INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 18, Number 6, Pages 811–833

A FULLY DISCRETE, DECOUPLED SCHEME WITH DIFFERENT TIME STEPS FOR APPROXIMATING NEMATIC LIQUID CRYSTAL FLOW

TING LI, PENGZHAN HUANG*, AND YINNIAN HE

Abstract. This paper designs a decoupled scheme for approximating nematic liquid crystal flow based on a fully discrete mixed finite element method, which allows different time steps for different physical fields. Besides, error estimates for velocity and macroscopic molecular orientation of the nematic liquid crystal flow are shown. Finally, numerical tests are provided to demonstrate efficiency of the scheme. It is found the presented scheme can save lots of computational time compared with common decoupled scheme.

Key words. Nematic liquid crystal flow, decoupled scheme, different time steps, error estimates.

1. Introduction

Liquid crystal is usually known as the fourth state of matter and is different to gas, liquid and solid. The simplest liquid crystal phase is the nematic liquid crystal. It is consisted of elongated rod-like molecules with similar size. The centers of mass of these molecules have no positional order, but tend to align along preferred direction. In recent decades, many studies are dealing with the nematic liquid crystal, due to the importance of related scientific and, engineering applications [2].

Ericksen-Leslie model, built by Ericksen [9, 10] and Leslie [18], can simulate the hydrodynamics of the nematic liquid crystal flow, and it is the macroscopic continuum description of the time evolution of both flow velocity and microscopic orientation. Further, a simplified Ericksen-Leslie model is derived by Lin [22] initially and its governing equations are written as follows [22, 1]:

$$\begin{aligned} &\mathbf{u}_t - \nu\Delta\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p + \lambda\nabla\cdot(\nabla\mathbf{d}\odot\nabla\mathbf{d}) = \mathbf{f},\\ &\mathbf{d}_t - \gamma\Delta\mathbf{d} + (\mathbf{u}\cdot\nabla)\mathbf{d} = \gamma|\nabla\mathbf{d}|^2\mathbf{d},\\ &\nabla\cdot\mathbf{u} = 0,\ |\mathbf{d}| = 1, \end{aligned} \tag{1}$$

for $(\mathbf{x},t)\in Q_T$, where $Q_T=\Omega\times(0,T)$ with a fixed $T\in(0,\infty)$. Here, $\mathbf{u}(\mathbf{x},t):Q_T\to\mathbb{R}^2$ and $p(\mathbf{x},t):Q_T\to\mathbb{R}$ denote the velocity field and the pressure of the flow, respectively. Besides, $\mathbf{d}(\mathbf{x},t):Q_T\to\mathbb{S}$ is the director, which represents the molecular orientation field of the nematic liquid crystal material and describes the average molecular alignment, where $\mathbb{S}\subset\mathbb{R}^2$ is a unit circle. In addition, $\mathbf{f}(\mathbf{x},t):Q_T\to\mathbb{R}^2$ represents a body force on the flow. Three parameters ν, λ and γ denote the kinematic viscosity, the competition between kinetic and potential energy, and the microscopic elastic relaxation time for the molecular orientation field, respectively. Hereafter, $|\nabla\mathbf{d}|$ or $|\mathbf{d}|$ denotes the Euclidean norm of $\nabla\mathbf{d}$ or $\mathbf{d}$, and $\nabla\mathbf{d}\odot\nabla\mathbf{d}$ is a 2×2 matrix whose (i,j)-the entry is written by $(\sum_{k=1}^{2}\frac{\partial d_k}{\partial x_i}\frac{\partial d_k}{\partial x_j})_{i,j}$. As in [1], in

Received by the editors July 10, 2020 and, in revised form, May 31, 2021.
2000 *Mathematics Subject Classification.* 65M60, 76A15, 76D05.
*Corresponding author.

this paper the system (1) is considered in conjunction with the following initial and boundary conditions:

$$\begin{aligned} &\mathbf{u}(\mathbf{x},0)=\mathbf{u}_0(\mathbf{x}), \quad \mathbf{d}(\mathbf{x},0)=\mathbf{d}_0(\mathbf{x}),\ \forall \mathbf{x}\in\Omega, \\ &\mathbf{u}|_{S_T}=0, \quad \partial_{\mathbf{n}}\mathbf{d}|_{S_T}=0, \end{aligned} \tag{2}$$

with $\nabla\cdot\mathbf{u}_0=0$ and $|\mathbf{d}_0|=1$, where $S_T=\partial\Omega\times(0,T)$ and $\mathbf{n}$ is the outer unit normal of $\partial\Omega$.

Although this simplified Ericksen-Leslie model neglects the Leslie stress in the Ericksen-Leslie model, it still retains some essential difficulties of the Ericksen-Leslie model and keeps the core of the mathematical structure, such as strong nonlinearities and constraints, as well as the physical structure, such as the anisotropic effect of the elasticity on the velocity field. Thus, the system (1)-(2) can be regarded as a nice initial step towards the theoretical and numerical analysis of the Ericksen-Leslie model.

Because the governing equations (1)-(2) of the simplified Ericksen-Leslie model include not only the incompressibility, the strong nonlinearity and the physical and nonconvex side constraint $|\mathbf{d}|=1$ but also the coupling between the harmonic map flow and the fluid equations of motion, which make it not easy to solve these equations effectively. Therefore, much effort has been throwing to the development of some efficient numerical methods for investigating this system [13, 6, 7, 27, 19, 16] and the references therein. Besides, Du et al. [8] have studied a Fourier-spectral method for the simplified Ericksen-Leslie system and established spectral accuracy. In [12], a linear fully discrete mixed scheme has been considered, using finite element method in space and a semi-implicit Euler scheme in time. In addition, Becker et al. [3] have constructed a fully discrete scheme, which uses low order finite elements and enjoys a discrete energy law. Based on explicit treatment of the unitary constraint for the director field, a fully splitting and decoupled in time linear algorithm has been designed [14]. Recently, An and Su [1] have shown optimal error estimates for an linearized semi-implicit Euler finite element scheme for the considered system.

In this paper, we design a fully discrete, decoupled finite element scheme for approximating the simplified Ericksen-Lesliel system (1)-(2). Since the system has many physical fields and is a multiphysics problem, we adopt different time step sizes for different physical fields. In fact, Ge and Ma [11] have proposed a multirate iterative scheme based on multiphysics discontinuous Galerkin method for a poroelasticity model, which is a fluid-solid interaction system at pore scale. Shi et al. [26, 25] have designed a multistep technique to overcome the instability mainly caused by the explicit treatment of the convection system and to enlarge the stability region such that the resulting scheme behaved like an unconditionally stable scheme. Besides, the differing time steps methods have been applied to the Stokes-Darcy model [24], the Navier-Stokes/Darcy model [17] and the Darcy-Brinkman problem [21].

2. A decoupled scheme with different time steps for the nematic liquid crystal flow

In this section, we describe some necessary definitions and inequalities, which will be frequently applied to following sections.

Firstly, we introduce standard notations for Lebesgue space $L^p(\Omega)$ and Sobolve space $W^{m,p}(\Omega)$, $1\le p\le\infty$, $m\in\mathbb{N}^+$. Then, their norms are denoted by $\|\cdot\|_{L^p(\Omega)}$ and $\|\cdot\|_{W^{m,p}(\Omega)}$, respectively. In particular, $H^m(\Omega)$ is used to represent the space $W^{m,2}(\Omega)$ and $\|\cdot\|_m$ denotes the norm in $H^m(\Omega)$. Besides, $L^2(\Omega)$ norm and its