

Numerics for Liquid Crystals with Variable Degree of Orientation

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Abstract

We consider the simplest one-constant model, put forward by J. Eriksen, for nematic liquid crystals with variable degree of orientation. The equilibrium state is described by a director field \mathbf{n} and its degree of orientation s , where the pair (\mathbf{n}, s) minimizes a sum of Frank-like energies and a double well potential. In particular, the Euler-Lagrange equations for the minimizer contain a degenerate elliptic equation for \mathbf{n} , which allows for line and plane defects to have finite energy. Using a special discretization of the liquid crystal energy, and a strictly monotone energy decreasing gradient flow scheme, we present a simulation of a plane-defect in three dimensions to illustrate our method.

1 INTRODUCTION

Complex fluids are ubiquitous in nature and industrial processes and are critical for modern engineering systems [20, 11]. Liquid crystals [27, 16, 14, 3, 2, 10, 6, 21, 22, 4, 26] are a relatively simple example of a material with microstructure that may or may not be immersed in a fluid with a free interface [30, 29].

Several numerical methods for liquid crystals have been proposed [5]. Some are based on harmonic mappings [7, 1, 15, 19, 23] where a unit vector field (called the director field) is used to represent the orientation of liquid crystal molecules; in these methods, they only model the equilibrium state. Some methods for the dynamics of liquid crystals can be found in [18, 24, 28].

The main result of our work is a finite element method (FEM) with provable stability and convergence properties, which we use to explore equilibrium configurations of liquid crystals via gradient flows. The equilibrium theory, found in [17, 16, 27], deals with a director field \mathbf{n} , that represents the orientation of liquid crystal molecules, and a scalar parameter s , $-1/2 < s < 1$, that represents the degree of alignment that molecules have with respect to \mathbf{n} . The main purpose of this model is to represent line and plane defects with finite elastic/free energy. Some related work can be found in [12, 13, 22, 21, 25, 4, 26]. The most relevant work that we know of is in [14, 7] which also considers the variable

degree-of-orientation s parameter. However, in both cases they regularize the model to avoid an inherent degeneracy introduced by the s parameter. The regularization is completely artificial and removes the ability to truly capture line and plane defects. The purpose of the regularization is purely mathematical. Our method builds on [8, 9] and consists of a special discrete energy that does *not* use any regularization, hence we can compute minimizers that exhibit line and plane defects.

In this proceedings paper, we only briefly review the continuous model and show some numerical results.

2 ERICKSEN’S ONE CONSTANT MODEL

In Ericksen’s model [17], the configuration of liquid crystals is described by the orientation of the liquid crystal \mathbf{n} and its degree of orientation s . Here, the director field $\mathbf{n} : \Omega \subset \mathbb{R}^d \rightarrow \mathbb{S}^{d-1}$ is a vector-valued function with unit length, and the degree of orientation $s : \Omega \subset \mathbb{R}^3 \rightarrow [-\frac{1}{2}, 1]$ is a real valued function. The case $s = 1$ represents the state of perfect alignment in which all molecules are parallel to \mathbf{n} . Likewise, $s = -1/2$ represents the state of microscopic order in which all molecules are orthogonal to the orientation \mathbf{n} . When $s = 0$, the molecules do not lie along any preferred direction which represent the state that the distribution of molecules is isotropic.

The equilibrium state of the liquid crystals is described by the pair (s, \mathbf{n}) minimizing a bulk-energy functional which in the simplest one-constant model reduces to

$$E[\Omega, s, \mathbf{n}] := \underbrace{\int_{\Omega} \kappa |\nabla s|^2 + s^2 |\nabla \mathbf{n}|^2 dx}_{:=E_1[\Omega, s, \mathbf{n}]} + \underbrace{\int_{\Omega} \psi(s) dx}_{:=E_2[\Omega, s]}, \quad (1)$$

with $\kappa > 0$, where the double well potential function ψ is a C^2 function defined on $-1/2 < s < 1$ (see [17]). The parameter κ depends on the material properties of the liquid crystal and captures the “elastic” energy associated with various modes of orientation, such as *splay*, *bend*, *twist*, and *saddle-splay* [27].

Note that when the degree of orientation s equals a non-zero constant, the energy (1) reduces to the standard Oseen-Frank energy [27]. The introduction of the degree of orientation relaxes the energy of defects. In fact, with finite energy $E[\Omega, s, \mathbf{n}]$, defects (discontinuity of \mathbf{n}) may still occur in the singular set

$$\mathcal{S} := \{x \in \Omega, s(x) = 0\}. \quad (2)$$

We develop a suitable discretization of the energy (1) and a gradient flow strategy to compute its discrete minimizer. We emphasize that our method can handle a singular set (of dimension 0, 1, or 2) without introducing any artificial parameters.

3 NUMERICAL EXPERIMENT: PLANE DEFECT IN 3-D

We simulate the gradient flow evolution of the liquid crystal director field toward a *plane* defect equilibrium state on a cube domain (Ω is the unit cube). This is motivated by

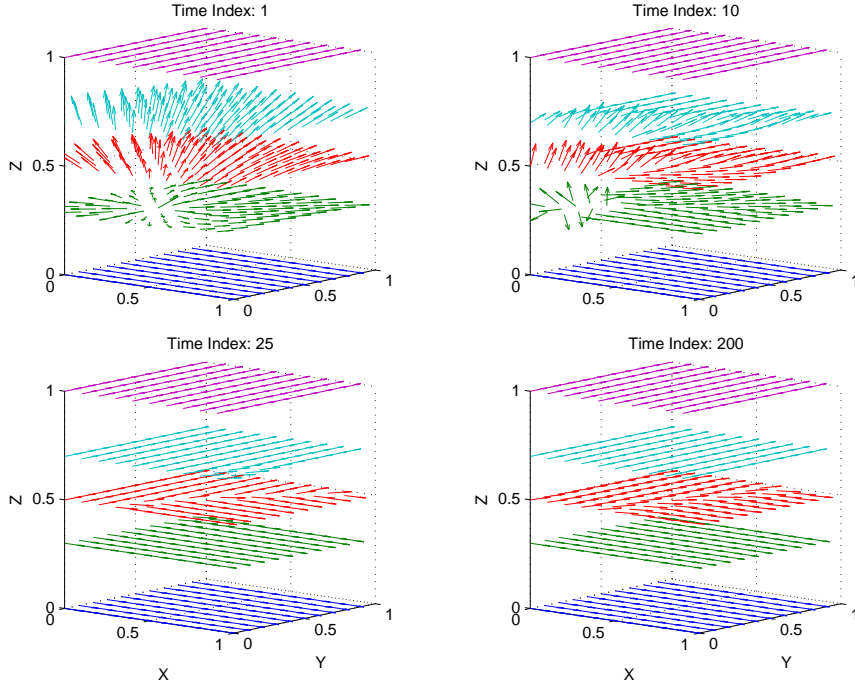


Figure 1: Evolution toward an (equilibrium) plane defect (Section 3). The director field \mathbf{n} is shown at five different horizontal slices. The time step used was $\delta t = 0.02$.

an exact solution found in [27, Sec. 6.4]. We set $\kappa = 0.2$ and *remove* the double well potential.

The following Dirichlet boundary conditions on $\overline{\partial\Omega} \cap (\{z = 0\} \cup \{z = 1\})$ are imposed for s and \mathbf{n} :

$$\begin{aligned} z = 0 : \quad s &= s^*, & \mathbf{n} &= (1, 0, 0), \\ z = 1 : \quad s &= s^*, & \mathbf{n} &= (0, 1, 0), \end{aligned} \tag{3}$$

where $s^* = 0.750025$, i.e. on the top and bottom faces of the cube, we set s to a fixed constant. We set the director field \mathbf{n} to point in the x (y) direction on the bottom (top) face. On the remaining four sides of the cube, we allow s and \mathbf{n} to vary freely (physically, there is no explicit forcing of the molecule's orientation). Initial conditions on Ω for the gradient flow are: $s = s^*$ and a regularized point defect away from the center of the cube. Figures 1 and 2 show our numerical results.

Figure 1 shows the evolution of the director field \mathbf{n} toward the plane defect. The exact solution corresponds to $\mathbf{n} = (1, 0, 0)$ on the bottom half of the cube $z < 0.5$, $\mathbf{n} = (0, 1, 0)$ on the top half of the cube $z > 0.5$, with a discontinuity at $z = 0.5$. Only a few slices are shown in Figure 1 because of the simple form of the equilibrium solution.

Figure 2 shows the components of \mathbf{n} evaluated along a one dimensional vertical slice. Clearly, the numerical solution approximates the exact solution well, except at the narrow transition region near $z = 0.5$.

4 CONCLUSION

We have presented numerical simulations of liquid crystal equilibrium states which minimize a discrete version of the energy (1). Our method is able to capture minimizers

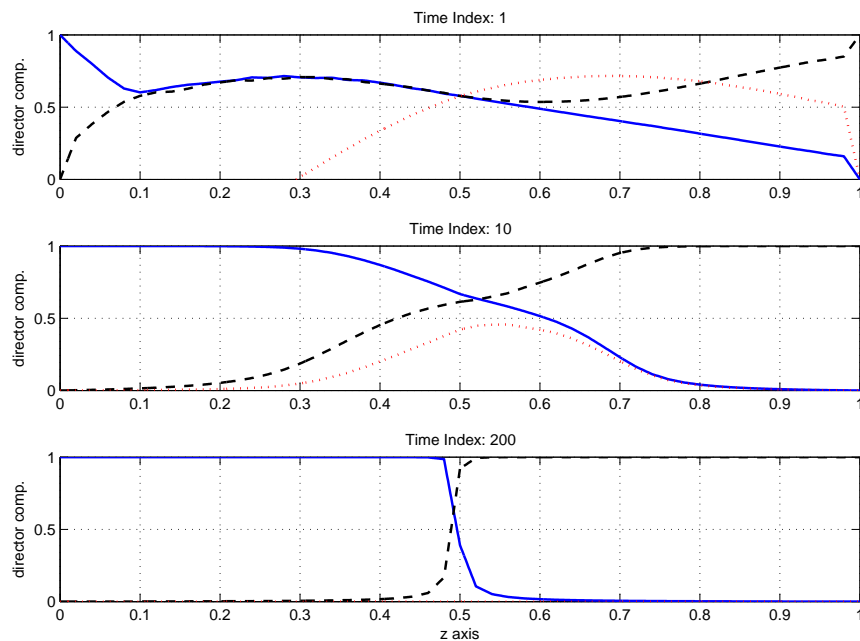


Figure 2: Evolution toward an (equilibrium) plane defect (Section 3). Plots of the three components of \mathbf{n} , evaluated along the vertical line $x = 0.5, y = 0.5$, are shown at three time indices. Legend: x -component of \mathbf{n} is the solid blue curve, y -component of \mathbf{n} is the dashed black curve, z -component of \mathbf{n} is the dotted red curve. One can see that, at equilibrium, \mathbf{n} is nearly piecewise constant with a narrow transition region around $z = 0.5$.

with defects of large dimension and finite energy, and is useful for exploring interesting configurations of liquid crystals. It is not clear at this time how close these configurations are to real structures; this will require further investigation and experiments. One extension of this work is to include external field effects (e.g. electric or magnetic) and see how that may affect the minimizers. Moreover, we could explore how the equilibrium shapes of liquid crystal *droplets* are affected by line and plane defects by including a free interface with surface tension in the problem.

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