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A Second-Order Length-Preserving and Unconditionally Energy Stable Rotational Discrete Gradient Method for Oseen-Frank Gradient Flows

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Abstract. We present a second-order strictly length-preserving and unconditionally energy-stable rotational discrete gradient (Rdg) scheme for the numerical approximation of the Oseen-Frank gradient flows with anisotropic elastic energy functional. Two essential ingredients of the Rdg method are reformulation of the length constrained gradient flow into an unconstrained rotational form and discrete gradient discretization for the energy variation. Besides the well-known mean-value and Gonzalez discrete gradients, we propose a novel Oseen-Frank discrete gradient, specifically designed for the solution of Oseen-Frank gradient flow. We prove that the proposed Oseen-Frank discrete gradient satisfies the energy difference relation, thus the resultant Rdg scheme is energy stable. Numerical experiments demonstrate the efficiency and accuracy of the proposed Rdg method and its capability for providing reliable simulation results with highly disparate elastic coefficients.

AMS subject classifications: 65N35, 65N22, 65F05, 35J05

Key words: Nematic liquid crystal, Oseen-Frank gradient flow, energy stability, length-preservation, rotational discrete gradient method.

1 Introduction

The dynamics of liquid crystals involve the evolution of local anisotropy generated by nonuniform orientational distribution. For uniaxial nematics, the equilibrium orienta-

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tional distribution is axisymmetric and is allowed to rotate freely as a whole. A simplified setting for the dynamics of uniaxial nematics is to assume that the local anisotropy is kept at the equilibrium state and only rotations of the state is allowed. Under this rationale, the local anisotropy is sufficiently described by a unit vector field $\boldsymbol{n}(\boldsymbol{x})$. The well-known Ericksen-Leslie model [14, 26] couples the velocity and the unit vector field. The evolution of the vector field is given by

$$\boldsymbol{n}\times\Big(\gamma_1\big(\boldsymbol{n}_t+\boldsymbol{v}\cdot\nabla\boldsymbol{n}-\overline{\overline{\Omega}}\cdot\boldsymbol{n}\big)+\gamma_2\overline{\overline{\tau}}\cdot\boldsymbol{n}+\frac{\delta\mathcal{F}[\boldsymbol{n}]}{\delta\boldsymbol{n}}\Big)=0, \tag{1.1a}$$

$$|\boldsymbol{n}|=1. \tag{1.1b}$$

In the above, $\overline{\overline{\Omega}}=(\nabla\boldsymbol{v}-\nabla\boldsymbol{v}^\intercal)/2$, and $\overline{\overline{\tau}}=(\nabla\boldsymbol{v}+\nabla\boldsymbol{v}^\intercal)/2$, where $\boldsymbol{v}$ is the velocity of the fluid governed by the Navier–Stokes equation that we do not write down here. The force by the interaction of local anisotropy is characterized by variational derivative of the Oseen–Frank energy [17, 31],

$$\begin{aligned}\mathcal{F}[\boldsymbol{n}]=\frac{1}{2}\int_\Omega & k_1(\nabla\cdot\boldsymbol{n})^2+k_2|\boldsymbol{n}\cdot(\nabla\times\boldsymbol{n})|^2+k_3|\boldsymbol{n}\times(\nabla\times\boldsymbol{n})|^2\\ &+(k_2+k_4)\big[\mathrm{tr}\big((\nabla\boldsymbol{n})^2\big)-(\nabla\cdot\boldsymbol{n})^2\big]dV.\end{aligned} \tag{1.2}$$

The first three terms can be explained as excess energy density for three typical deformations specifically for unit vector fields: splay, twist and bend [9]. Therefore, it is the three constants k_1,k_2,k_3 that characterize the elasticity of a certain material. They are closely related to physical parameters, whose relative magnitudes may vary in a wide range by previous experimental or theoretical results [3, 11, 18, 21, 23, 24, 27, 30, 35, 40–43]. The last term can be rewritten as a surface integral, which is usually not considered as it vanishes under periodic or some other commonly adopted boundary conditions.

When the velocity is small, one may approximate by assuming $\boldsymbol{v}=0$, so that the Ericksen-Leslie model is reduced to

$$\boldsymbol{n}\times\boldsymbol{n}_t=-\boldsymbol{n}\times\frac{\delta\mathcal{F}[\boldsymbol{n}]}{\delta\boldsymbol{n}}, \tag{1.3a}$$

$$|\boldsymbol{n}|=1, \tag{1.3b}$$

where γ_1 is also eliminated with suitable rescaling. This equation can be interpreted as a gradient flow driven by the Oseen–Frank energy with an explicit length constraint, which we shall clarify later. Notably, it is desirable for a numerical scheme to keep the vector length and the energy dissipation. In particular, the deviation of vector length would bring ambiguity when explaining the results because the pictures of splay, twist and bend terms are no longer valid for vector fields with varying lengths. However, both the k_i terms and the length constraint give rise to strong nonlinearity that is not easy to handle.