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Simulations of singularity dynamics in liquid crystal flows: A C^0 finite element approach

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Abstract

In this paper, we present a C^0 finite element method for a 2D hydrodynamic liquid crystal model which is simpler than existing C^1 element methods and mixed element formulation. The energy law is formally justified and the energy decay is used as a validation tool for our numerical computation. A splitting method combined with only a few fixed point iteration for the penalty term of the director field is applied to reduce the size of the stiffness matrix and to keep the stiffness matrix time-independent. The latter avoids solving a linear system at every time step and largely reduces the computational time, especially when direct linear system solvers are used. Our approach is verified by comparing its computational results with those obtained by C^1 elements and by mixed formulation. Through numerical experiments of a few other splittings and explicit–implicit strategies, we recommend a fast and reliable algorithm for this model. A number of examples are computed to demonstrate the algorithm.

MSC: 65M60; 76A15

Keywords: Liquid crystal flow; Finite element approximation; Splitting method

1. Introduction

There are growing interests about the theory and computation of liquid crystals among physicists and mathematicians. Liquid crystal materials not only see many important industrial applications [5,8], they can also be considered to be simple examples of elastic complex fluids. The hydrodynamical and rheological properties of the materials reflect the competition between the kinetic and elastic energies, through the transport of the orientational order parameter. The motivation of this paper is to develop an effective and robust numerical tool to illustrate and investigate such competitions.

Liquid crystal materials do not show a single transition from solid to liquid, but rather a cascade of transitions involving new phases. Classical Oseen–Frank theory suggests that the nematic phase of liquid crystals

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can be described by an orientational order parameter or a director field $\mathbf{d}$, which minimizes so called Oseen–Frank elastic energy functional. The energy dictates the tendency of the orientational director being aligned to each other. This macroscopic orientational order parameter can also be derived through the microscopic kinetic equation as the eigenvector of the second moment [8]. Mathematical analysis and computation for some special cases of Oseen–Frank model may be found in [1,3,4,8,10–13]. To describe liquid crystal flows we need not only the orientation, as represented by the director field $\mathbf{d}$, but also a macroscopic motion, represented by the velocity field $\mathbf{u}$. Ericksen and Leslie derive a hydrodynamic model for nematic liquid crystals. A nematic flow behaves like a regular liquid with molecules of similar size. However, it displays anisotropic properties due to the molecule alignment described by the local director field $\mathbf{d}$. In order to understand Ericksen–Leslie theory from the analysis point of view, Lin and Liu [14] proposed to consider a simplified model which retains most mathematical and physical significance of the original system and at the same time is possible for rigorous analysis. The model also emphasizes the special coupling between the director and the flow field. The model reads

$$\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u} - \nu\nabla\cdot D(\mathbf{u}) + \nabla p + \lambda\nabla\cdot((\nabla\mathbf{d})^{\mathrm{T}}\nabla\mathbf{d}) = 0, \tag{1.1}$$

$$\nabla\cdot\mathbf{u} = 0, \tag{1.2}$$

$$\mathbf{d}_t + (\mathbf{u}\cdot\nabla)\mathbf{d} - \gamma(\Delta\mathbf{d} - \mathbf{f}(\mathbf{d})) = 0 \tag{1.3}$$

with initial and boundary conditions

$$\mathbf{u}|_{t=0} = \mathbf{u}_0, \quad \mathbf{d}|_{t=0} = \mathbf{d}_0, \quad \mathbf{u}|_{\partial\Omega} = \mathbf{u}_0|_{\partial\Omega} = \mathbf{g}_{\mathbf{u}}, \quad \mathbf{d}|_{\partial\Omega} = \mathbf{d}_0|_{\partial\Omega} = \mathbf{g}_{\mathbf{d}}.$$

Here, $\mathbf{u}$ represents the velocity of the liquid crystal flow, p the pressure, and $\mathbf{d}$ the orientation of the liquid crystal molecules, $\mathbf{u}, \mathbf{d}$: $\Omega\times\mathscr{R}^+ \to \mathscr{R}^n$, p: $\Omega\times\mathscr{R}^+ \to \mathscr{R}$ and $\Omega\subset\mathscr{R}^n$. In our computation, we will only consider $n = 2$, i.e. two-dimensional cases. Also, the strain rate $D(\mathbf{u}) = (1/2)(\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}})$, the gradients of the director field take the standard notation as

$$(\nabla\mathbf{d})_{ij} = \mathbf{d}_{i,j} = \frac{\partial d_i}{\partial x_j}$$

and $\mathbf{f}(\mathbf{d}) = (1/\epsilon^2)(—\mathbf{d}|^2 - 1)\mathbf{d}$ is a penalty function used to approximate the constraint $|\mathbf{d}| = 1$ which is due to liquid crystal molecules being of similar size. $\mathbf{f}(\mathbf{d})$ is the gradient of the scalar valued function $F(\mathbf{d}) = (1/4\epsilon^2)(|\mathbf{d}|^2 - 1)^2$. The divergence operator of a matrix is defined as

$$(\nabla\cdot A)_i = a_{ij,j} = \sum_j \frac{\partial a_{ij}}{\partial x_j}.$$

The first equation in the system is the equation for the conservation of linear momentum (the force balance equation). It combines a usual equation describing the flow of an isotropic fluid and an extra nonlinear coupling term which is anisotropic. This extra term is the induced elastic stress from the elastic energy through the transport in the third equation. The second equation represents incompressibility of the liquid. The third equation is associated with conservation of the angular momentum. We want to point out the choice of the transport of the director, $\mathbf{d}_t + (\mathbf{u}\cdot\nabla)\mathbf{d}$, reflects the assumption that the molecule is small and only the transport of the center of the mass is taken into account.

It is expected that the flow velocity will influence the alignment of the molecule $\mathbf{d}$ by the transport of the vector. And the converse is also true, i.e. the change in alignment may induce velocity through the induced elastic stress. Even if the initial velocity is zero the evolution of the director field may induce a velocity (the phenomena having been coined as back-flow), and the velocity may in turn affect the evolution of the director field. Such special coupling makes the theoretical discussion, especially explicit analytical expression of the solutions, rather difficult for this complicated model (as will also be indicated in our later numerical examples). Numerical simulation of these phenomena is then interesting, or even necessary, to researchers in this area.

Some properties of the system of equations may be used to justify the correctness of simulation results. For instance, the director field satisfies the maximum principle, that is, its magnitude will not achieve a maximum