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A coupled Ericksen/Allen–Cahn model for liquid crystal droplets

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ABSTRACT

We present a model and discretization that couples the Ericksen model of liquid crystals with variable degree of orientation to the Allen–Cahn equations with a mass constraint. The coupled system models liquid crystal droplets with anisotropic surface tension effects due to the liquid crystal molecular alignment. The total energy consists of the Ericksen energy, phase-field (Allen–Cahn) energy, and a weak anchoring energy that couples the liquid crystal to the diffuse interface. We describe our discretization of the total energy along with a method to compute minimizers via a discrete gradient flow algorithm which has a strictly monotone energy decreasing property. Numerical experiments are given in three dimensions that illustrate a wide variety of droplet shapes that result from their interaction with defects.

1. Introduction

This paper presents a method for solving the Ericksen model coupled to the Allen–Cahn equations [1–3] in order to model the equilibrium shapes of nematic liquid crystal (**LC**) droplets with anisotropic surface tension [4–6]. LCs have a variety of applications, e.g. electronic displays [7–9], in addition to a host of potential applications in material science [10–25]. To the best of our knowledge, coupling Ericksen to Allen–Cahn has never been done. The main contributions of the paper are the numerical method and the three-dimensional simulations of LC droplets that illustrate the coupled model.

Nematic droplets have been studied at the continuum level, including experiments [26,27], modeling [28–32], and shape minimization of LC droplets [33]. Numerically, molecular dynamics approaches [34,22] and PDE techniques [35–39] have been used to simulate LC droplets at equilibrium as well as dynamics. The above references use either a (regularized) Oseen–Frank type of model or the Landau–deGennes model (**Q**-tensor) [40,6]. Our paper, and [41], is the first to consider the Ericksen model in the context of LC droplets.

Initial studies of dynamics and numerics for the Ericksen model can be found in [42,43]. More recently, a method was developed in [44–46] to solve the Ericksen model without any ad hoc regularization term. The method was justified via Γ-convergence, and simulations were shown in three dimensions illustrating novel defect structures.

In this paper, we present a coupled model that combines the Ericksen model with anisotropic surface tension to model energy minimizing shapes of LC droplets. The rest of the paper is organized as follows. In Section 2, we present the coupled model at the continuous level, and Section 3 describes our discretization of the continuous model using a finite element

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method. Section 4 presents a gradient flow method for computing minimizers of the discrete energy, and numerical examples in three dimensions are presented in Section 5. We conclude with some discussion in Section 6.

2. Coupled model

We couple two energetic models (Ericksen and Allen–Cahn) to obtain an equilibrium model of LC droplets. The Allen–Cahn energy [2,3] models the separation of two immiscible LC phases with anisotropic surface tension between the phases [4,40,47–49,36,35]. The Ericksen energy models the elasticity of the LC medium [5,40,6,42] in each phase.

2.1. Phase field representation

Suppose we have a fixed hold-all domain $\Omega \subset \mathbb{R}^d$ that partitions into two "phases". For simplicity, we assume both phases contain liquid crystal material, i.e. $\Omega \equiv \text{int}\left(\overline{\Omega_{\text{lc}}^1} \cup \overline{\Omega_{\text{lc}}^2}\right)$, where Ω_{lc}^i is the ith liquid crystal phase ($i = 1, 2$). In order to avoid dealing with sharp interfaces, we use a phase field function $\phi : \Omega \to [-1, +1]$ to represent the coexistence of the two phases, i.e. $\phi \approx +1$ in Ω_{lc}^1 and $\phi \approx -1$ in Ω_{lc}^2 [50].

2.2. Ericksen's model

The state of the liquid crystal is modeled by a director field $\mathbf{n} : \Omega \subset \mathbb{R}^d \to \mathbb{S}^{d-1}$ with unit length, and a scalar field $s : \Omega \subset \mathbb{R}^d \to (-\frac{1}{2}, 1)$ called the *degree-of-orientation* [40,46]. Essentially, $\mathbf{n}$ specifies the averaged *orientation* of LC molecules, and s represents how well the individual LC molecules are aligned with $\mathbf{n}$. The equilibrium state $(s, \mathbf{n})$ is assumed to minimize a "one-constant" energy.

2.2.1. Ericksen's one-constant energy

The equilibrium state $(s, \mathbf{n})$ of the liquid crystal is assumed to minimize the following energy functional:

$$\begin{aligned} E_{\text{erk}}(s, \mathbf{n}) &:= \int_\Omega \left(\kappa |\nabla s|^2 + s^2 |\nabla \mathbf{n}|^2\right) dx, \\ E_{\text{bulk}}(s) &:= \int_\Omega \omega(s) dx, \end{aligned} \tag{1}$$

where $\kappa > 0$. The function ω is C^2, defined on $-1/2 < s < 1$, and satisfies [5,51,52]

1. $\lim_{s\to 1}\omega(s) = \lim_{s\to -1/2}\omega(s) = \infty$,
2. $\omega(0) > \omega(s^*) = \min_{s\in[-1/2,1]}\omega(s) = 0$ for some $s^* \in (0, 1)$,
3. $\omega'(0) = 0$.

2.2.2. Theoretical framework

The initial theory for minimizers (and regularity) of (1) was developed in [51,52], where they introduced an auxiliary variable $\mathbf{u} = s\mathbf{n}$ which allows for rewriting the energy $E_{\text{erk}}(s, \mathbf{n})$ as

$$E_{\text{erk}}(s, \mathbf{n}) = \widetilde{E}_1(s, \mathbf{u}) := \int_\Omega \left((\kappa - 1)|\nabla s|^2 + |\nabla \mathbf{u}|^2\right) dx, \tag{2}$$

which derives from the identity $\mathbf{n}^T \nabla \mathbf{n} = \mathbf{0}^T$ because of the unit length constraint $|\mathbf{n}| = 1$. This suggests the following admissible class of solutions (minimizers) to be [51,52]:

$$\mathcal{K} := \{(s, \mathbf{u}) : \Omega \to (-1/2, 1) \times \mathbb{R}^d : (s, \mathbf{u}) \in [H^1(\Omega)]^{d+1},\ \mathbf{u} = s\mathbf{n}, \mathbf{n} \in \mathbb{S}^{d-1}\}. \tag{3}$$

Note: we use an abuse of notation and write $(s, \mathbf{n})$ in $\mathcal{K}$ to be equivalent to $(s, \mathbf{u})$ in $\mathcal{K}$ with $\mathbf{u} = s\mathbf{n}$.

Enforcing boundary conditions on $(s, \mathbf{u})$ is done in the following way. Let $(\Gamma_s, \Gamma_{\mathbf{u}})$ be open subsets of $\partial\Omega$ where we set Dirichlet boundary conditions for $(s, \mathbf{u})$. This yields the following restricted admissible class

$$\mathcal{K}(g, \mathbf{r}) := \left\{(s, \mathbf{u}) \in \mathcal{K} : s|_{\Gamma_s} = g, \quad \mathbf{u}|_{\Gamma_{\mathbf{u}}} = \mathbf{r}\right\}, \tag{4}$$

for some given functions $(g, \mathbf{r}) \in [W_\infty^1(\mathbb{R}^d)]^{d+1}$ that satisfy the following in a neighborhood of $\partial\Omega$: $-1/2 < g < 1$ and $\mathbf{r} = g\mathbf{q}$, for some $\mathbf{q} \in \mathbb{S}^{d-1}$. If we further assume

$$g \geq \delta_0 \quad \text{on } \partial\Omega, \quad \text{for some } \delta_0 > 0, \tag{5}$$

then $\mathbf{n}$ is H^1 in a neighborhood of $\partial\Omega$ and satisfies $\mathbf{n} = g^{-1}\mathbf{r} = \mathbf{q} \in \mathbb{S}^{d-1}$ on $\partial\Omega$.

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