A Finite Element Method for a Phase Field Model of Nematic Liquid Crystal Droplets

Amanda E. Diegel[1] and Shawn W. Walker[1,*]

[1] *Department of Mathematics, Louisiana State University, Baton Rouge, LA 70803-4918, USA.*

Abstract. We develop a novel finite element method for a phase field model of nematic liquid crystal droplets. The continuous model considers a free energy comprised of three components: the Ericksen's energy for liquid crystals, the Cahn-Hilliard energy representing the interfacial energy of the droplet, and an anisotropic weak anchoring energy that enforces a condition such that the director field is aligned perpendicular to the interface of the droplet. Applications of the model are for finding minimizers of the free energy and exploring gradient flow dynamics. We present a finite element method that utilizes a special discretization of the liquid crystal elastic energy, as well as mass-lumping to discretize the coupling terms for the anisotropic surface tension part. Next, we present a discrete gradient flow method and show that it is monotone energy decreasing. Furthermore, we show that global discrete energy minimizers Γ-converge to global minimizers of the continuous energy. We conclude with numerical experiments illustrating different gradient flow dynamics, including droplet coalescence and break-up.

1 Introduction

The purpose of this paper is to couple Ericksen's model for nematic liquid crystals to an interfacial energy (modeled via the Cahn-Hilliard equation) in order to model liquid crystal droplets. Interest in developing numerical methods for modeling liquid crystals or complex fluids involving liquid crystals has grown in recent years, [2, 5, 20, 28, 34, 35, 40, 41, 54]. One driver for this development is the large host of technological applications of liquid crystals [1, 4, 8, 9, 29, 36, 38, 42, 45, 49, 55]. Popular models representing liquid crystal substances include the Q-tensor model, the Oseen-Frank model, and Ericksen's model with a variable degree of orientation. A common issue in any of these methods

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*Corresponding author. *Email addresses:* `diegel@math.lsu.edu` (A. E. Diegel), `walker@math.lsu.edu` (S. W. Walker)

is capturing defects. For instance, in [5], Barrett et al. presents a fully discrete finite element method for the evolution of uniaxial nematic liquid crystals with variable degree of orientation. An advantage of their method is that they are able to provide convergence results. However, in order to avoid the degeneracy introduced by the degree of orientation variable s, they use a regularization of Ericksen's model.

The use of diffuse interface theory to describe the mixing of complex fluids has likewise grown in popularity and the research group which includes J. Zhao, X. Yang, Q. Wang, J. Shen (among others) has released several papers on this subject [57–62]. Their models may be described as energy minimizing models whereby their energy functionals are composed of a kinetic energy and a free energy. The kinetic energy is based on fluid velocity coming from a fluid model, such as Stoke's flow. The free energy is then broken down into three parts: the mixing energy, the bulk free energy for liquid crystals, and an anchoring energy. For instance, in [62], Zhao et. al. develop an energy-stable scheme for a binary hydrodynamic phase field model of mixtures of nematic liquid crystals and viscous fluids where they use the Cahn-Hilliard energy to describe the mixing energy and the Oseen-Frank energy to describe the bulk free energy for liquid crystals. Defects are effectively regularized by penalizing the unit length constraint.

The work presented herein is unique in the following sense: the Cahn-Hilliard energy is combined directly with Ericksen's energy in order to develop a phase field model for nematic liquid crystal droplets in a pure liquid crystal substance. In this way, the model we present herein should be considered as a first approximation to modeling deformable colloids in liquid crystalline substances. We therefore make the assumption that the liquid crystal properties are congruent across the interface of the droplet. The model considers a free energy which is comprised of three components: the Ericksen's energy for liquid crystals, the Cahn-Hilliard energy representing the interfacial energy of the droplet, and an anisotropic weak anchoring energy that enforces a condition such that the director field is aligned perpendicular to the interface of the droplet. The goal is to find minimizers of this free energy. To this end, we present a finite element discretization of the energy and apply a modified time-discrete gradient flow method to compute minimizers. The numerical scheme considered herein combines the finite element approximation of the Ericksen model of nematic liquid crystals in [40], which captures point and line defects and requires no regularization, and the technique considered in [24] which follows a convex splitting gradient flow strategy for modeling the Cahn-Hilliard equation.

An outline of the paper is as follows. Section 2 describes the continuous energy model for the liquid crystal/surface tension system. In Section 3, we present a discretization of the total energy (2.12) followed by the development of a discrete gradient flow strategy in Section 4. In Section 5, we present a fully discrete finite element scheme based on the gradient flow strategy and prove its stability. In Section 6, we demonstrate that the discrete energy converges to the continuous energy using the tools of Γ-convergence. We conclude with several numerical experiments in Section 7, and some discussion in Section 8.