega)}^2 + \frac{1}{2} \| \nabla \underline{d}_h^k \|_h^2 - \underline{E}^k \right) \mathrm{d}t \le 0 .
\end{aligned}
\tag{51}
$$

Since $\phi \ge 0$ for all $t \in [0,T]$, the second term can be estimated from below by zero. We observe that the terms $\left(\overline{T_{Dh}}^k ; (\nabla \overline{v}_h^k)_{\mathrm{sym}} \right)$ are non-negative and quadratic in $\nabla \overline{v}_h^k$ such that they are convex and weakly-lower continuous. Furthermore, we observe that

$$
-\left([\mathscr{R}_h \nabla \underline{d}_h^k]^T [\overline{\underline{d}}_h^k \times (\overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_h^k)], \mathscr{Q}_h \overline{\tilde{v}}^k \right)_h = \left(\overline{\underline{d}}_h^k \times [\mathscr{R}_h \nabla \underline{d}_h^k] \mathscr{Q}_h \overline{\tilde{v}}^k, \overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_h^k \right)_h ,
$$

and from inequality (31) that $\left\| \nabla \underline{d}_h^k \right\|_{L^2(\Omega)}^2 \ge \left\| \mathscr{R}_h \nabla \underline{d}_h^k \right\|_h^2$ such that we may find

$$
\begin{aligned}
&\left(\overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_h^k, \overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_h^k \right)_h + \mathscr{K}(\mathscr{Q}_h \overline{\tilde{v}}^k) \frac{1}{2} \| \nabla \underline{d}_h^k \|_{L^2(\Omega)}^2 \\
&\quad - \left([\mathscr{R}_h \nabla \underline{d}_h^k]^T [\overline{\underline{d}}_h^k \times (\overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_h^k)], \mathscr{Q}_h \overline{\tilde{v}}^k \right)_h \\
&= \left\| (\overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_h^k) + \frac{1}{2} \overline{\underline{d}}_h^k \times [\mathscr{R}_h \nabla \underline{d}_h^k] \mathscr{Q}_h \overline{\tilde{v}}^k \right\|_h^2 \\
&\quad + \frac{1}{4} \| \mathscr{Q}_h \overline{\tilde{v}}^k \|_{L^\infty(\Omega)}^2 \| \mathscr{R}_h \nabla \underline{d}_h^k \|_h^2 - \frac{1}{4} \| \overline{\underline{d}}_h^k \times [\mathscr{R}_h \nabla \underline{d}_h^k] \mathscr{Q}_h \overline{\tilde{v}}^k \|_h^2 \\
&= \left\| \mathscr{I}_h (\overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_h^k) + \frac{1}{2} \mathscr{I}_h (\overline{\underline{d}}_h^k \times [\mathscr{R}_h \nabla \underline{d}_h^k] \mathscr{Q}_h \overline{\tilde{v}}^k) \right\|_{L^2(\Omega)}^2 \\
&\quad + \frac{1}{4} \int_\Omega \mathscr{I}_h \left[\left(\| \mathscr{Q}_h \overline{\tilde{v}}^k \|_{L^\infty(\Omega)}^2 I - \mathscr{Q}_h \overline{\tilde{v}}^k \otimes \mathscr{Q}_h \overline{\tilde{v}}^k \right) [\mathscr{R}_h \nabla \underline{d}_h^k]^T [\mathscr{R}_h \nabla \underline{d}_h^k] \right] \mathrm{d}x \\
&\quad + \frac{1}{4} \int_\Omega \mathscr{I}_h \left[\left(\overline{\underline{d}}_h^k \cdot [\mathscr{R}_h \nabla \underline{d}_h^k] \mathscr{Q}_h \overline{\tilde{v}}^k \right)^2 \right] \mathrm{d}x .
\end{aligned}
$$

By writing $\|\boldsymbol{a}\|^2_{L^\infty(\Omega)} I - \boldsymbol{a} \otimes \boldsymbol{a} = \left(\sqrt{\|\boldsymbol{a}\|^2_{L^\infty(\Omega)} - |\boldsymbol{a}|} \right)^2 I + \left(|\boldsymbol{a}| I - \frac{\boldsymbol{a} \otimes \boldsymbol{a}}{|\boldsymbol{a}|} \right)^2$ for $\boldsymbol{a} \in L^\infty(\Omega)$, we may use (23) to infer

$$\int_\Omega \mathscr{I}_h \left[\left(\|\mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k\|^2_{L^\infty(\Omega)} I - \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k \otimes \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k \right) [\mathscr{R}_h \nabla \underline{d}_h^k]^T [\mathscr{R}_h \nabla \underline{d}_h^k] \right] \mathrm{d}x$$

$$+ \int_\Omega \mathscr{I}_h \left[\left(\overline{\underline{d}}_h^k \cdot [\mathscr{R}_h \nabla \underline{d}_h^k] \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k \right)^2 \right] \mathrm{d}x$$

$$\geq \left\| \sqrt{\|\mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k\|^2_{L^\infty(\Omega)} - |\mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k|} [\mathscr{R}_h \nabla \underline{d}_h^k] \right\|^2_h$$

$$+ \left\| \left(|\mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k| I - \frac{\mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k \otimes \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k}{|\mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k|} \right) [\mathscr{R}_h \nabla \underline{d}_h^k] \right\|^2_h + \left\| \overline{\underline{d}}_h^k \cdot [\mathscr{R}_h \nabla \underline{d}_h^k] \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k \right\|^2_h$$

$$\geq \left\| \mathscr{I}_h \left[\sqrt{\|\mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k\|^2_{L^\infty(\Omega)} - |\mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k|^2} [\mathscr{R}_h \nabla \underline{d}_h^k] \right] \right\|^2_{L^2(\Omega)}$$

$$+ \left\| \mathscr{I}_h \left[\left(|\mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k| I - \frac{\mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k \otimes \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k}{|\mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k|} \right) [\mathscr{R}_h \nabla \underline{d}_h^k] \right] \right\|^2_{L^2(\Omega)}$$

$$+ \left\| \mathscr{I}_h \left[\overline{\underline{d}}_h^k \cdot [\mathscr{R}_h \nabla \underline{d}_h^k] \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k \right] \right\|^2_{L^2(\Omega)}.$$

From (46), we already know that $\mathscr{I}_h(\overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_h^k) \rightharpoonup \boldsymbol{d} \times \Delta \boldsymbol{d}$ in $L^2(\Omega \times (0, T))$. Additionally, we observe that

$$\mathscr{I}_h(\overline{\underline{d}}_h^k \times [\mathscr{R}_h \nabla \underline{d}_h^k] \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k) \rightharpoonup \boldsymbol{d} \times \nabla \boldsymbol{d} \cdot \overline{\tilde{\boldsymbol{v}}}^k \quad \text{in } L^2(\Omega \times (0, T))$$

for all $\overline{\tilde{\boldsymbol{v}}}^k \in \mathscr{C}([0, T]; H^2(\Omega) \cap H^1_{0,\sigma}(\Omega))$ by observing that for all $\boldsymbol{\varphi} \in \mathscr{C}^\infty_c(\Omega)$ and a.e. $t \in (0, T)$, it holds

$$\left(\mathscr{I}_h(\overline{\underline{d}}_h^k \times [\mathscr{R}_h \nabla \underline{d}_h^k] \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k), \boldsymbol{\varphi} \right)$$

$$= \left(\overline{\underline{d}}_h^k \times [\mathscr{R}_h \nabla \underline{d}_h^k] \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k, \widetilde{\mathscr{I}}_h(\boldsymbol{\varphi}) \right)_h$$

$$= \left([\mathscr{R}_h \nabla \underline{d}_h^k]; \mathscr{I}_h \left[[\overline{\underline{d}}_h^k]^T_\times \widetilde{\mathscr{I}}_h(\boldsymbol{\varphi}) \otimes \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k \right] \right)_h$$

$$= \left(\nabla \underline{d}_h^k; \mathscr{I}_h \left[[\overline{\underline{d}}_h^k]^T_\times \widetilde{\mathscr{I}}_h(\boldsymbol{\varphi}) \otimes \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k \right] \right)$$

$$= \left(\nabla \underline{d}_h^k; [\overline{\underline{d}}_h^k]^T_\times \widetilde{\mathscr{I}}_h(\boldsymbol{\varphi}) \otimes \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k \right) + \left(\nabla \underline{d}_h^k; (\mathscr{I}_h - I) \left[[\overline{\underline{d}}_h^k]^T_\times \widetilde{\mathscr{I}}_h(\boldsymbol{\varphi}) \otimes \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k \right] \right)$$

$$\leq \left(\nabla \underline{d}_h^k; [\overline{\underline{d}}_h^k]^T_\times \widetilde{\mathscr{I}}_h(\boldsymbol{\varphi}) \otimes \overline{\tilde{\boldsymbol{v}}}^k \right)$$

$$+ \|\nabla \underline{d}_h^k\|_{L^2(\Omega)} \left\| \overline{\underline{d}}_h^k \right\|_{L^\infty(\Omega)} \left\| \widetilde{\mathscr{I}}_h(\boldsymbol{\varphi}) \right\|_{L^2(\Omega)} \left\| (I - \mathscr{Q}_h) \overline{\tilde{\boldsymbol{v}}}^k \right\|_{L^\infty(\Omega)}$$

$$+ \|\nabla \underline{d}_h^k\|_{L^2(\Omega)} \left\| (\mathscr{I}_h - I) \left[[\overline{\underline{d}}_h^k]^T_\times \widetilde{\mathscr{I}}_h(\boldsymbol{\varphi}) \otimes \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k \right] \right\|_{L^2(\Omega)}.$$

The first equality holds due to the definition of the interpolation operator in (28). The second equality is a transformation and the third is the definition of (30). In the fourth equation, a zero is added and the last inequality follows from Hölder's inequality. Furthermore, we estimate the second term on the right-hand side of the previous inequality by

$$
\left\| (\mathscr{I}_h - I) \left[[\underline{\bar{d}}_h^k]_\times^T \widetilde{\mathscr{I}}_{\mathrm{h}}(\boldsymbol{\varphi}) \otimes \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k \right] \right\|_{L^2(\Omega)}^2
$$

$$
\leq C h^4 \sum_{K \in \mathscr{T}_h} \left\| \nabla^2 \left[[\underline{\bar{d}}_h^k]_\times^T \widetilde{\mathscr{I}}_{\mathrm{h}}(\boldsymbol{\varphi}) \otimes \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k \right] \right\|_{L^2(K)}^2
$$

$$
\leq C h^4 \sum_{K \in \mathscr{T}_h} \left(\left\| \left[[\nabla \underline{\bar{d}}_h^k]_\times^T \nabla \widetilde{\mathscr{I}}_{\mathrm{h}}(\boldsymbol{\varphi}) \otimes \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k + [\nabla \underline{\bar{d}}_h^k]_\times^T \widetilde{\mathscr{I}}_{\mathrm{h}}(\boldsymbol{\varphi}) \otimes \nabla \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k \right] \right\|_{L^2(K)} \right)^2
$$

$$
+ C h^4 \sum_{K \in \mathscr{T}_h} \left(\left\| \left[[\underline{\bar{d}}_h^k]_\times^T \nabla \widetilde{\mathscr{I}}_{\mathrm{h}}(\boldsymbol{\varphi}) \otimes \nabla \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k + [\underline{\bar{d}}_h^k]_\times^T \widetilde{\mathscr{I}}_{\mathrm{h}}(\boldsymbol{\varphi}) \otimes \nabla^2 \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k \right] \right\|_{L^2(K)} \right)^2
$$

$$
\leq C \left(h \left[\left\| \underline{\bar{d}}_h^k \right\|_{L^\infty(\Omega)} + \left\| \nabla \underline{\bar{d}}_h^k \right\|_{L^2(\Omega)} \right] \left\| \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k \right\|_{H^2(\Omega)} \left\| \widetilde{\mathscr{I}}_{\mathrm{h}}(\boldsymbol{\varphi}) \right\|_{L^\infty(\Omega)} \right)^2 .
$$

The first inequality follows from the local estimate of the interpolation error (*cf.* Lemma 2.10) and the quasi-uniformity of the mesh. In order to infer the second inequality, we calculate the derivatives via the product rule and observe that the second derivative vanishes for all functions in $[Z_h]^3$. In the third estimate, we use Hölder's inequality and local inverse estimates.

We note that the interpolation $\widetilde{\mathscr{I}}_{\mathrm{h}}$ converges in $\mathscr{C}(\overline{\Omega})$ (*cf.* Lemma 2.12). Moreover, from (21) and Gagliardo–Nirenberg's inequality [48] we infer

$$
\| \tilde{\boldsymbol{v}} - \mathscr{Q}_h \tilde{\boldsymbol{v}} \|_{L^\infty(\Omega)} \leq C \| \tilde{\boldsymbol{v}} - \mathscr{Q}_h \tilde{\boldsymbol{v}} \|_{H^1(\Omega)}^{1/2} \| \tilde{\boldsymbol{v}} - \mathscr{Q}_h \tilde{\boldsymbol{v}} \|_{H^2(\Omega)}^{1/2} \leq C h^{1/2} \| \tilde{\boldsymbol{v}} - \mathscr{Q}_h \tilde{\boldsymbol{v}} \|_{H^2(\Omega)}
$$

for all $\tilde{\boldsymbol{v}} \in H^2(\Omega) \cap H^1_{0,\sigma}(\Omega)$. The weak convergence (45) and the strong convergence (48) implies the weak convergence

$$
\mathscr{I}_h(\underline{\bar{d}}_h^k \times [\mathscr{R}_h \nabla \underline{d}_h^k] \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k) \rightharpoonup \boldsymbol{d} \times (\nabla \boldsymbol{d} \cdot \tilde{\boldsymbol{v}}) \quad \text{in } L^2(\Omega \times (0, T); \mathbb{R}^3) .
$$

In a similar fashion, we may infer the convergences

$$
\mathscr{I}_h \left[\sqrt{\| \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k \|_{L^\infty(\Omega)}^2 - |\mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k|} [\mathscr{R}_h \nabla \underline{d}_h^k] \right] \rightharpoonup \sqrt{\| \tilde{\boldsymbol{v}} \|_{L^\infty(\Omega)}^2 - |\tilde{\boldsymbol{v}}|} \nabla \boldsymbol{d} ,
$$

$$
\mathscr{I}_h \left[\left(|\mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k| I - \frac{\mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k \otimes \mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k}{|\mathscr{Q}_h \overline{\tilde{\boldsymbol{v}}}^k|} \right) [\mathscr{R}_h \nabla \underline{d}_h^k] \right] \rightharpoonup \left(|\tilde{\boldsymbol{v}}| I - \frac{\tilde{\boldsymbol{v}} \otimes \tilde{\boldsymbol{v}}}{|\tilde{\boldsymbol{v}}|} \right) \nabla \boldsymbol{d} ,
$$

$$
\mathscr{I}_h \left[\underline{\bar{d}}_h^k \cdot [\mathscr{R}_h \nabla \underline{d}_h^k] \mathscr{Q}_h \tilde{\boldsymbol{v}}^k \right] \rightharpoonup \boldsymbol{d} \cdot (\nabla \boldsymbol{d} \tilde{\boldsymbol{v}})
$$

in $L^2(\Omega \times (0,T); \mathbb{R}^{3\times 3})$ and $L^2(\Omega \times (0,T); \mathbb{R})$, respectively. The weakly-lower semi-continuity of the $L^2(\Omega)$ norm implies

$$
\liminf_{k,h\to 0} \int_0^T \overline{\phi}^k \Big[\big(\overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_h^k, \overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_h^k \big)_h
$$

$$
+ \mathscr{K}(\overline{\tilde{v}}^k) \frac{1}{2} \|\nabla \underline{d}_h^k\|_{L^2(\Omega)}^2 - \big([\mathscr{R}_h \nabla \underline{d}_h^k]^T [\overline{\underline{d}}_h^k \times (\overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_h^k)], \overline{\tilde{v}}^k \big)_h \Big] dt
$$

$$
\geq \int_0^T \phi \Big[\Big\| d \times \Delta d + \frac{1}{2} d \times (\nabla d\tilde{v}) \Big\|_{L^2(\Omega)}^2 + \frac{1}{4} \Big\| \sqrt{\|\tilde{v}\|_{L^\infty(\Omega)}^2 - |\tilde{v}|} \nabla d \Big\|_{L^2(\Omega)}^2 \Big] dt
$$

$$
+ \frac{1}{4} \int_0^T \phi \Big[\Big\| \Big(|\tilde{v}| I - \frac{\tilde{v} \otimes \tilde{v}}{|\tilde{v}|} \Big) \nabla d \Big\|_{L^2(\Omega)}^2 + \|d \cdot \nabla d\tilde{v}\|_{L^2(\Omega)}^2 \Big] dt
$$

$$
= \int_0^T \phi \Big[\|d \times \Delta d\|_{L^2(\Omega)}^2 + (d \times \Delta d, d \times (\nabla d\tilde{v})) \Big] dt
$$

$$
+ \frac{1}{4} \int_0^T \phi \Big[\|d \times (\nabla d\tilde{v})\|_{L^2(\Omega)}^2 + \int_\Omega \big(\|\tilde{v}\|_{L^\infty(\Omega)}^2 - |\tilde{v}|^2 \big) I : [\nabla d^T] \nabla d \, dx \Big] dt
$$

$$
+ \int_0^T \phi \int_\Omega \big[\big(|\tilde{v}|^2 I - \tilde{v} \otimes \tilde{v} \big) [\nabla d^T] \nabla d + (d \cdot \nabla d\tilde{v})^2 \big] dx dt
$$

$$
= \int_0^T \phi \Big[\|d \times \Delta d\|_{L^2(\Omega)}^2 + (d \times \Delta d, d \times (\nabla d\tilde{v})) + \frac{1}{4} \|\tilde{v}\|_{L^\infty(\Omega)}^2 \|\nabla d\|_{L^2(\Omega)}^2 \Big] dt .
$$

The pointwise convergence of $\underline{E}_h^k \to E$ allows passing to the limit in the occurring terms, even though the prefactors are possibly negative. In all other terms, the quantities in (51) $(\nabla v_h^j, \nabla d_h^j, \mathscr{I}_h(\overline{\underline{d}}_h^k \times \Delta_h \overline{\underline{d}}_h^k))$ only occur linearly and can thus, be handled in a standard fashion. The switch from mass-lumping to the L^2 inner product and the convergence of the projection of the gradient can be dealt with as in the previous section.

Passing to the limit in (51) leads to the formulation

$$
- \int_0^T \phi'(E - \int_\Omega v \cdot \tilde{v} dx) dt - \int_0^T \phi \mathscr{K}(\tilde{v}) (E - \mathscr{E}(v,d)) dt
$$

$$
+ \int_0^T \phi \int_\Omega v \cdot \partial_t \tilde{v} - (v \cdot \nabla) v \cdot \tilde{v} + (d \times \Delta d) \cdot (d \times (\nabla d\tilde{v})) \, dx dt
$$

$$
+ \int_0^T \phi \int_\Omega \big((\mu_1 + \lambda^2)(d \cdot (\nabla v)_{sym} d)(d \otimes d) + \mu_4 (\nabla v)_{sym} \big) (\nabla v - \nabla \tilde{v}) dx dt
$$

$$
+ \int_0^T \phi \int_\Omega (\mu_5 + \mu_6 - \lambda^2)(d \otimes (\nabla v)_{sym} d)_{sym} (\nabla v - \nabla \tilde{v}) + |d \times \Delta d|^2 dx dt
$$

$$
+ \int_s^t \int_\Omega \big(\lambda [d \otimes [d]_x^T [d]_x \cdot \Delta d]_{sym} + [d \otimes \Delta d]_{skw} \big) : \nabla \tilde{v} dx d\tau \leq 0 .
$$

From Lemma (2.7), we infer the formulation (5) with $\mathscr{K}(\tilde{v}) = \frac{1}{2} \|\tilde{v}\|_{L^\infty(\Omega)}^2$ and

$$
\langle T_1^E(d), v \rangle = \int_\Omega (d \times \Delta d) \cdot (d \times (\nabla d\tilde{v})) \, dx
$$

as given in Definition 2.1.

4 Computational Studies

An efficient implementation of our discrete scheme (33a)–(33b) faces two challenges: The non-linearity in scheme (33a)–(33b) does not allow us to rely on well-known and effective solvers for the resulting linear systems. Secondly, all equations are coupled which leads to a high-dimensional mixed problem formulation. Therefore, by fully linearizing and decoupling all equations we make use of an iterative fixed-point algorithm which was presented in [49, ch. 5] and follows the ideas of [45, Algorithm A_1].

This approach can be described by the following scheme.

Scheme 52 (1) *Let* $(v^{j,0}, d_\circ^{j,0})^T = (v^{j-1}, d_\circ^{j-1})^T \in U_h$ *for* $j > 1$. *For* $j = 1$ *let the initial values be given by* $(v^0, d^0) = (\mathcal{Q}_h v_0, \mathcal{I}_h d_0)$.
(2) *For* $1 \le l \le J$ *and* $(v^{j,l-1}, d^{j,l-1}) \in U_h$, *we want to find* $(v^{j,l}, d_\circ^{j,l}) \in U_h$, *such that*

$$
\begin{aligned}
&(d_t v^{j,l}, a) + ((v^{j-1} \cdot \nabla) v^{j,l}, a) + \frac{1}{2}((\nabla \cdot v^{j-1}) v^{j,l}, a) + (T_L^{j,l}, \nabla a) \\
&\quad - v_{el} A([\mathcal{R}_h \nabla d^{j-1}]^T [d^{j-1/2,l-1} \times (d^{j-1/2,l-1} \times \Delta_h d^{j-1/2,l-1})], a)_h = 0
\end{aligned}
\tag{52a}
$$

$$
\begin{aligned}
&(d_t d^{j,l}, c)_h + v_{el}(d^{j-1/2,l-1} \times [\mathcal{R}_h \nabla d^{j-1} v^{j,l-1}], d^{j-1/2,l} \times c)_h \\
&\quad - A(d^{j-1/2,l-1} \times \Delta_h d^{j-1/2,l-1}, d^{j-1/2,l} \times c)_h \\
&\quad - v_{el}((\nabla v^{j,l-1})_{skw} d^{j-1/2,l}, c)_h \\
&\quad + v_{el}\lambda(d^{j-1/2,l-1} \times [(\nabla v^{j,l-1})_{sym} d^{j-1/2,l-1}], d^{j-1/2,l} \times c)_h = 0,
\end{aligned}
\tag{52b}
$$

for all $(a, c) \in U_h$, *where the constants* v_{el}, A *describe the intensity of the coupling of the different physical properties.*
(3) *Stop if* $\|v^{j,l} - v^{j,l-1}\|_{L^2(\Omega)} + \|d^{j,l} - d^{j,l-1}\|_{H^1(\Omega)} \le \theta$, *where* θ *describes the tolerance of the fixpoint-solver.*

For the above scheme, one would solve the discrete Laplace equation computationally after solving (52a) and (52b). This is possible since (52b) does not depend on $\Delta_h d^{j,l}$. Note that (52a) and (52b) could even be solved in parallel. The Leslie stress tensor is thereby discretized as

$$
\begin{aligned}
T_L^{j,l} :=& v_{el}(\mu_1 + \lambda^2)(d^{j,l-1} \cdot (\nabla v^{j,l})_{sym} d^{j,l-1})(d^{j,l-1} \otimes d^{j,l-1}) + \mu_4 (\nabla v^{j,l})_{sym} \\
& + v_{el}(\mu_5 + \mu_6 - \lambda^2)(d^{j,l-1} \otimes (\nabla v^{j,l})_{sym} d^{j,l-1})_{sym} \\
& + \lambda v_{el} A[d^{j-1/2,l-1} \otimes [d^{j-1/2,l-1}]_x^T [d^{j-1/2,l-1}]_x \cdot \Delta_h d^{j-1/2,l-1}]_{sym} \\
& + v_{el} A[d^{j-1/2,l-1} \otimes \Delta_h d^{j-1/2,l-1}]_{skw}.
\end{aligned}
$$

Any fixed-point of scheme (52a)–(52b) solves the highly non-linear scheme (33a)–(33b). By standard arguments, one can derive conditional convergence of our fixpoint algorithm, i.e. $u^{j,l} \to u^j \in U_h$ as $l \to \infty$ for a sufficiently small k, h. For more details, we refer to [49]. Since we introduced the constants v_{el}, A for the physical coupling of the quantities, the energy law changes slightly and we rescale the total energy to

$$
\mathcal{E}(v, d) := \frac{1}{2}\|v\|_{L^2(\Omega)}^2 + \frac{A}{2}\|\nabla d\|_{L^2(\Omega)}^2 .
$$

Table 1 Parameter choices for the experiments

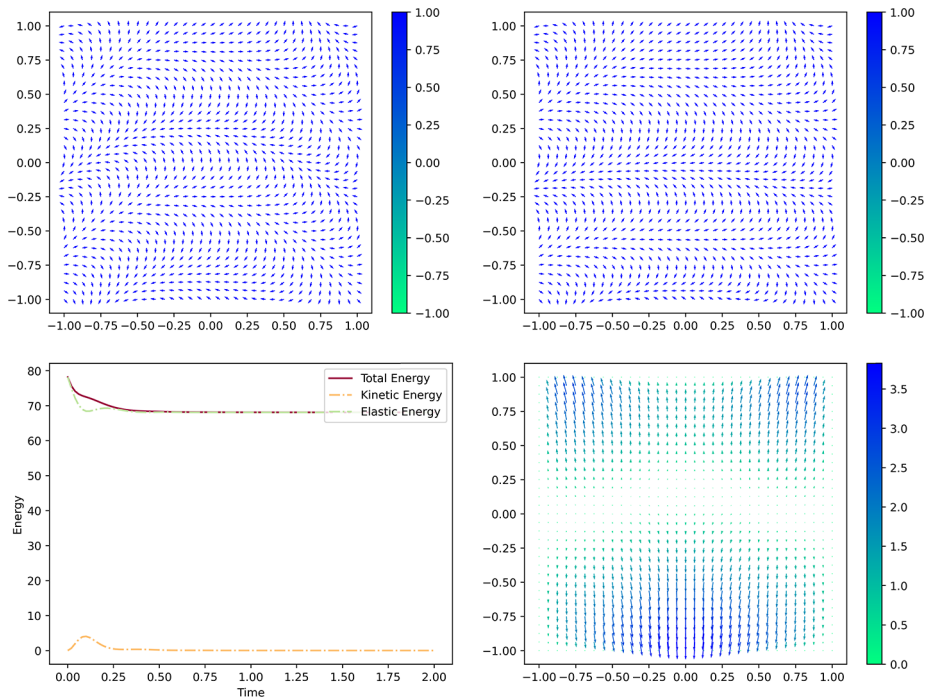|	Ω	h	k	μ_1	μ_4	ν	μ_5, μ_6, λ	A	ν_{el}
Experiment 1	$(-1,1)^2$	2^{-5}	0.00025	1	0.1	0.1	1	1	1
Experiment 2	$(-0.5, 0.5)^3$	2^{-4}	0.00025	1	1	1	1	1	0.25
Experiment 3	$(-0.5, 0.5)^3$	2^{-4}	0.00025	1	1	1	1	0.1	1

Fig. 2 Experiment 4.1, simplified model (53): Evolution of the director at time $t = 0, 2.0$ (from left to right), evolution of the energy (bottom left), velocity field at times $t = 0.2$ (bottom right). The colour marks the magnitude of the vectors. (Color figure online)

The computational studies consist of three numerical experiments which have been standard benchmarks for past numerical methods of nematic liquid crystals (see e.g. [17, 22–24]). As a simplified version of our discrete scheme, we consider one analogous to the Ericksen–Leslie interactions in [24] and similar to [23, Algorithm 4.1]. The simplified scheme is attained by choosing a reduced (discrete) version of the Leslie stress tensor, *i.e.*

$$(T_L^j, a) = \nu(\nabla v^j, \nabla a). \tag{53}$$

Accordingly, the fourth and last term in the director equation (33b) of our scheme are also neglected. Both schemes can be solved by the fixed-point iteration described above. The tolerance of the iterative fixpoint solver was set to $\theta = 10^{-6}$. The python implementation of the fixed-point solver relies on the API of the finite element package FEniCS (*cf.* [50, 51]). The implementation can be found in [52].
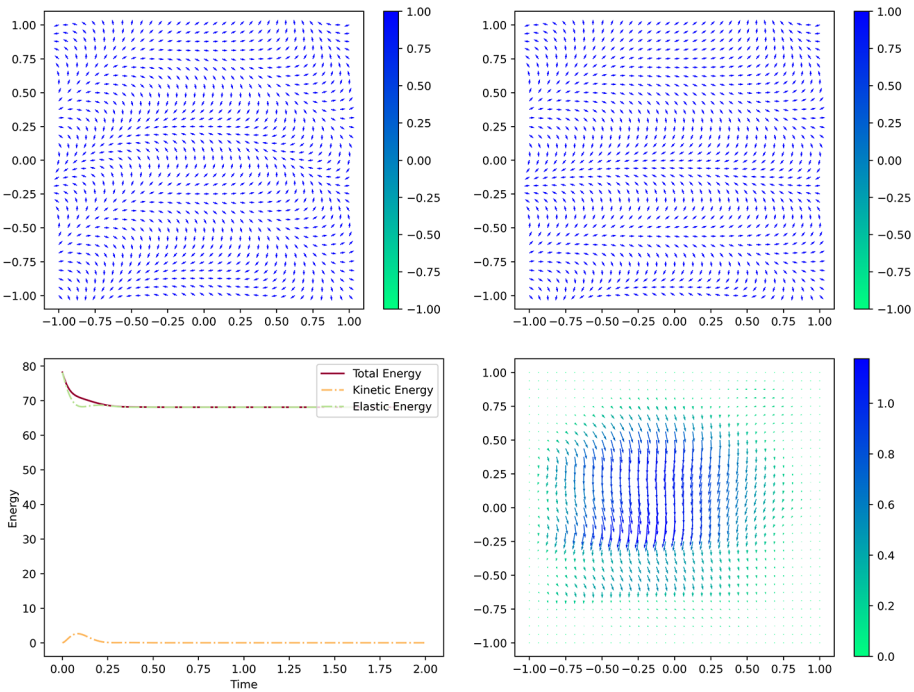
Fig. 3 Experiment 4.1, model (33a)–(33b): Evolution of the director at time $t = 0, 2.0$ (from left to right), evolution of the energy (bottom left), velocity field at times $t = 0.2$ (bottom right). The colour marks the magnitude of the vectors. (Color figure online)

If not mentioned otherwise, we employ homogeneous Dirichlet boundary (no-slip) conditions for the velocity and non-homogeneous Dirichlet boundary conditions for the director prescribed constantly in time by the initial condition. The parameter choices for the following experiments can be found in Table 1. Our choice of parameters is rather exemplary and analogous to the experiments considered in [17, 22–24]. In particular, regarding the choice of μ, other choices are most definitely conceivable. Note that the dissipative character of the system is fulfilled, *i.e.,* $\mu_4 > 0$, $\mu_5 + \mu_6 - \lambda^2 > 0$, $\mu_1 + \lambda^2 > 0$. Further, $\nu = \mu_4$ is fulfilled which shall allow a comparison of the models. Since the convergence of our fixed-point solver relies on a contraction property, a smaller choice of our temporal discretization parameter k might sometimes still lead to faster computation time, if this leads to fewer total iterations of the fixed-point solver itself.

4.1 A Smooth Example in Two Spatial Dimensions

We consider the domain $\Omega = (-1, 1)^2$ equipped with the initial conditions

$$d_0(x) = \begin{pmatrix} \sin\left(2\pi\left(\cos(x_1) - \sin(x_2)\right)\right) \\ \cos\left(2\pi\left(\cos(x_1) - \sin(x_2)\right)\right) \end{pmatrix} \text{ for } x \in \Omega,$$

$$v_0 = 0.$$

Although the above analysis is only done for three spatial dimensions, the results can be transferred to the two-dimensional case as well. In this case, the cross product has to be
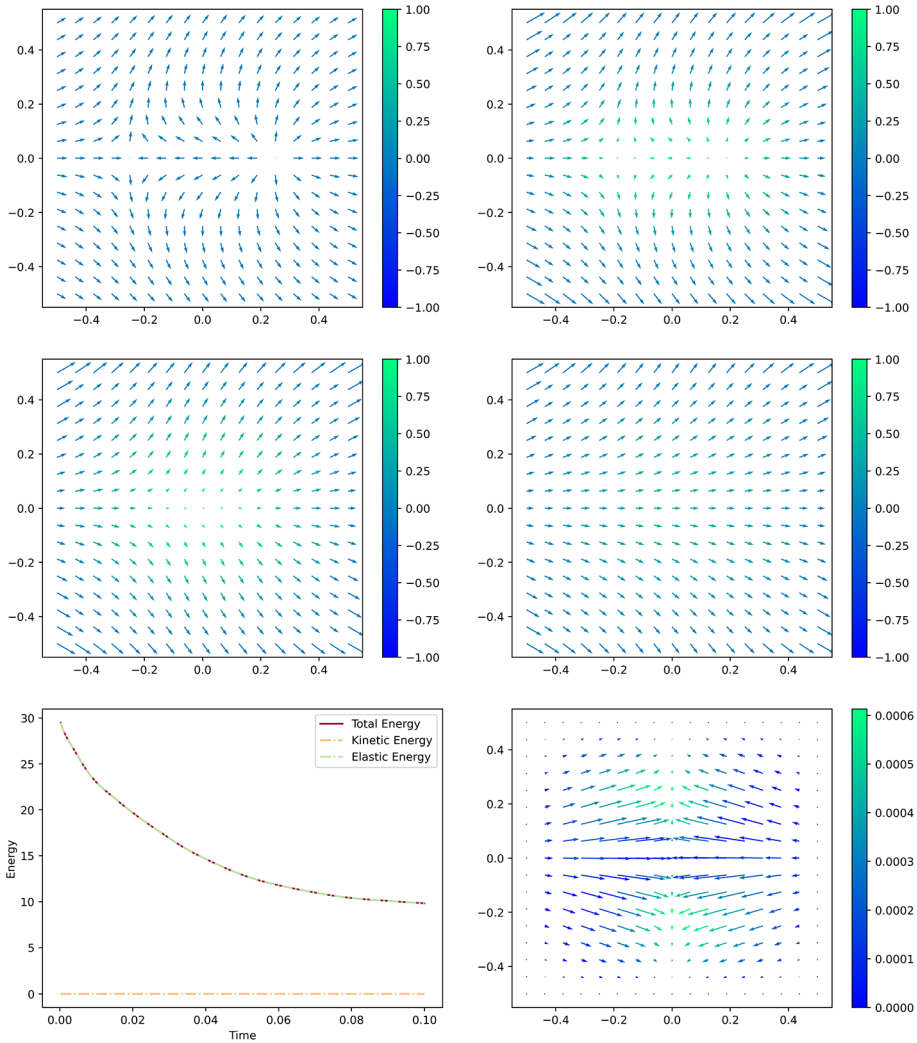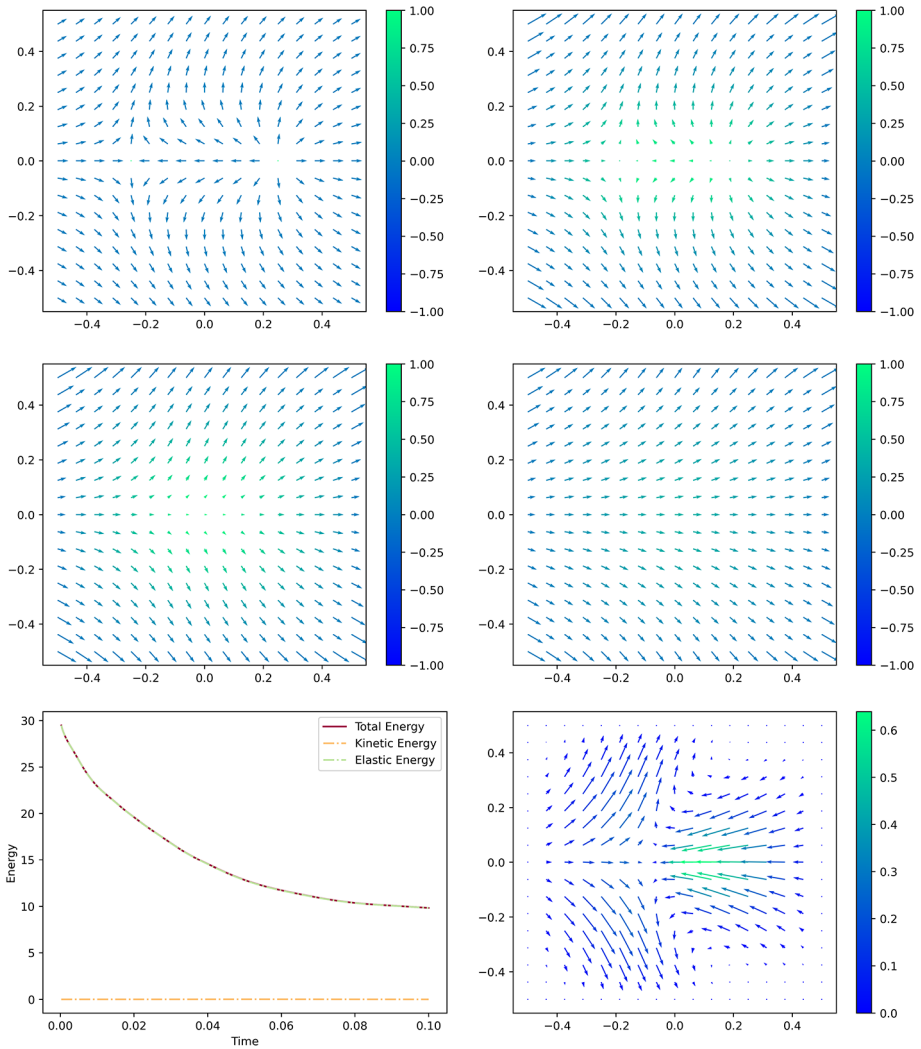
Fig. 4 Experiment 4.2, simplified model (53): Evolution of the director in the plane $x_3 = 0$ at time $t = 0, 0.03, 0.05, 0.1$ (from left to right, from top to bottom), evolution of the energy (bottom left), velocity field in the plane $x_3 = 0$ at time $t = 0.05$ (bottom right). The colour marks the (absolute) value of the z-component. (Color figure online)

understood in the sense of the matrix $I - d \otimes d$ (see (6)), which in three dimensions fulfills $I - d \otimes d = [d]_x^T [d]_x$. In this setting, at least for the simplified model, a smooth solution exists except for finitely many points in time (*cf.* [9, Thm. 1.3]). The results for our simplified model (see (53), Fig. 2) deviate from the results of previous authors (*cf.* [23]) due to our Dirichlet boundary conditions. The director exhibits a long-term self-alignment which causes a fluid flow. In opposite to e.g. [23], this alignment of the director is not uniform. The same holds for our full Ericksen–Leslie model (see Fig. 3) except for the fact that the induced velocity field exhibits less symmetry due to the anisotropic dynamics of our Leslie-stress tensor.

Fig. 5 Experiment 4.2, model (33a)–(33b): Evolution of the director in the plane $x_3 = 0$ at time $t = 0, 0.03, 0.05, 0.1$ (from left to right, from top to bottom), evolution of the energy (bottom left), velocity field in the plane $x_3 = 0$ at time $t = 0.05$ (bottom right). The colour marks the (absolute) value of the z-component. (Color figure online)

4.2 Annihilation of Two Defects

On the three-dimensional domain $\Omega = (-0.5, 0.5)^3$, we set the initial director to

$$d_0 = \begin{cases} \dfrac{\tilde{d}_0(x)}{\left\| \tilde{d}_0(x) \right\|}, & \text{if } \left\| \tilde{d}_0(x) \right\| > 0 \\ (0, 0, 1)^T, & \text{otherwise}, \end{cases}$$

for $\tilde{d}_0(x) = (4x_1^2 + 4x_2^2 - 0.25, 2x_2, 0)^T$,
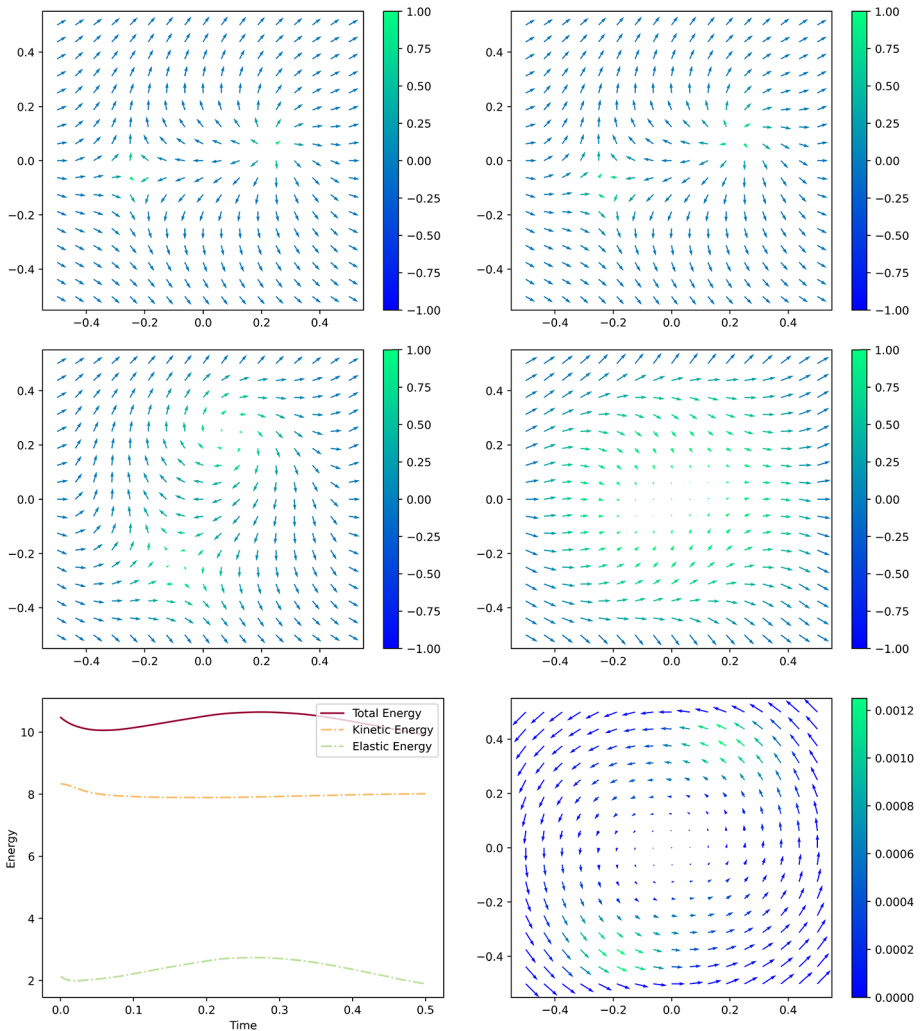
Fig. 6 Annihilation in a rotating flow, simplified model (53): Evolution of the director in the plane $x_3 = 0$ at time $t = 0.03, 0.05, 0.15, 0.5$, evolution of the energy, velocity field in the plane $x_3 = 0$ at time $t = 0.15$ (from top left to bottom right). The colour marks the (absolute) value of the z-component. (Color figure online)

where the locations with $\boldsymbol{d}_0 = (0, 0, 1)^T$ are considered *defects* of the liquid crystal. The initial velocity is set to $\boldsymbol{v}_0 = 0$.

It can be observed that for both models the defects slowly annihilate by rotation of the director (see Fig. 4 and Fig. 5). This causes rough swirls to develop in the velocity field. The evolution of the director qualitatively agrees with the results in [17, 22–24].[1] For the full Ericksen–Leslie model, we observe again anisotropic dynamics transferred to the velocity field as well.

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[1] Since the norm conservation is fulfilled precisely at every node in our case, we cannot simulate this experiment in two dimensions as done in [23] because the defects would otherwise be conserved.
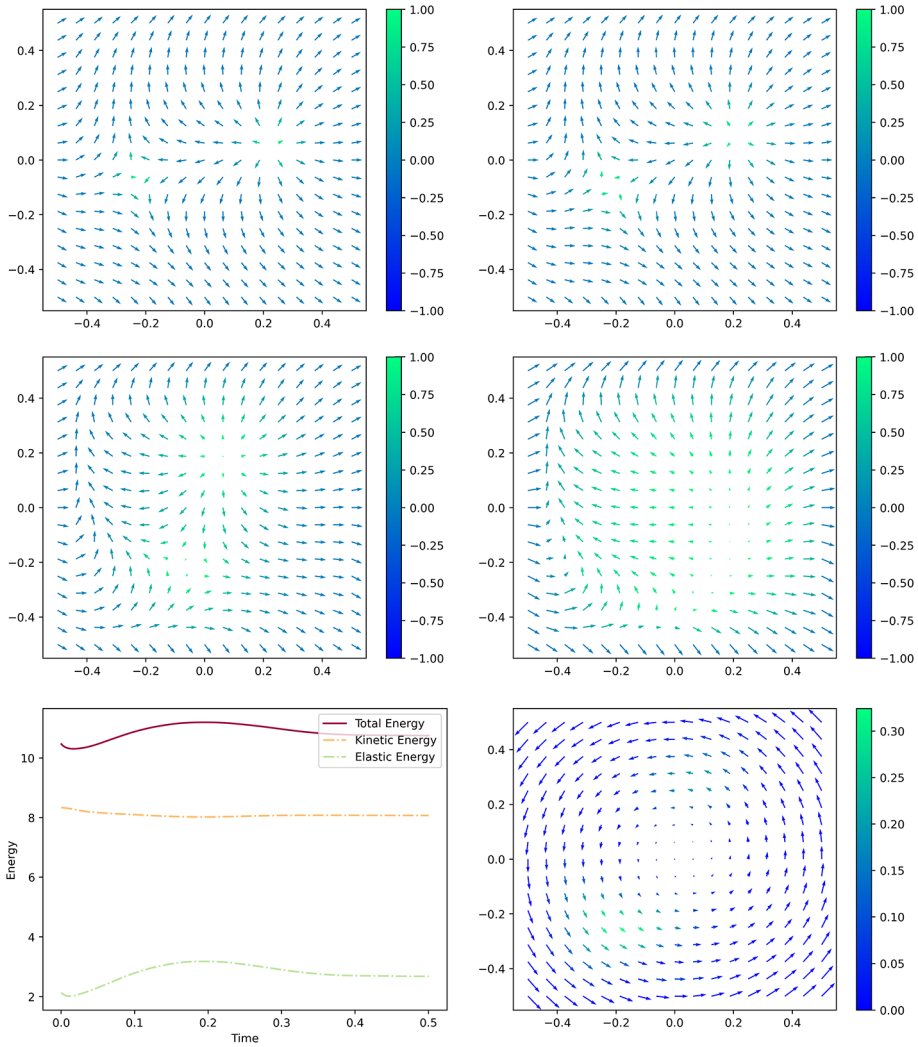
Fig. 7 Annihilation in a rotating flow, model (33a)–(33b): Evolution of the director in the plane $x_3 = 0$ at time $t = 0.03, 0.05, 0.15, 0.5$, evolution of the energy, velocity field in the plane $x_3 = 0$ at time $t = 0.15$ (from top left to bottom right). The colour marks the (absolute) value of the z-component. (Color figure online)

4.3 Annihilation of Two Defects in a Rotating Flow

The setting of the experiment equals the setting of the one before except for the choice of the initial condition and boundary condition of the velocity. Instead, we choose

$$\boldsymbol{v}_0 = 10(-x_2, x_1, 0)^T \text{ for all } x \in \Omega,$$

$$\boldsymbol{v} = 10(-x_2, x_1, 0)^T \text{ for all } x \in \partial\Omega.$$

Note that the inhomogeneous Dirichlet boundary conditions for the velocity are a deviation from our so far considered setting such that we can only expect the energy law (38) to hold

with a modified right-hand side accounting for the boundary conditions (see Fig. 6). In Fig. 6 we can observe that in the simplified model the defects are swirled anticlockwise around the center by the velocity field before annihilation. This is in qualitative agreement with the results obtained by [17, 24] and also holds for the more general model (see Fig. 7).

Declarations

Competing Interests The authors have no competing interests to declare that are relevant to the content of this article.

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