Available online at www.sciencedirect.com
ScienceDirect
Journal of Computational Physics 225 (2007) 2069–2082
JOURNAL OF COMPUTATIONAL PHYSICS
www.elsevier.com/locate/jcp

An adaptive homotopy multi-grid method for molecule orientations of high dimensional liquid crystals

Ping Lin [a], Thomas Richter [b,*]

[a] Department of Mathematics, The National University of Singapore, Singapore 117543, Singapore
[b] Department for Aeronautics and Astronautics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA

Received 14 September 2006; accepted 9 March 2007
Available online 24 March 2007

Abstract

The liquid crystal molecule orientation is arranged by minimizing the so-called Oseen–Frank energy functional. For a better understanding of these complicated orientation singularities, simplified models resulting from specific choices of elastic constants are always of interest. In this paper a pseudo Newton method together with a multi-grid linear system solver or preconditioner is used to compute the orientation of liquid crystal molecules based on a simplified Oseen–Frank energy functional. The penalty method is used to deal with the unit-length constraint of liquid crystal molecules. The Newton and multi-grid methods do not converge when some parameters are small. A homotopy algorithm combined with mesh refinement strategies in order to deal with small parameter cases is studied and is found to be very robust in computing the solution of the model. The method is implemented to compute the orientation of liquid crystal molecules in domains of typical shapes and with various rotational boundary conditions in 2D and 3D. Interesting singularity patterns are observed.

MSC: 65H20; 65N55; 65N30; 76A20

Keywords: Multigrid; Homotopy; Liquid crystals; Adaptivity

1. Introduction

Liquid crystals are a phase of matter whose order is intermediate between that of a liquid and that of a crystal. The molecules are typically rod-shaped with a fixed length and their ordering is important to characterize their microstructure. The nematic phase, for example, is characterized by the orientational order of the constituent molecules. Nematics are the most commonly used phase in liquid crystal displays (LCDs), with many such devices using the twisted nematic geometry.

* Corresponding author. Tel.: +1 617 997 7107.
E-mail addresses: matlinp@math.nus.edu.sg (P. Lin), trichter@mit.edu (T. Richter).

0021-9991/$ - see front matter © 2007 Elsevier Inc. All rights reserved.
doi:10.1016/j.jcp.2007.03.009

There is growing interest in the theory of liquid crystals among physicists and mathematicians due to their broad applications. There exists a number of phases in liquid crystals. The study of phases and transition phenomenon between them (e.g. from nematic to smectic-A) is thus an important topic in the theory of liquid crystals (see [10,11]). Classical Oseen–Frank theory (cf. [13]) suggests that the nematic phase of liquid crystals can be described by a director field $\mathbf{n}$, which minimizes the following Oseen–Frank energy functional

$$\mathscr{W}(\mathbf{n}) = \int_\Omega W(\mathbf{n}, \nabla\mathbf{n})\,\mathrm{d}\mathbf{x},$$

where $\Omega \subset \mathbf{R}^i$, $i = 2$ or 3, is a bounded domain occupied by the liquid crystal sample, and

$$W(\mathbf{n}, \nabla\mathbf{n}) = \frac{k_1}{2}|\nabla\cdot\mathbf{n}|^2 + \frac{k_2}{2}|\mathbf{n}\cdot\nabla\times\mathbf{n}|^2 + \frac{k_3}{2}|\mathbf{n}\times\nabla\times\mathbf{n}|^2 + \frac{k_2+k_4}{2}[tr(\nabla\mathbf{n})^2 - (\nabla\cdot\mathbf{n})^2].$$

Here the k_i are elastic constants and $k_1, k_2, k_3 > 0$ are splay, twist and bend constants, respectively. The molecular orientation can be controlled with applied forces on the boundary. So we shall consider Dirichlet boundary conditions. The last term $[tr(\nabla\mathbf{n})^2 - (\nabla\cdot\mathbf{n})^2]$ will be dropped, since it is a divergence term and can be reduced to a surface integral via integration by parts (see [17], Lemma 1.2). So we only need to consider

$$W(\mathbf{n}, \nabla\mathbf{n}) = \frac{k_1}{2}|\nabla\cdot\mathbf{n}|^2 + \frac{k_2}{2}|\mathbf{n}\cdot\nabla\times\mathbf{n}|^2 + \frac{k_3}{2}|\mathbf{n}\times\nabla\times\mathbf{n}|^2. \tag{1}$$

As pointed out in [11] the full form of (1) is still too complex to be of practical use – either because the relative values of the three elastic constants k_i are unknown, or because the equilibrium equations derived from (1) are prohibitively difficult to solve. Indeed, no theoretical analysis has been done to the general Oseen–Frank functional. In such cases, a further simplification based on specific choices of elastic constants is often useful to understand the orientation pattern. There are two typical simplifications. If $k_1 = k_2 = k_3 = 1$ then the Oseen–Frank energy becomes

$$\mathscr{W}(\mathbf{n}) = \frac{1}{2}\int_\Omega |\nabla\mathbf{n}|^2\,\mathrm{d}\mathbf{x}. \tag{2}$$

Together with a fixed length condition, say $|\mathbf{n}| = 1$, the solution is also called harmonic map from a 2D or 3D compact manifold to a 2D circle or 3D sphere, respectively. Some basic numerical results and techniques have been reported in [1,8,9,15]. It is also related to phase field models in dealing with moving interface and image processing problems if changing $\mathbf{n}$ to a scalar phase field variable. There are also other studies on the coupling of the simplified model (2) with flow field in 2D (see, e.g. [12,20,21]). If $k_2 = k_3 = k + k_1$, we can have another simplification

$$\mathscr{W}(\mathbf{n}) = \frac{1}{2}\int_\Omega [k_1|\nabla\mathbf{n}|^2 + k|\nabla\times\mathbf{n}|^2]\,\mathrm{d}\mathbf{x}. \tag{3}$$

Although the assumption on the ratio of parameters k_i may not be quantitatively true in various practical situations, this simpler form of (1) resulting from the assumption is often a valuable tool to reach a qualitative insight into material properties such as molecule orientations. It is expected that, as $k \to \infty$, the asymptotic behavior of minimizers of (3) under suitable boundary conditions will provide a mathematical representation of the phase transition process of liquid crystals from nematic phase to smectic-A phase (see [16,19]). Some mathematical analysis for the limiting case of (3) is discussed in [2,3,17,18,22]. That is why we are particularly interested in considering the limiting case that $k \gg k_1$. It is also very challenging to design appropriate numerical methods in this case since the ellipticity of the operator is largely reduced. Some initial numerical results in simple 2D cases are reported in [14] where the direct method is used to solve the resulting linear system.

In this paper we will focus on the simplified model (3) since not many theoretical and numerical results are available. We will mainly consider three dimensional cases with $k \gg k_1$. In 3D and, in particular, when more nodes are needed due to the orientation singularities there is no hope to use a direct method to solve the linear system resulted from the Newton's iteration of this nonlinear problem. We shall use the multigrid method to solve the linear system or use it as a pre-conditioner for an iterative linear system solver