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CONSTRAINT-PRESERVING ENERGY-STABLE SCHEME FOR THE 2D SIMPLIFIED ERICKSEN-LESLIE SYSTEM*

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Abstract

Here we consider the numerical approximations of the 2D simplified Ericksen-Leslie system. We first rewrite the system and get a new system. For the new system, we propose an easy-to-implement time discretization scheme which preserves the sphere constraint at each node, enjoys a discrete energy law, and leads to linear and decoupled elliptic equations to be solved at each time step. A discrete maximum principle of the scheme in the finite element form is also proved. Some numerical simulations are performed to validate the scheme and simulate the dynamic motion of liquid crystals.

Mathematics subject classification: 52B10, 65D18, 68U05, 68U07.
Key words: Nematic liquid crystal, Ericksen-Leslie system, Constraint preserving, Finite element.

1. Introduction

Here we consider the 2D simplified Ericksen-Leslie system which models the hydrodynamics of nematic liquid crystals. The system is a simplified version of the Ericksen-Leslie system introduced by Ericksen [12] and Leslie [20]. Since the full Ericksen-Leslie system is too complicated, Lin [21] proposed this simplified version in 1989. The model is derived as the following coupled system:

$$\mathbf{d}_t + (\mathbf{u}\cdot\nabla)\mathbf{d} = \Delta\mathbf{d} + |\nabla\mathbf{d}|^2\mathbf{d}, \tag{1.1}$$

$$|\mathbf{d}| = 1, \tag{1.2}$$

$$\mathbf{u}_t + \mathbf{u}\cdot\nabla\mathbf{u} + \nabla P = \Delta\mathbf{u} - \nabla\cdot((\nabla\mathbf{d})^T\nabla\mathbf{d}), \tag{1.3}$$

$$\nabla\cdot\mathbf{u} = 0. \tag{1.4}$$

Here, Ω is a bounded domain in $\mathbb{R}^2$, the given time $T > 0$. $\mathbf{u}, \mathbf{d} : \Omega \times [0,T] \to \mathbb{R}^2$ are the fluid velocity and the mean orientation of the molecules respectively, $P : \Omega \times [0,T] \to \mathbb{R}$ is the fluid pressure. Equation (1.3) is the Navier-Stokes equation [31] coupled with the extra term

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$\nabla \cdot ((\nabla \mathbf{d})^T \nabla \mathbf{d})$, and equation (1.1) is the harmonic map heat flow with the convection term $(\mathbf{u} \cdot \nabla)\mathbf{d}$ [25].

We will investigate the system with homogeneous Dirichlet boundary conditions for the velocity field and homogeneous Neumann boundary conditions for the director field:

$$\mathbf{u} = 0, \quad \frac{\partial \mathbf{d}}{\partial \mathbf{n}} = \mathbf{0}, \quad \text{on} \quad \partial\Omega \times (0, T), \tag{1.5}$$

where $\mathbf{n}$ denotes the outer normal vector on the boundary.

The initial conditions are used as follows:

$$\mathbf{d}(\mathbf{x}, 0) = \mathbf{d}_0(\mathbf{x}), \quad \mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), \quad \text{in} \quad \Omega, \tag{1.6}$$

where $\mathbf{u}_0 : \Omega \to \mathbb{R}^2$ satisfying $\nabla \cdot \mathbf{u}_0 = 0$, and $\mathbf{d}_0 : \Omega \to \mathbb{R}^2$ satisfying $|\mathbf{d}_0| = 1$ are given functions. Under the boundary conditions mentioned above, the system (1.1)–(1.4) satisfies the following energy law:

$$\frac{d}{dt}\left(\frac{1}{2}\|\mathbf{u}\|^2 + \frac{1}{2}\|\nabla \mathbf{d}\|^2\right) + \|\nabla \mathbf{u}\|^2 + \|\Delta \mathbf{d} + |\nabla \mathbf{d}|^2 \mathbf{d}\|^2 = 0, \tag{1.7}$$

where $\|\cdot\|$ denotes the L^2 norm in Ω.

It requires that $\mathbf{d}$ must have the unit length, i.e., $|\mathbf{d}| = 1$ almost everywhere. From the numerical point of view, this constraint makes it difficult to manage since we can not imply the sphere constraint at the nodes via interpolation. In addition, the presence of the extra term $\nabla \cdot ((\nabla \mathbf{d})^T \nabla \mathbf{d})$ causes strong coupling [27]. Hence, a penalty function such as the Ginzburg-Landau approximation is widely used to overcome these difficulties [22], and the general penalty version reads as follows:

$$\mathbf{d}_t + (\mathbf{u} \cdot \nabla)\mathbf{d} + \frac{1}{\epsilon^2}\mathbf{f}(\mathbf{d}) - \Delta \mathbf{d} = \mathbf{0}, \tag{1.8}$$

$$\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u} + \nabla P = \Delta \mathbf{u} - \nabla \cdot \Big((\nabla \mathbf{d})^T \nabla \mathbf{d}\Big), \tag{1.9}$$

$$\nabla \cdot \mathbf{u} = 0, \tag{1.10}$$

where $\epsilon > 0$ is the penalty parameter, $\mathbf{f}(\mathbf{d})$ is the Ginzburg-Landau approximation of the constraint $|\mathbf{d}| = 1$ for small ϵ. The penalty function is the gradient of a scalar-valued function $F(\mathbf{d})$, i.e., $\mathbf{f}(\mathbf{d}) = \nabla_{\mathbf{d}} F(\mathbf{d})$, where,

$$F(\mathbf{d}) = \begin{cases} \frac{1}{4}(|\mathbf{d}|^2 - 1)^2, & \text{if } |\mathbf{d}| \leqslant 1, \\ (|\mathbf{d}|^2 - 1)^2, & \text{if } |\mathbf{d}| > 1. \end{cases} \tag{1.11}$$

It is still an open problem that whether weak solutions $(\mathbf{u}_\epsilon, \mathbf{d}_\epsilon)$ of the system (1.8)–(1.10) with Dirichlet boundary conditions weakly converge to that of the system (1.1)–(1.4) as $\epsilon \to 0$ [27]. It has been proved that, up to a subsequence, $(\mathbf{u}_\epsilon, \mathbf{d}_\epsilon)$ weakly converge to $(\mathbf{u}, \mathbf{d})$ which satisfies a system the same as (1.1)–(1.4) except for an additional measure-valued tensor in the equation (1.3) [24].

In [22], Lin and Liu proved the global existence of the solution of (1.8)–(1.10) with Dirichlet boundary conditions in the dimension two and three. Later, Lin and Liu in [23] proved partial regularity of weak solutions to the system in the dimension three. Since the Ericksen-Leslie system with $|\mathbf{d}| = 1$ is complicated, it was a challenging problem to prove global existence of