First-Order, Unconditionally Stable, Fully Decoupled Methods for the Penalty Ericksen-Leslie System with Variable Density

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Abstract. In this paper, we propose two first-order, unconditionally stable, fully decoupled methods based on the Gauge-Uzawa method for solving the penalty Ericksen-Leslie system with variable density. The first method is based on the scalar auxiliary variable method for explicitly handling the nonlinear part, and the Gauge-Uzawa method for decoupling the velocity and pressure. The second method is formulated by introducing an auxiliary intermediate velocity variable for decoupling the director field computation from the velocity field, and then combining it with the Gauge-Uzawa method and the convex splitting method. Thus, two highly efficient, fully decoupled schemes are built. Furthermore, we use the finite element method to give an efficient implementation of the schemes. Then, we prove that both two schemes are unconditionally stable. Finally, numerical examples are provided to verify the convergence rate, unconditional stability, and computational efficiency. The proposed methods also provide a solution for establishing numerical schemes for other highly nonlinear variable-density coupled systems.

AMS subject classifications: 65N12, 65N30

Key words: Ericksen-Leslie, fully decoupled, unconditionally stable, variable density, Gauge-Uzawa method.

1 Introduction

This paper focuses on the numerical approximation of the two-dimensional penalty Ericksen-Leslie system with variable density [1, 2], which provides a phenomenological description of the hydrodynamics of nematic liquid crystals from a macroscopic point

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of view [3–6]. The governing equations are as follows

$$\rho_t + \nabla \cdot (\rho \mathbf{u}) = 0 \qquad \text{in } \Omega_T, \tag{1.1a}$$

$$\rho(\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u}) + \nabla p - \mu \triangle \mathbf{u} - \lambda (\nabla \mathbf{d})^t \mathbf{w} = 0 \qquad \text{in } \Omega_T, \tag{1.1b}$$

$$\mathbf{d}_t + \mathbf{u} \cdot \nabla \mathbf{d} + \gamma \mathbf{w} = \mathbf{0} \qquad \text{in } \Omega_T, \qquad (1.1c)$$

$$-\Delta \mathbf{d} + f(\mathbf{d}) - \mathbf{w} = \mathbf{0} \qquad \text{in } \Omega_T, \qquad (1.1d)$$

$$\nabla \cdot \mathbf{u} = 0 \qquad \text{in } \Omega_T. \tag{1.1e}$$

Here, $\Omega_T = \Omega \times (0,T]$, where Ω is a bounded open subset of \mathbb{R}^2 with smooth boundary $\partial \Omega$, and T > 0 is the final time. The parameter $\gamma > 0$ is a relaxation time constant, $\mu > 0$ is a constant depending on the fluid viscosity, and $\lambda > 0$ is an elasticity constant. $\mathbf{d}: \Omega_T \to \mathbb{R}^2$ is the orientation of the molecules, $\mathbf{w}: \Omega_T \to \mathbb{R}^2$ is a chemical potential, $\mathbf{u}: \Omega_T \to \mathbb{R}^2$ is the fluid velocity, and $p: \Omega_T \to \mathbb{R}$ is the fluid pressure. Moreover, $(\nabla \mathbf{d})^t$ denotes the transposed matrix of $\nabla \mathbf{d} = (\partial_j \mathbf{d}_i)_{i,j}$. $f(\mathbf{d})$ is the penalty function related to the constraint $|\mathbf{d}| = 1$. Its specific form is as follows

$$f(\mathbf{d}) = \frac{1}{\varepsilon^2} (|\mathbf{d}|^2 - 1) \mathbf{d},$$

where $\varepsilon > 0$ is the penalty parameter. It is easy to see that f is the gradient of the Ginzburg–Landau potential

$$F(\mathbf{d}) = \frac{1}{4\varepsilon^2} (|\mathbf{d}|^2 - 1)^2,$$

that is, $f(\mathbf{d}) = \nabla_{\mathbf{d}} F(\mathbf{d})$ for all \mathbf{d} .

Next, we provide the boundary and initial conditions for the system (1.1)

$$\begin{cases} \mathbf{u}(x,0) = \mathbf{u}_0(x), & \mathbf{u}(x,t)|_{\Gamma} = \mathbf{g}, \\ \rho(x,0) = \rho_0(x), & \rho(x,t)|_{\Gamma_{in}} = a(x,t), \\ \mathbf{d}(x,0) = \mathbf{d}_0(x), & \partial_{\mathbf{n}} \mathbf{d}(x,t) = \mathbf{0}. \end{cases}$$

Here, $\Gamma = \partial \Omega$ is boundary of Ω . Γ_{in} represents the inflow boundary, which is defined as $\Gamma_{in} = \{x \in \Gamma : \mathbf{g} \cdot \mathbf{n} < 0\}$. \mathbf{n} represents the outward unit normal vector on boundary Γ . For simplicity, as shown in [7], we see the boundary as impermeable, i.e., $\Gamma_{in} = \emptyset$ and $\mathbf{g} = 0$. ρ_0 is the initial value of ρ , which is bounded and away from zero. There exist two constants $\rho_{\min}^0 > 0$ and $\rho_{\max}^0 > 0$ such that

$$\rho_{\min}^0 \le \rho_0(x) \le \rho_{\max}^0 \quad \text{in } \Omega, \tag{1.2}$$

which implies that the system is not in a vacuum state within Ω . The initial values \mathbf{d}_0 and \mathbf{u}_0 satisfy the compatibility condition $|\mathbf{d}_0| = 1$ and $\nabla \cdot \mathbf{u}_0 = 0$.

In recent years, there has been a great interest in the numerical approximation of liquid crystal flows. The reason for this is that liquid crystals are limited by geometrical boundary conditions, which cannot be easily studied from experimental observations.