Advances in Applied Mathematics and Mechanics
Adv. Appl. Math. Mech., Vol. **16**, No. 4, pp. 952-979

DOI: 10.4208/aamm.OA-2023-0121
August 2024

Error Analysis of a Pressure Penalty Scheme for the Reformulated Ericksen-Leslie System with Variable Density

Xin Zhang[1], Danxia Wang[1,2,*], Jianwen Zhang[1,2] and Hongen Jia[1,2]

[1] *School of Mathematics, Taiyuan University of Technology, Jinzhong, Shanxi 030600, China*
[2] *Shanxi Key Laboratory for Intelligent Optimization Computing and Blockchain Technology, Taiyuan, Shanxi 030024, China*

Received 28 April 2023; Accepted (in revised version) 4 June 2023

Abstract. Numerical approximation of the Ericksen-Leslie system with variable density is considered in this paper. The spherical constraint condition of the orientation field is preserved by using polar coordinates to reformulate the system. The equivalent new system is computationally cheaper because the vector function of the orientation field is replaced by a scalar function. An iteration penalty method is applied to construct a numerical scheme so that stability is improved. We first prove that the scheme is uniquely solvable and unconditionally stable in energy. Then we show that this scheme is of first-order convergence rate by rigorous error estimation. Finally, some numerical simulations are performed to illustrate the accuracy and effectiveness of the scheme.

AMS subject classifications: 65M12, 65M60
Key words: Variable density, constraint-preserving, Ericksen-Leslie, error analysis.

1 Introduction

In recent years, more and more scholars are interested in the theory of liquid crystals. Liquid crystals are materials that show the intermediate phase between solid and liquid. This implies that liquid crystals conjoin the characteristics of both solids and isotropic liquids. Nematic is the simplest phase of liquid crystals. In this case, molecules are provided with ordered orientation, but disordered in position configuration. In the 1960s, Ericksen [9] and Leslie [18] first introduced the Ericksen-Leslie system, which models the hydrodynamics of nematic liquid crystals. Under the influence of flow velocity and

*Corresponding author.
Email: 2621259544@qq.com (D. Wang)

microscopic orientation configurations, this system describes the macroscopic temporal evolution of liquid crystal materials.

Lin [21] proposed a simplified version because the original Ericksen-Leslie system is too complicated. Major mathematical difficulties remain, although the simplified version ignores the Leslie tension. This system consists of a Navier-Stokes equation [29] coupled with the extra term $\nabla\cdot(\nabla\mathbf{d}\odot\nabla\mathbf{d})$ and a harmonic map heat flow with the convection term $(\mathbf{u}\cdot\nabla)\mathbf{d}$ [22], read as:

$$\mathbf{u}_t+\mathbf{u}\cdot\nabla\mathbf{u}+\nabla P-\mu\Delta\mathbf{u}+\nabla\cdot(\nabla\mathbf{d}\odot\nabla\mathbf{d})=0, \tag{1.1a}$$

$$\mathbf{d}_t+(\mathbf{u}\cdot\nabla)\mathbf{d}-\Delta\mathbf{d}-|\nabla\mathbf{d}|^2\mathbf{d}=0, \tag{1.1b}$$

$$|\mathbf{d}|=1, \tag{1.1c}$$

$$\nabla\cdot\mathbf{u}=0, \tag{1.1d}$$

where $\mathbf{u}$, $\mathbf{d}$ and P are the fluid velocity, the mean orientation of the molecules and the fluid pressure, respectively. Coefficient μ of $\Delta\mathbf{u}$ represents the viscosity of the fluid. Some descriptions of operators in this system are given as follows. The gradient operator $\nabla\mathbf{u}=(\partial_j u_i)_{i,j}$; the Laplacian operator $\Delta\mathbf{u}=\sum_{i=1}^{M}\partial_{ii}\mathbf{u}$; the convective operator $(\mathbf{u}\cdot\nabla)\mathbf{d}=\sum_{i=1}^{M}u_i\partial_i\mathbf{d}$. Moreover, $|\mathbf{d}|$ is the Euclidean norm in $\mathbf{R}^M$. The term $\nabla\mathbf{d}\odot\nabla\mathbf{d}$ is a 2×2 matrix whose (i,j)-the entry is given by $(\nabla_i\mathbf{d})\cdot(\nabla_j\mathbf{d})$. Henceforth, we denote

$$\nabla\mathbf{d}\odot\nabla\mathbf{d}=(\nabla\mathbf{d})^T\nabla\mathbf{d},$$

where $(\nabla\mathbf{d})^T$ denotes the transpose of $\nabla\mathbf{d}$.

For the system (1.1), Lin et al. [26] proposed a C_0 finite element scheme for simulating the kinematic effects in liquid crystal dynamics. To obtain a flow equation without $\Delta\mathbf{d}$, they reformulated the flow equation by using the orientation field equation. In addition, they proved the discrete energy law. An and Su [3] investigated the time-dependent nematic liquid crystal flows by semi-implicit Galerkin method. They showed the temporal and the spatial error estimates. We refer the reader to [4, 13] and reference therein.

There are two main difficulties in studying the system (1.1). The spherical constraint condition $|\mathbf{d}|=1$ is difficult to implement at the discrete level. Specifically, we can not imply the spherical constraint at nodes by interpolation. Moreover, the extra term $\nabla\cdot((\nabla\mathbf{d})^T\nabla\mathbf{d})$ causes strong coupling. Therefore, a Ginzburg-Landau penalty method is proposed to overcome the difficulty of $|\mathbf{d}|=1$ [23]. By introducing a Ginzburg-Landau penalty function $\frac{1}{\epsilon^2}\mathbf{f}(\mathbf{d})$ to replace $|\nabla\mathbf{d}|^2\mathbf{d}$, the constraint $|\mathbf{d}|=1$ is relaxed. The general penalty version reads as follows:

$$\mathbf{u}_t+\mathbf{u}\cdot\nabla\mathbf{u}+\nabla P=\mu\Delta\mathbf{u}-\nabla\cdot((\nabla\mathbf{d}^T)\nabla\mathbf{d}), \tag{1.2a}$$

$$\mathbf{d}_t+(\mathbf{u}\cdot\nabla)\mathbf{d}+\frac{1}{\epsilon^2}\mathbf{f}(\mathbf{d})-\Delta\mathbf{d}=0, \tag{1.2b}$$

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