ENERGY STABLE NUMERICAL SCHEMES FOR A HYDRODYNAMIC MODEL OF NEMATIC LIQUID CRYSTALS∗

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Abstract. We develop a first-order and a second-order, coupled, energy stable numerical schemes for a modified Ericksen–Leslie hydrodynamic model for nematic liquid crystals. We then discuss two ways to develop decoupled schemes for the model and show that they are energy stable as well. The coupled schemes are implemented in 2-dimensional space, with which we study defect dynamics in flows of nematic liquid crystals. Comparisons of our model predictions with that of a reduced model previously studied, which used the material derivative in place of the time invariant derivative in the Ericksen–Leslie model, are made, demonstrating quite different, but more realistic orientational dynamics in flows of nematic liquid crystals.

Key words. liquid crystals, energy stable schemes, finite difference, hydrodynamics, phase field theory

AMS subject classifications. 65M06, 65M12, 65Z05

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1. Introduction. The liquid crystal is an intermediate phase between the conventional liquid and solid. For instance, a liquid crystal can flow like a liquid, but due to its anisotropic microstructures, it also exhibits a partial order in the mesoscopic scale normally observed in a solid phase. One of the simple phases of liquid crystals is the nematic phase, where the calamitic or rod-shaped molecules have no positional order, but demonstrate a long-range orientational order formed by their long axes. Readers are referred to [19] for a review on dynamic phenomena in liquid crystal materials.

One of the most well-known continuum theories for flows of liquid crystals is the Ericksen–Leslie theory. The hydrodynamic theory for liquid crystals by Ericksen and Leslie dates back to 1960s [6, 7, 8, 14]. In this theory, an order parameter, a unit vector known as the director field \( \mathbf{d} \), is employed to describe the nematic order in space and time. Given an open and bounded domain \( \Omega \in \mathbb{R}^d \) (\( d \) is the dimension, equal to 2 or 3) with smooth boundary \( \partial \Omega \), we define \( \Omega_T = (0, T) \times \Omega \). For any \( (x, t) \in \Omega_T \), we summarize the dimensionless governing system of equations in the

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Ericksen–Leslie model with the one constant approximation as follows [3, 5]:

\[
\begin{aligned}
\partial_t u + u \cdot \nabla u &= -\nabla p + \eta \Delta u + \nabla \cdot \left( -\frac{a}{2}(dh + hd) + \frac{1}{2}(dh - hd) \right) - h \nabla d, \\
\nabla \cdot u &= 0, \\
\partial_t d + u \cdot \nabla d - W \cdot d - a(D \cdot d - d d d) &= M(h + |\nabla d|^2 d), \\
|d| &= 1, \quad h = \Delta d,
\end{aligned}
\]

where \( D_{\alpha \beta} = \frac{1}{2}(\partial_{\beta} u_{\alpha} + \partial_{\alpha} u_{\beta}) \) is the rate of strain tensor, \( W_{\alpha \beta} = \frac{1}{2}(\partial_{\beta} u_{\alpha} - \partial_{\alpha} u_{\beta}) \) is the vorticity tensor, \( p \) is the hydrostatic pressure, \( a \) is a geometry parameter of liquid crystal molecules, \( M \) is a dimensionless parameter proportional to the reciprocal of the Ericksen number, and \( \eta \) is the dimensionless parameter for viscosity. However, due to the nonconvex constraint \(|d| = 1\), one experiences many problems in either the numerical analysis or algorithmic design. A penalty term can be added to enforce the constraint \(|d| = 1\) softly via a potential, which leads to the modified Ericksen–Leslie model:

\[
\begin{aligned}
\partial_t u + u \cdot \nabla u &= -\nabla p + \eta \Delta u + \nabla \cdot \left( -\frac{a}{2}(dh + hd) + \frac{1}{2}(dh - hd) \right) - h \nabla d, \\
\nabla \cdot u &= 0, \\
\partial_t d + u \cdot \nabla d - W \cdot d - aD \cdot d &= Mh, \\
\h &= \Delta d - \frac{1}{\varepsilon}(|d|^2 - 1)d.
\end{aligned}
\]

Readers are referred to [15] for a survey on recent progress on the existence, regularity, uniqueness, and large time asymptotic behavior in flows of nematic liquid crystals. Some analytical results of the Ericksen–Leslie model are given in [24], where they studied the asymptotic behavior of global classical solutions of the hydrodynamic system. The regularity and existence of global solutions of the Ericksen–Leslie system in \( \mathbb{R}^2 \) are studied in [11]. The modified Ericksen–Leslie model has been extended to study mixtures of liquid crystals and viscous fluids [31, 32, 33] as well as some biological phenomena [12].

In numerical analysis, an overview of the most recent numerical development in the field of nematic liquid crystals can be found in [1]. Liu and Walkington developed a mixed method in [17] for a simplified Ericksen–Leslie model, which we refer to as the reduced model in this paper in the following. A finite element approximation was discussed in [2] for a similar model. We notice that all the current numerical analyses are based on the assumption that the elastic stress in the liquid crystal system given by \((-\frac{a}{2}(dh + hd) + \frac{1}{2}(dh - hd))\) in the momentum equation and the key component of the time invariant derivative consisting of the term \(-W \cdot d - aD \cdot d\) in the transport equation of \( d \) were neglected for technical convenience, which led to a much simpler model. With the omission of the key terms, the Ericksen–Leslie model (1.1) reduces to

\[
\begin{aligned}
\partial_t u + u \cdot \nabla u &= -\nabla p + \eta \Delta u - h \nabla d, \\
\nabla \cdot u &= 0, \\
\partial_t d + u \cdot \nabla d &= Mh, \\
|d| &= 1, \quad h = \Delta d + |\nabla d|^2 d,
\end{aligned}
\]
and the modified Ericksen–Leslie model (1.2) reduces to

\[
\begin{aligned}
\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} &= -\nabla p + \eta \Delta \mathbf{u} - h \nabla d, \\
\nabla \cdot \mathbf{u} &= 0, \\
\partial_t d + \mathbf{u} \cdot \nabla d &= Mh, \\
h &= \Delta d - \frac{1}{\varepsilon^2}(|d|^2 - 1)d.
\end{aligned}
\]  

(1.4)

Apparently, the reduced models are physically incorrect for flows of liquid crystals since they do not obey the frame-invariant principle nor include the elastic stress in the liquid crystal flow system. One may argue that the reduced models may be acceptable when the velocity gradient is small and the elastic stress is weak at the same time. But, in general, these two effects can rarely be weak simultaneously. Hence, the reduced models have very limited applicability to real liquid crystal flows. As we will show at the end of this paper, the reduced models and the full model predict quite different orientational dynamics in liquid crystal flows, revealing the fallout of using an incorrect time invariant derivative and omitting the elastic stress in the model.

It is common sense in continuum mechanics that time derivatives of any internal variables must be frame indifferent or invariant with respect to translation and rigid body rotation. For instance, the invariant time derivative of the director vector \( \mathbf{d} \) must contain two parts: the part transporting the center of mass (\( \partial_t \mathbf{d} + \mathbf{v} \cdot \nabla \mathbf{d} \), material derivative) and the part rotating the vector due to the fluid vorticity (\( -\mathbf{W} \cdot \mathbf{d} \)). In addition, if we consider the kinematic change (stretching or compressing of the molecule due to the flow), we must add the extra term (\( -a \mathbf{D} \cdot \mathbf{d} \)) for a flexible/extensible molecule or (\( -a \mathbf{D} \cdot \mathbf{d} + a \mathbf{D} : \mathbf{d} \mathbf{d} \)) for rigid molecule. In short, the two pairs of models (\((1.1) \text{ and } (1.3)\)) and (\((1.2) \text{ and } (1.4)\)) indeed describe different physics due to different equation components. There have been some rare studies that demonstrate the difference numerically (see references in [16, 29]). However, that seemed to have not deterred people from using the reduced models to predict liquid crystal flow behavior even today.

This motivates us to bring this critical issue up again for awareness. In this paper, we design several semidiscrete, energy stable, numerical schemes for the modified Ericksen–Leslie model (1.2) to study flows of liquid crystals. These energy stable schemes include both fully coupled and decoupled ones. We then use one of the fully coupled schemes to study defect dynamics in liquid crystal flows and to make a comparison between the full model and the reduced ones mentioned above. These new numerical methods demonstrate how to numerically treat the time invariant derivatives in the transport equation of the director field \( \mathbf{d} \) and the corresponding elastic stress in the momentum balance equation consistently, enabling one to use the correct hydrodynamic model to study flows of liquid crystals in the future.

The rest of the paper is organized as follows. In section 2, we briefly discuss the modified Ericksen–Leslie model and show its energy dissipation property. In section 3, we present several semidiscrete numerical schemes for the model and prove their energy stability. In section 4, we conduct several numerical studies on the mesh-refinement test to confirm the numerical accuracy and defect dynamics of liquid crystals. We then conclude in the last section.

In this section, we briefly discuss the modified Ericksen–Leslie model with a penalty term (1.2) and show its energy dissipation property. Notice that this model is derived
using a variational approach coupled with the Onsager theory for dissipative systems [27, 28]. So, an energy dissipation is expected. For simplicity, we will work with the model in its dimensionless form.

We use \( \mathcal{E} \) to denote the sum of the kinetic and Helmholtz free energy, which we term as the total energy in this paper,

\[
\mathcal{E} = E_{\text{kin}} + E,
\]

where \( E_{\text{kin}} \) is the kinetic energy and \( E \) is the free energy, given, respectively, by

\[
E_{\text{kin}} = \int_{\Omega} \frac{1}{2} |\mathbf{u}|^2 d\mathbf{x}, \quad E = \int_{\Omega} \left( \frac{1}{2} |\nabla d|^2 + g(d) \right) d\mathbf{x}.
\]

More precisely, it should be identified as the total free energy. Here \( g(d) = \frac{1}{4\varepsilon^2}(|d|^2 - 1)^2 \) is the Landau–De Gennes bulk energy with a model parameter \( \varepsilon \) measuring the size of the defect core. Intuitively, \( g(d) \) penalizes any departure of \( d \) from a unit vector while resuming a maximum value at the potential defect where \( d = 0 \).

The governing equations in the modified Ericksen–Leslie model consist of the following:

\[
\begin{align*}
\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} &= -\nabla p + \eta \Delta \mathbf{u} + \nabla \cdot \left( -\frac{\mathbf{g}}{2}(\mathbf{h}^2 + \mathbf{hd}) + \frac{\gamma}{2}(\mathbf{d}^2 - \mathbf{hd}) \right) - \mathbf{h} \nabla d, \\
\nabla \cdot \mathbf{u} &= 0, \\
\partial_t d + \mathbf{u} \cdot \nabla d - \mathbf{W} \cdot d - aD \cdot d &= M h,
\end{align*}
\]

where \( h \) is the molecular field given by

\[
h = \frac{\delta E}{\delta d} = \Delta d - \nabla d g(d).
\]

Consistent with no energy generation or dissipation at the boundary, we assume the following boundary conditions at the fixed boundary \( \partial \Omega \):

\[
\begin{align*}
\mathbf{u} |_{\partial \Omega} &= 0, \\
\mathbf{n} \cdot \nabla d |_{\partial \Omega} &= 0,
\end{align*}
\]

where \( \mathbf{n} \) is the unit outward normal of the domain \( \Omega \).

We remark that the theorems that we will prove in this paper are valid for both the physical boundary conditions listed above as well as the periodic boundary condition. It is easy to show the energy dissipation law of the modified Ericksen–Leslie model.

**Theorem 2.1 (continuous energy dissipation law).** Model (2.3) with boundary condition (2.5) satisfies the following energy dissipation law

\[
\frac{d\mathcal{E}}{dt} = -\int_{\Omega} (\eta |\nabla \mathbf{u}|^2 + M |h|^2) d\mathbf{x}.
\]

**Proof.** The time rate change of the total energy is calculated as follows:

\[
\frac{d\mathcal{E}}{dt} = \frac{dE_{\text{kin}}}{dt} + \frac{dE}{dt} = \int_{\Omega} \mathbf{x} \left[ \frac{\delta E_{\text{kin}}}{\delta \mathbf{u}} \frac{\partial \mathbf{u}}{\partial t} + \frac{\delta E}{\delta \mathbf{d}} \frac{\partial \mathbf{d}}{\partial t} \right] = \int_{\Omega} \mathbf{x} \left[ \mathbf{u} \frac{\partial \mathbf{u}}{\partial t} - \mathbf{h} \frac{\partial \mathbf{d}}{\partial t} \right].
\]
From (2.3), it follows that

\begin{align}
\partial_t u &= -u \cdot \nabla u - \nabla p + \nabla \cdot \left( -\frac{\eta}{2} (dh + hd) + \frac{1}{2} (dh - hd) \right) - h \nabla d, \\
\partial_t d &= -u \cdot \nabla d + W \cdot d + aD \cdot d + Mh. 
\end{align}

Therefore, substituting (2.8) into (2.7), we obtain

\begin{align}
\frac{d\mathcal{E}}{dt} &= \int_\Omega d x \left[ u \left( -u \cdot \nabla u - \nabla p + \nabla \cdot \left( -\frac{a}{2} (dh + hd) + \frac{1}{2} (dh - hd) \right) \right) \\
&\quad - h \left( -u \cdot \nabla d + W \cdot d + aD \cdot d + Mh \right) \\
&= \int_\Omega d x \left[ -\nabla \cdot \left( \frac{|u|^2}{2} \right) + \frac{|u|^2}{2} \nabla \cdot u - \nabla \cdot (pu) + p \nabla \cdot u + \nabla \cdot (\eta u \nabla u) - \eta |\nabla u|^2 \\
&\quad + \nabla \cdot \left( -\frac{a}{2} (dh + hd) u + \frac{1}{2} (dh - hd) u \right) - M|h|^2 \right].
\end{align}

Applying \( u \mid_{\partial \Omega} = 0 \) and \( \nabla \cdot u = 0 \), we end up with

\begin{align}
\frac{d\mathcal{E}}{dt} &= -\int_\Omega (\eta |\nabla u|^2 + M|h|^2) d x. \quad \Box
\end{align}

3. Semidiscrete numerical schemes. Now that the modified Ericksen–Leslie model obeys the energy dissipation law, one would like to design numerical schemes to approximate the continuum model as accurately as possible and in the meantime obey consistent energy dissipation laws at the discrete level. By any measure, this is a good indication of a fine time discretization for the continuum dissipative system as it preserves an important property for the partial differential equation system.

In this section, we will derive several energy stable numerical schemes, based on the stabilization technique [21, 26, 30] and convex splitting strategy [9, 20, 23] for the modified Ericksen–Leslie model. These schemes address the following numerical issues in the governing system of equations:

- the coupling of the velocity and the pressure through the incompressible condition;
- the stiffness in the director equation associated with the defect core size parameterized by \( \varepsilon \);
- the nonlinear coupling between the momentum balance equation and the director transport equation.

Specifically, we will propose a first-order and a second-order energy stable schemes for the modified model, respectively. Then, we will discuss the decoupling strategy and provide two linearly decoupled energy stable schemes for the same model. The proof of the theorems on the stability of the schemes will be given in details in the following.

To prove energy stability of the scheme for model (2.3), we have to assume some properties for the bulk potential function \( g(d) \) technically, i.e., they satisfy the following conditions: (i) \( g \) has a continuous second-order derivative, (ii) there exists a constant \( L \) such that

\begin{align}
\max_{|d|_{\mathbb{R}^3}} |\nabla g(d)| \leq L,
\end{align}
where $H(d)$ is the Hessian matrix of $g(d)$. In practice, the properties can be readily met provided we modify the given function of $g$ far away from the origin to meet the conditions. For example, one can modify the potential $g(d) = \frac{1}{4\varepsilon^2}(|d|^2 - 1)^2$ outside $[-1,1]$ to a potential with a quadratic growth without affecting the solution if the maximum norm of the initial condition $d^0$ is bounded by 1 [4, 13, 21]. In [25], they used a modified $\tilde{g}$ defined by

$$
\tilde{g}(d) = \begin{cases} 
\frac{1}{\varepsilon^2}(|d| - 1)^2, & |d| > 1, \\
\frac{1}{\varepsilon^2}(|d|^2 - 1)^2, & |d| \leq 1.
\end{cases}
$$

Then, we can easily calculate

$$
\nabla_d \tilde{g} = \begin{cases} 
\frac{2}{\varepsilon^2}(|d| - 1)\frac{d}{|d|}, & |d| > 1, \\
\frac{1}{\varepsilon^2}(|d|^2 - 1)d, & |d| \leq 1,
\end{cases}
$$

and

$$
\partial_d \partial_d \tilde{g} = \begin{cases} 
\frac{2}{\varepsilon^2} \left( \delta_{ij} - \frac{\delta_{ij}|d|^2 - \delta_{ij}|d|^2}{|d|^2} \right), & |d| > 1, \\
\frac{1}{\varepsilon^2} (2d_id_j + (|d|^2 - 1)\delta_{ij}), & |d| \leq 1.
\end{cases}
$$

It satisfies the condition on the Hessian alluded to earlier. We note that, for the Landau–De Gennes bulk potential $g(d) = \frac{1}{4\varepsilon^2}(|d|^2 - 1)^2$, $L$ is on the order of $\frac{1}{\varepsilon^2}$. In the following, we drop the tilde $\tilde{\bullet}$ and assume $g$ satisfies conditions (i) and (ii) above.

In addition, we can also use the convex-splitting strategy [9] to develop energy stable schemes for the model (2.3) without truncating the bulk potential. In particular, the bulk potential $g(d) = \frac{1}{4\varepsilon^2}(|d|^2 - 1)^2$ could be split into the difference between two convex functions $g_e(d)$ and $g_c(d)$, i.e.,

$$
g(d) = g_c(d) - g_e(d),
$$

where

$$
g_e(d) = \frac{1}{4\varepsilon^2}|d|^4, \quad g_c(d) = \frac{1}{4\varepsilon^2}(|d|^2 - 1).
$$

To simplify our presentation, we introduce the following notations:

$$
\begin{align*}
 u^{n+\frac{1}{2}} &= \frac{1}{2}(u^{n+1} + u^n), \quad d^{n+\frac{1}{2}} = \frac{1}{2}(d^{n+1} + d^n), \\
\bar{u}^{n+\frac{1}{2}} &= \frac{3}{2}u^n - \frac{1}{2}u^{n-1}, \quad \bar{d}^{n+\frac{1}{2}} = \frac{3}{2}d^n - \frac{1}{2}d^{n-1}.
\end{align*}
$$

During the following discussion, we consider a smooth domain $\Omega$. For any two vector functions $f = (f_1, f_2, \ldots, f_d)$ and $g = (g_1, g_2, \ldots, g_d)$, where $d$ is a positive integer denoting the dimension of the vector function, the inner product and norm are defined by

$$
(f, g) = \sum_{i=1}^{d} \int_{\Omega} f_i g_i dx, \quad ||f|| = \sqrt{(f, f)}.
$$
We use $E^n$ to denote the discrete free energy at time step $t^n$,

$$E^n = \left( \frac{1}{2} |\nabla d^n|^2 + g(d^n), 1 \right).$$  

For convenience, we introduce the following simplified notations:

$$g(d) = \nabla d g, \quad g''(d) = H(d),$$

where $H(d)$ is the Hessian matrix of $g(d)$. Sometimes, to better explain the proof, we will use index notation. When there are repeated index, we follow Einstein’s convention, i.e., a repeated index implies the summation over all possible values of the index.

### 3.1. Preliminaries

Instead of presenting the schemes and proving their energy stability in a long proof, we first prove some lemmas to assist readers in navigating through the details of the proofs of the theorems.

**Lemma 3.1.** The following equalities hold for any $d$-dimensional vectors $d^n$ and $d^{n+1}$:

$$2(d^{n+1} - d^n, d^{n+1}) = ||d^{n+1}||^2 - ||d^n||^2 + ||d^{n+1} - d^n||^2,$$

$$2(d^{n+1} - d^n, d^n) = ||d^{n+1}||^2 - ||d^n||^2 - ||d^{n+1} - d^n||^2,$$

$$2(\nabla d^{n+1} - \nabla d^n, \nabla d^{n+1}) = ||\nabla d^{n+1}||^2 - ||\nabla d^n||^2 + ||\nabla d^{n+1} - \nabla d^n||^2,$$

$$2(\nabla d^{n+1} - \nabla d^n, \nabla d^n) = ||\nabla d^{n+1}||^2 - ||\nabla d^n||^2 - ||\nabla d^{n+1} - \nabla d^n||^2.$$

**Proof.** We obtain the equalities by expanding the inner product on the right-hand side and then combining the corresponding terms. \hfill \Box

**Lemma 3.2.** Let $g \in C^2(\mathbb{R}^d)$, where $d$ is the dimension of the space.

(i) If

$$\max_{x \in \mathbb{R}^d} |H(x)| < L,$$

where $H(x)$ is the Hessian matrix of $g(x)$, then $\forall x^{n+1}, x^n \in \mathbb{R}^d$, the following inequality holds:

$$\langle x^{n+1} - x^n, \nabla x g(x^n) \rangle \geq (g(x^{n+1}) - g(x^n), 1) - L\|x^{n+1} - x^n\|^2.$$

(ii) If $g$ is a convex function, i.e., $H(x)$ is positive definite $\forall x \in \mathbb{R}^d$, the following two inequalities hold:

$$\langle x^{n+1} - x^n, \nabla x g(x^n) \rangle \geq - (g(x^{n+1}) - g(x^n), 1),$$

$$\langle x^{n+1} - x^n, \nabla x g(x^{n+1}) \rangle \geq (g(x^{n+1}) - g(x^n), 1).$$

**Proof.** From the Taylor expansion, $\forall x^n, x^{n+1} \in \mathbb{R}^d$, there exist $\zeta_1, \zeta_2 \in \mathbb{R}^d$, such that

$$g(x^{n+1}) - g(x^n) = \langle \nabla x g(x^n), x^{n+1} - x^n \rangle + (x^{n+1} - x^n, H(\zeta_1)(x^{n+1} - x^n)), \quad (g(x^n) - g(x^{n+1}), 1)$$

$$= \langle \nabla x g(x^{n+1}), x^n - x^{n+1} \rangle + (x^n - x^{n+1}, H(\zeta_2)(x^n - x^{n+1})).$$

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(i) If (3.12) holds, from (3.16), it follows that

\[(3.18) \quad (x^{n+1} - x^n, \nabla_x g(x^n)) \geq (g(x^{n+1}) - g(x^n), 1) - L\|x^{n+1} - x^n\|^2.\]

(ii) If \(g\) is a convex function, i.e., \(\mathcal{H}(x)\) is positive definite, from (3.16), it reads

\[(3.19) \quad -(x^{n+1} - x^n, \nabla_x g(x^n)) \geq -(g(x^{n+1}) - g(x^n), 1).\]

Analogously, from (3.17), we can derive

\[(3.20) \quad (x^{n+1} - x^n, \nabla_x g(x^{n+1})) \geq (g(x^{n+1}) - g(x^n), 1).\]

**Lemma 3.3.** Define the space

\[(3.21) \quad H = \{v \in L^2(\Omega), \ \nabla \cdot v = 0, \ v \cdot n |_{\partial \Omega} = 0\}.\]

For any \(u \in H^1(\Omega)\) and \(v \in H\), the following identity holds:

\[(3.22) \quad (v \cdot \nabla u, u) = 0.\]

For this lemma, users should refer to [22] for details.

**Lemma 3.4.** Given \(u, d, h \in H^1(\Omega)\) and \(u|_{\partial \Omega} = 0\), it follows that

\[(3.23) \quad \left(\nabla \cdot \left(\frac{1-a}{2} dh - \frac{1+a}{2} hd\right), u\right) = \left(h, (W + aD) \cdot d\right),\]

where \(D = \frac{1}{2} (\nabla u + \nabla u^T)\) and \(W = \frac{1}{2} (\nabla u - \nabla u^T)\).

**Proof.** Using the index notation, we write the left-hand side of (3.23) as follows:

\[(3.24) \quad \left(\nabla \cdot \left(\frac{1-a}{2} dh - \frac{1+a}{2} hd\right), u\right) = \left(\partial_j \left(\frac{1-a}{2} d_i h_j - \frac{1+a}{2} h_i d_j\right), u_i\right) = \left(\partial_j \left(\frac{1-a}{2} d_i h_j u_i - \frac{1+a}{2} h_i d_j u_i\right), 1\right) - \left(\frac{1-a}{2} d_i h_j - \frac{1+a}{2} h_i d_j, \partial_j u_i\right)
= -\left(\frac{1-a}{2} d_i h_j - \frac{1+a}{2} h_i d_j, \partial_j u_i\right),\]

provided \(u|_{\partial \Omega} = 0\).
Similarly, we write the right-hand side of (3.23) as follows:

\[
\left( h_i (W + aD) \cdot d \right) = \left( h_i, \frac{1}{2} (\partial_j u_i - \partial_i u_j) d_j + \frac{a}{2} (\partial_j u_i + \partial_i u_j) d_j \right)
\]

\[
= - \left( \frac{1 - a}{2} d_i h_j - \frac{1 + a}{2} h_i d_j, \partial_j u_i \right).
\]

From (3.24) and (3.25), it follows that

\[
(3.26) \quad \nabla \cdot \left( \frac{1 - a}{2} dh - \frac{1 + a}{2} hd \right), u = \left( h, (W + aD) \cdot d \right).
\]

### 3.2. Linearly first-order unconditionally energy stable scheme.

We first present a first-order linear scheme. Then we show that this scheme is unconditionally energy stable [18].

**Algorithm 3.1.** Set \( d^0 = d_0, u^0 = u_0, \) and \( p^0 = 0. \) Repeat for \( 1 \leq n \leq N = T/\tau - 1: \)

1. **Step 1:** Find \((d^{n+1}, u^{n+1}_r)\) as the solution of

\[
\begin{align*}
\frac{d^{n+1} - d^n}{\tau} + u^{n+1}_r \cdot \nabla d^n - W^{n+1}_r \cdot d^n - aD^{n+1} \cdot d^n &= Mh^{n+1}, \\
h^{n+1} &= -C_1(d^{n+1} - d^n) + \Delta d^{n+1} - g(d^n), \\
\frac{u^{n+1}_r - u^n}{\tau} + (u^n \cdot \nabla) u^{n+1}_r &= \eta \Delta u^{n+1}_r - \nabla p^n - h^{n+1} \nabla d^n \\
+ \nabla \cdot \left( -\frac{a}{2} (d^n h^{n+1} + h^{n+1} d^n) + \frac{1}{2} (d^n h^{n+1} - h^{n+1} d^n) \right), \\
u^{n+1}_r|_{\partial \Omega} = 0, \quad \frac{\partial d^{n+1}}{\partial n}|_{\partial \Omega} = 0,
\end{align*}
\]

where

\[
(3.28) \quad W^{n+1}_r = \frac{1}{2} (\nabla u^{n+1}_r - (\nabla u^{n+1}_r)^T), \quad D^{n+1}_r = \frac{1}{2} (\nabla u^{n+1}_r + (\nabla u^{n+1}_r)^T).
\]

2. **Step 2:** Find \((u^{n+1}, p^{n+1})\) as the solution of

\[
(3.29) \quad \begin{cases} 
\frac{u^{n+1} - u^n}{\tau} = -\nabla (p^{n+1} - p^n), \\
\nabla \cdot u^{n+1} = 0, \quad u^{n+1} \cdot n|_{\partial \Omega} = 0.
\end{cases}
\]

**Remark 3.1.** Here, \( C_1 \) is the coefficient of the stabilizer added and \( \tau \) is the time step. It introduces a first-order error, consistent with the accuracy order of the scheme.

**Remark 3.2.** Scheme (3.29) can be decoupled into two steps. First, we calculate \( p^{n+1} \) via

\[
(3.30) \quad \begin{cases} 
-\Delta p^{n+1} = \Delta p^n + \frac{1}{\tau} \nabla \cdot u^{n+1}_r, \\
\frac{\partial p^{n+1}}{\partial n} = 0,
\end{cases}
\]

and then we update \( u^{n+1} \) using

\[
(3.31) \quad u^{n+1} = -\tau \nabla (p^{n+1} - p^n) + u^{n+1}_r.
\]
Remark 3.3. In scheme (3.27)–(3.29), we use the first-order pressure correction scheme to discretize the Navier–Stokes equation. This scheme is thus first order. We notice a coupling between \( \mathbf{d}^{n+1} \) and \( \mathbf{u}^{n+1}_* \), which means that we have to solve these two equations simultaneously. We will design schemes to decouple them in the next subsection.

Lemma 3.5. Define
\[
\mathbf{h}^{n+1} = \Delta \mathbf{d}^{n+1} - g'(\mathbf{d}^n) - C_1(\mathbf{d}^{n+1} - \mathbf{d}^n).
\]
Then, the following inequality holds:
\[
-(\mathbf{d}^{n+1} - \mathbf{d}^n, \mathbf{h}^{n+1}) \geq E^{n+1} - E^n,
\]
provided \( C_1 > L \), where \( E^{n+1} \) and \( E^n \) are the discrete free energy defined in (3.9).

Proof. If \( C_1 > L \), according to Lemma 3.2, we easily obtain
\[
-(\mathbf{d}^{n+1} - \mathbf{d}^n, \mathbf{h}^{n+1}) = C_1||\mathbf{d}^{n+1} - \mathbf{d}^n||^2
+ \frac{1}{2}(\|\nabla\mathbf{d}^{n+1}\|^2 - \|\nabla\mathbf{d}^n\|^2 + \|\nabla\mathbf{d}^{n+1} - \nabla\mathbf{d}^n\|^2) + (\mathbf{d}^{n+1} - \mathbf{d}^n, g'(\mathbf{d}^n))
\]
\[
\geq C_1||\mathbf{d}^{n+1} - \mathbf{d}^n||^2
+ \frac{1}{2}(\|\nabla\mathbf{d}^{n+1}\|^2 - \|\nabla\mathbf{d}^n\|^2) + (g(\mathbf{d}^{n+1}) - g(\mathbf{d}^n), 1) - L||\mathbf{d}^{n+1} - \mathbf{d}^n||^2
\geq E^{n+1} - E^n.
\]

Theorem 3.1. Under the condition \( C_1 \geq L \), Algorithm 3.1 is unconditionally stable in the sense that, for all \( \tau > 0 \) and \( 0 \leq n \leq T/\tau - 1 \), the following discrete energy law holds:
\[
\frac{1}{2}\|\mathbf{u}_*^{n+1}\|^2 + E^{n+1} + \frac{\tau^2}{2}\|\nabla \mathbf{p}^{n+1}\|^2 + \tau(\eta\|\nabla \mathbf{u}_*^{n+1}\|^2 + M\|\mathbf{h}^{n+1}\|^2)
\leq \frac{1}{2}\|\mathbf{u}_*^{n}\|^2 + E^n + \frac{\tau^2}{2}\|\nabla \mathbf{p}^n\|^2.
\]

Proof. Taking the inner product of (3.27) with \( 2\tau\mathbf{u}_*^{n+1} \), we obtain
\[
\|\mathbf{u}_*^{n+1}\|^2 - \|\mathbf{u}_*^{n}\|^2 + \|\mathbf{u}_*^{n+1} - \mathbf{u}_*^{n}\|^2 + 2\eta\tau\|\nabla \mathbf{u}_*^{n+1}\|^2 + 2\tau(\nabla \mathbf{p}^n, \mathbf{u}_*^{n+1})
+ 2\tau(\mathbf{h}_*^{n+1} \nabla \mathbf{d}^n, \mathbf{u}_*^{n}) - 2\tau \left( \nabla \cdot \left( \frac{1-a}{2} \mathbf{d}^n \mathbf{h}_*^{n+1} + \frac{1+a}{2} \mathbf{h}_*^{n+1} \mathbf{d}^n \right), \mathbf{u}_*^{n} \right) = 0.
\]

To deal with the pressure term, we take the inner product of (3.29) with \( 2\tau^2 \nabla \mathbf{p}^n \) to arrive at
\[
\tau^2(\|\nabla \mathbf{p}^{n+1}\|^2 - \|\nabla \mathbf{p}^n\|^2 - \|\nabla \mathbf{p}^{n+1} - \nabla \mathbf{p}^n\|^2) = 2\tau(\mathbf{u}_*^{n+1}, \nabla \mathbf{p}^n).
\]
Taking the inner product of (3.29) with \( 2\tau\mathbf{u}_*^{n+1} \), we have
\[
\|\mathbf{u}_*^{n+1}\|^2 + \|\mathbf{u}_*^{n+1} - \mathbf{u}_*^{n}\|^2 = \|\mathbf{u}_*^{n+1}\|^2.
\]
It follows from (3.29) directly that
\[
\tau^2\|\nabla \mathbf{p}^{n+1} - \nabla \mathbf{p}^n\|^2 = \|\mathbf{u}_*^{n+1} - \mathbf{u}_*^{n}\|^2.
\]
Combining (3.36)–(3.39), we have

\begin{equation}
\|u^{n+1}\|^2 - \|u_n^{\ast}\|^2 + \|u_n^{\ast} - u^n\|^2 + \delta t^2 (\|\nabla p^{n+1}\|^2 - \|\nabla p^n\|^2) + 2\eta \tau \|\nabla u_n^{\ast}\|^2 + 2\eta \tau \|\nabla^2 u_n\|_1^2 = 0.
\end{equation}

If we take the inner product of (3.27) with \(2\delta t h^{n+1}\), we obtain

\begin{equation}
2\tau M\|h^{n+1}\|^2 - 2\tau (\|u^{n+1}_\ast \cdot \nabla\|d^n\| - 2(\|d^{n+1}_\ast - d^n, h^{n+1}\| + 2\tau (h^{n+1}, (W_n^{n+1} + M\|h^{n+1}\|_1^2) = 0.
\end{equation}

From Lemma 3.4, it follows that

\begin{equation}
(3.42) \quad \left(\nabla \cdot \left(\frac{1-a}{2} d^n h^{n+1} - \frac{1+a}{2} h^{n+1} d^n\right), u_n^{\ast}\right) = (h^{n+1}, (W_n^{n+1} + M\|h^{n+1}\|_1^2).
\end{equation}

Using (3.42) and combing (3.40) and (3.41), we conclude that

\begin{equation}
\|u^{n+1}\|^2 - \|u_n^{\ast}\|^2 + \|u_n^{\ast} - u^n\|^2 + \delta t^2 (\|\nabla p^{n+1}\|^2 - \|\nabla p^n\|^2) - 2(\|d^{n+1}_\ast - d^n, h^{n+1}\| + 2\tau \|\nabla u_n^{\ast}\|^2 + 2\tau M\|h^{n+1}\|^2) = 0.
\end{equation}

Applying Lemma 3.5, we finally arrive at

\begin{equation}
\frac{1}{2}\|u^{n+1}\|^2 + E^{n+1} + \frac{\tau}{2}\|\nabla p^{n+1}\|^2 + \tau (\|\nabla u_n^{\ast}\|^2 + M\|h^{n+1}\|_1^2)
\end{equation}

\begin{equation}
\leq \frac{1}{2}\|u^n\|^2 + E^n + \frac{\tau}{2}\|\nabla p^n\|^2. \quad \Box
\end{equation}

### 3.3. Second-order unconditionally energy stable scheme

In this section, we present two second-order schemes. These two proposed schemes are all unconditionally energy stable, but nonlinear.

**Algorithm 3.2.** Set \(d^0 = d_0, u^0 = u_0\), and \(p^0 = 0\). Calculate \((d^1, u^1, p^1)\) using the first-order scheme (3.27)–(3.29). Repeat for \(1 \leq n \leq N = T/\tau - 1\) the following:

1. **Step 1:** Solve the following equations for \((d^{n+1}, u_n^{\ast+1})\):

\begin{equation}
\begin{cases}
\frac{d^{n+1}_\ast - d^n}{\tau} + u_n^{\ast+\frac{1}{2}} \cdot \nabla d^{n+\frac{1}{2}} - W_n^{n+\frac{1}{2}} \cdot d^{n+\frac{1}{2}} - a D_n^{n+\frac{1}{2}} \cdot d^{n+\frac{1}{2}} = M h^{n+\frac{1}{2}},
\\
h^{n+\frac{1}{2}} = \Delta d^{n+\frac{1}{2}} - \frac{1}{2} a (d^n, d^{n+1}),
\\
\frac{u^{n+1}_n - u^n}{\tau} + (\nabla u_n^{\ast+\frac{1}{2}}) = \eta \Delta u_n^{\ast+\frac{1}{2}} - \nabla p^n - h^{n+\frac{1}{2}} \nabla d^{n+\frac{1}{2}}
\\
+ \nabla \cdot \left(\frac{1}{2} a d^{n+\frac{1}{2}} h^{n+\frac{1}{2}} + h^{n+\frac{1}{2}} \nabla d^{n+\frac{1}{2}}\right),
\\
u_n^{\ast+1}|_{\partial \Omega} = 0, \quad \frac{\partial u_n^{\ast+1}}{\partial n}|_{\partial \Omega} = 0,
\end{cases}
\end{equation}

where

\begin{equation}
W_n^{n+1} = \frac{1}{2} (\nabla u_n^{\ast+1} - (\nabla u_n^{\ast+1})^T), \quad D_n^{n+1} = \frac{1}{2} (\nabla u_n^{\ast+1} + (\nabla u_n^{\ast+1})^T).
\end{equation}

Here \(g'(d^n, d^{n+1})\) is a second-order approximation for \(g'(d)\) at time step \(n+\frac{1}{2}\). We will give a detailed discussion on the choices of \(g'(d^n, d^{n+1})\).
2. Step 2: Solve the following equations for \((u^{n+1}, p^{n+1})\):

\[
\begin{aligned}
\frac{u^{n+1} - u^n}{\tau} &= -\frac{1}{\tau} \nabla (p^{n+1} - p^n), \\
\nabla \cdot u^{n+1} &= 0, \quad u^{n+1} \cdot n|\partial \Omega = 0.
\end{aligned}
\]

**Lemma 3.6.** If we define

\[
h^{n+\frac{1}{2}} = \Delta d^{n+\frac{1}{2}} - g'(d^n, d^{n+1}),
\]


where

\[
g'(d^n, d^{n+1}) = \begin{cases}
g(\frac{d^{n+1} - d^2}{d^{n+1} - d^n}), & d^{n+1} \neq d^n, \\
g'(d^n), & d^{n+1} = d^n,
\end{cases}
\]

then

\[
-(d^{n+1} - d^n, h^{n+\frac{1}{2}}) = E^{n+1} - E^n.
\]

**Proof.** We take the inner product of (3.48) with \(d^{n+1} - d^n\). Then, it follows that

\[
-(d^{n+1} - d^n, h^{n+\frac{1}{2}}) = \frac{1}{2} |\nabla d^{n+1}|^2 - |\nabla d^n|^2, 1) + (g(d^{n+1}) - g(d^n), 1) = E^{n+1} - E^n.
\]

**Theorem 3.2.** Given

\[
g'(d^n, d^{n+1}) = \begin{cases}
g(\frac{d^{n+1} - d^2}{d^{n+1} - d^n}), & d^{n+1} \neq d^n, \\
g'(d^n), & d^{n+1} = d^n,
\end{cases}
\]

the scheme defined by (3.45)–(3.47) obeys the discrete energy law

\[
\frac{1}{2} \|u^{n+1}\|^2 + E^{n+1} + \frac{\tau}{8} \|\nabla p^{n+1}\|^2 + \tau (\eta \|\nabla u^{n+\frac{1}{2}}\|^2 + M \|h^{n+\frac{1}{2}}\|^2) 
\[
\leq \frac{1}{2} \|u^n\|^2 + E^n + \frac{\tau}{8} \|\nabla p^n\|^2,
\]

where \(E^n\) and \(E^{n+1}\) are defined by (3.9).

**Proof.** We denote \(u^{n+\frac{1}{2}} = \frac{1}{2} (u^{n+1} + u^n)\). Taking the inner product of (3.45) with \(2\tau u^{n+\frac{1}{2}}\), we obtain

\[
\|u^{n+1}\|^2 - \|u^n\|^2 + 2\eta \|\nabla u^{n+\frac{1}{2}}\|^2 + 2\tau (\nabla p^n, u^{n+\frac{1}{2}}) + 2\tau (h^{n+\frac{1}{2}} \nabla d^{n+\frac{1}{2}} - d^n, u^{n+\frac{1}{2}})
\]

\[
\quad - 2\tau \left( \nabla \cdot \left( \frac{1}{2} d^{n+\frac{1}{2}} h^{n+\frac{1}{2}} - \frac{1}{2} h^{n+\frac{1}{2}} d^{n+\frac{1}{2}} \right), u^{n+\frac{1}{2}} \right) = 0.
\]

To deal with the pressure term, we take the inner product of (3.47) with \(2\tau^2 \nabla p^n\):

\[
\frac{\tau^2}{4} (\|\nabla p^{n+1}\|^2 - \|\nabla p^n\|^2 - \|\nabla p^{n+1} - \nabla p^n\|^2) = \tau (u^{n+1}, \nabla p^n).
\]
Taking the inner product of (3.47) with $2\tau u^{n+1}$, we have
\[(3.56) \quad \|u^{n+1}\|^2 + \|u^{n+1} - u_{*}^{n+1}\|^2 = \|u_{*}^{n+1}\|^2.\]
It follows from (3.47) that
\[(3.57) \quad \frac{\tau^2}{4}\|\nabla p^{n+1} - \nabla p^n\|^2 = \|u_{*}^{n+1} - u^{n+1}\|^2.\]
Since $(\nabla p, u^n) = 0$, it implies
\[(3.58) \quad 2\tau(\nabla p^n, u_{*}^{n+\frac{1}{2}}) = \tau(\nabla p^n, u_{*}^{n+1}).\]
Combining (3.54)–(3.57), we have
\[(3.59) \quad \|u^{n+1}\|^2 - \|u_{*}^{n+1}\|^2 = \|u_{*}^{n+1} - u^n\|^2 + \frac{\delta t^2}{4}(\|\nabla p^{n+1}\|^2 - \|\nabla p^n\|^2)\]
\[+ 2\eta\tau\|\nabla u_{*}^{n+1}\|^2 + 2\tau(h^{n+\frac{1}{2}}, d^{n+\frac{1}{2}}, u_{*}^{n+\frac{1}{2}})\]
\[\quad - 2\tau \left(\nabla \cdot \left(\frac{1-a}{2} d^{n+\frac{1}{2}} h^{n+\frac{1}{2}} - \frac{1+a}{2} h^{n+\frac{1}{2}} d^n \right), u_{*}^{n+1}\right) = 0.\]
Taking the inner product of (3.45) with $2\tau h^{n+\frac{1}{2}}$, we arrive at
\[(3.60) \quad 2\tau M\|h^{n+\frac{1}{2}}\|^2 - 2\tau(h^{n+\frac{1}{2}}, (u_{*}^{n+\frac{1}{2}} - \nabla) d^n) - 2(d^{n+1} - d^n, h^{n+\frac{1}{2}})\]
\[\quad + 2\tau \left(h^{n+1}, (W_{*}^{n+\frac{1}{2}} + aD_{*}^{n+\frac{1}{2}}) \cdot d^n\right) = 0.\]
Adding up (3.59), (3.60) and applying Lemma 3.5, we have
\[(3.61) \quad \left(\nabla \cdot \left(\frac{1-a}{2} d^{n+\frac{1}{2}} h^{n+\frac{1}{2}} - \frac{1+a}{2} h^{n+\frac{1}{2}} d^n \right), u_{*}^{n+\frac{1}{2}}\right)\]
\[\quad = \left(h^{n+\frac{1}{2}}, (W_{*}^{n+\frac{1}{2}} + aD_{*}^{n+\frac{1}{2}}) \cdot d^{n+\frac{1}{2}}\right)\]
and
\[(3.62) \quad \|u^{n+1}\|^2 - \|u_{*}^{n+1}\|^2 + \|u_{*}^{n+1} - u^n\|^2 + \frac{\delta t^2}{4}(\|\nabla p^{n+1}\|^2 - \|\nabla p^n\|^2)\]
\[\quad + 2\eta\tau\|\nabla u_{*}^{n+1}\|^2 + 2\tau M\|h^{n+\frac{1}{2}}\|^2 - 2(d^{n+1} - d^n, h^{n+\frac{1}{2}}) = 0.\]
From Lemma 3.6, it follows that
\[(3.63) \quad -(d^{n+1} - d^n, h^{n+\frac{1}{2}}) = E^{n+1} - E^n.\]
Finally, we conclude that
\[(3.64) \quad \frac{1}{2}\|u^{n+1}\|^2 + E^{n+1} + \frac{\tau^2}{8}\|\nabla p^{n+1}\|^2 + \tau(\eta\|\nabla u_{*}^{n+\frac{1}{2}}\|^2 + M\|h^{n+\frac{1}{2}}\|^2)\]
\[\quad \leq \frac{1}{2}\|u^n\|^2 + E^n + \frac{\tau^2}{8}\|\nabla p^n\|^2.\]
Remark 3.4. Here, \( g'(d^n, d^{n+1}) \) is a second order approximation of \( g'(d) \) at time step \( n + \frac{1}{\tau} \). For \( g(d) = \frac{1}{4\epsilon^2}(|d|^2 - 1)^2 \), it follows that
\[
(3.65) \quad g'(d^n, d^{n+1}) = \frac{1}{4\epsilon^2}(|d^{n+1}|^2 + |d^n|^2 - 2)(d^{n+1} + d^n).
\]

Remark 3.5. Unlike in Theorem 3.1, there is no constraint on \( C_1 \) in Theorem 3.2. This is due to the implicit treatment of the bulk potential.

We can take advantage of the convex splitting strategy [10] to rewrite \( g(d) \) given in (3.2) as a convex function minus another convex function (3.6). This leads to the following lemma and theorem.

**Lemma 3.7.** Given \( g(d) = g_c(d) - g_e(d) \) with convex functions \( g_c \) and \( g_e \) given in (3.6). We define
\[
(3.66) \quad h^{n+\frac{1}{2}} = \Delta d^{n+\frac{1}{2}} - g'(d^n, d^{n+1}),
\]
where
\[
(3.67) \quad g'(d^n, d^{n+1}) = g'_c(d^{n+1})(d^{n+1} - d^n) - g'(d^n) - \frac{1}{2}g'_c(d^n)(d^{n+1} - d^n).
\]

Then,
\[
(3.68) \quad -(d^{n+1} - d^n, h^{n+\frac{1}{2}}) \geq E^{n+1} - E^n.
\]

**Proof.** Taking the inner product of (3.66) with \( d^{n+1} - d^n \), we have
\[
(3.69) \quad -(d^{n+1} - d^n, h^{n+\frac{1}{2}})
\]
\[
= \frac{1}{2}(|\nabla d^{n+1}|^2 - |\nabla d^n|^2, 1) + (g'_c(d^{n+1}), d^{n+1} - d^n) - (g'_c(d^n), d^{n+1} - d^n)
\]
\[
+ \frac{1}{2}(g''_c(d^{n+1}), (d^{n+1} - d^n)^2) + \frac{1}{2}(g''_c(d^n), (d^{n+1} - d^n)^2)
\]
\[
\geq \frac{1}{2}(|\nabla d^{n+1}|^2 - |\nabla d^n|^2, 1) + (g'_c(d^{n+1}), d^{n+1} - d^n) - (g'_c(d^n), d^{n+1} - d^n),
\]
since \( g_c \) and \( g_e \) are convex functions. Using Lemma 3.2, we conclude that
\[
(3.70) \quad -(d^{n+1} - d^n, h^{n+\frac{1}{2}})
\]
\[
\geq \frac{1}{2}(|\nabla d^{n+1}|^2 - |\nabla d^n|^2, 1) + (g'_c(d^{n+1}) - g_e(d^{n+1}), 1)
\]
\[
- (g'_c(d^n) - g_e(d^n), 1)
\]
\[
= E^{n+1} - E^n.
\]

**Theorem 3.3.** If we define
\[
(3.71) \quad g'(d^n, d^{n+1}) = g'_c(d^{n+1})(d^{n+1} - d^n) - g'_c(d^n) - \frac{1}{2}g''_c(d^n)(d^{n+1} - d^n),
\]
where \( g_c \) and \( g_d \) are defined in (3.6), the scheme defined by (3.45)–(3.47) obeys the discrete energy law
\[
(3.72) \quad \frac{1}{2}||u^{n+1}||^2 + E^{n+1} + \frac{\tau^2}{8}||\nabla p^{n+1}||^2 + \tau(\eta)||\nabla u^{n+\frac{1}{2}}||^2 + M||h^{n+\frac{1}{2}}||^2
\]
\[
\leq \frac{1}{2}||u^n||^2 + E^n + \frac{\tau^2}{8}||\nabla p^n||^2.
\]
Proof. This proof is similar to the one given in Theorem 3.2 except that we need to use Lemma 3.7 instead of Lemma 3.6. We thus omit the details. □

3.4. Linearly first-order decoupled energy stable schemes. Next, we discuss two ways to design decoupled energy stable schemes. First, we present a first-order, quasi-energy-stable scheme. This scheme is easy to implement, but does not strictly preserve the energy dissipation property. In fact, it preserves the energy dissipation property up to an $O(\tau^4)$ error term. Thus, we name it a quasi-energy-stable scheme in this paper. Then, we present a true energy stable scheme.

Algorithm 3.3. Set $d^0 = d_0$, $u^0 = u_0$, and $p^0 = 0$. Repeat for all $1 \leq n \leq T/\tau - 1$:

1. Step 1: Solve for $d^{n+1}$:

$$
\begin{align*}
\frac{d^{n+1} - d^n}{\tau} + u^n \cdot \nabla d^n - W^n \cdot d^n - aD^n \cdot d^n &= Mh^{n+1}, \\
\frac{h^{n+1} = -C_1(d^{n+1} - d^n) + \Delta d^{n+1} - g'(d^n)}{\partial d^n/\partial n}|_{\partial \Omega} &= 0,
\end{align*}
\tag{3.73}
$$

where

$$
W^n = \frac{1}{2}(\nabla u^n - (\nabla u^n)^T), \quad D^n = \frac{1}{2}(\nabla u^n + (\nabla u^n)^T).
\tag{3.74}
$$

2. Step 2: Solve for intermediate variable $u^n$, $\Gamma^n$:

$$
\begin{align*}
\beta^n &= \left\| -h^{n+1} \nabla d^n + \nabla \left( \frac{1 - a}{2}d^n h^{n+1} - \frac{1 + a}{2}h^{n+1}d^n \right) \right\|, \\
u^n &= u^n - \tau h^{n+1} \nabla d^n + \tau \nabla \left( \frac{1 - a}{2}d^n h^{n+1} - \frac{1 + a}{2}h^{n+1}d^n \right), \\
\Gamma^n &= -\frac{\tau(\beta^n)^2}{\|u^n\|^2}u^n.
\end{align*}
\tag{3.75}
$$

3. Step 3: Solve for $u^{n+1}$:

$$
\begin{align*}
\frac{u^{n+1} - u^n}{\tau} + (u^n \cdot \nabla)\hat{u}^{n+1} &= \eta \Delta \hat{u}^{n+1} - \nabla p^n - h^{n+1} \nabla d^n + \Gamma^n \\
+ \nabla \cdot \left( -\frac{a}{2}(d^n h^{n+1} + h^{n+1}d^n) + \frac{a}{2}(d^n h^{n+1} - h^{n+1}d^n) \right), \\
\hat{u}^{n+1}|_{\partial \Omega} &= 0.
\end{align*}
\tag{3.76}
$$

$$
\begin{align*}
\frac{u^{n+1} - u^n}{\tau} &= -\nabla (p^{n+1} - p^n), \\
\nabla \cdot u^{n+1} &= 0, \quad u^{n+1} \cdot n|_{\partial \Omega} = 0.
\end{align*}
\tag{3.77}
$$

Theorem 3.4. If $C_1 > L$, the scheme defined by (3.73)-(3.77) satisfies the following semidiscrete energy dissipation law

$$
\begin{align*}
\frac{1}{2}\|u^{n+1}\|^2 + E^{n+1} + \frac{\tau^2}{2}\|\nabla p^{n+1}\|^2 &+ \tau \left( \eta \|\nabla \hat{u}^{n+1}\|^2 + M\|h^{n+1}\|^2 \right) \\
&\leq \frac{1}{2}\|u^n\|^2 + E^n + \frac{\tau^2}{2}\|\nabla p^n\|^2 + \tau^4 C^{n+1},
\end{align*}
\tag{3.78}
$$
where
\[
C^{n+1} = \frac{\| - h^{n+1} \nabla d^n + \nabla \cdot (\frac{1-a}{2} d^n h^{n+1} - \frac{1+a}{2} d^n h^{n+1} d^n) \|}{\| u^n - \tau h^{n+1} \nabla d^n + \tau \nabla \cdot (\frac{1-a}{2} d^n h^{n+1} - \frac{1+a}{2} h^{n+1} d^n) \|}^4.
\]

**Proof.** From the definition of \( u^n \) in (3.75), we rewrite the momentum equation as follows:
\[
\frac{\hat{u}^{n+1} - u^n}{\tau} + (u^n \cdot \nabla) \hat{u}^{n+1} - \eta \nabla u^{n+1} + \nabla p^n = 0,
\]
where
\[
u^n = u^n - \tau h^{n+1} \nabla d^n + \tau \nabla \cdot (\frac{1-a}{2} d^n h^{n+1} - \frac{1+a}{2} h^{n+1} d^n).
\]

Taking the inner product of (3.73) with \( 2 \nu^n \), we obtain
\[
2 \tau M \| h^{n+1} \|^2 - 2 \tau (h^{n+1}, (u^n \cdot \nabla) d^n)
- 2(d^{n+1} - d^n, h^{n+1}) + 2 \tau (h^{n+1}, (W^n + aD^n) \cdot d^n) = 0.
\]

Taking the inner product of (3.75) with \( 2 u^n \), we have
\[
\| u^n \|^2 - \| u^n \|^2 - \| u^n \|^2 + 2 \tau (h^{n+1} \nabla d^n, u^n)
- \tau (\nabla \cdot (\frac{1-a}{2} d^n h^{n+1} - \frac{1+a}{2} h^{n+1} d^n), u^n) = 0.
\]

Adding (3.82) to (3.83) and noticing the fact that
\[
\nabla \cdot (\frac{1-a}{2} d^n h^{n+1} - \frac{1+a}{2} h^{n+1} d^n), u^n = 0,
\]
we conclude that
\[
\| u^n \|^2 - \| u^n \|^2 + \| u^n \|^2 + 2 \tau M \| h^{n+1} \|^2 - 2(d^{n+1} - d^n, h^{n+1}) = 0.
\]

It follows from
\[
u^n = u^n - \tau \Gamma^n
\]
that
\[
\| u^n \|^2 = \left( 1 - \frac{\tau^2 (\beta^n)^2}{\| u^n \|^2} \right)^2 \| u^n \|^2,
\]
i.e.,
\[
\| u^n \|^2 - \| u^n \|^2 + \tau^2 (\beta^n)^2 + \tau^2 (\beta^n)^2 \left( 1 - \frac{\tau^2 (\beta^n)^2}{\| u^n \|^2} \right) = 0.
\]

Noticing the fact that \( \tau^2 (\beta^n)^2 = \| u^n \|^2 - \| u^n \|^2 \) and denoting
\[
C^{n+1} = \frac{\| - h^{n+1} \nabla d^n + \nabla \cdot (\frac{1-a}{2} d^n h^{n+1} - \frac{1+a}{2} h^{n+1} d^n) \|}{\| u^n - \tau h^{n+1} \nabla d^n + \tau \nabla \cdot (\frac{1-a}{2} d^n h^{n+1} - \frac{1+a}{2} h^{n+1} d^n) \|}^4.
\]
we arrive at

\begin{equation}
\|u^*_n\|^2 - \|u^n\|^2 + 2\|u^*_n - u^n\|^2 - C^{n+1}r^4 = 0.
\end{equation}

Taking the inner product of (3.80) with $2\tau \hat{u}^{n+1}$, we have

\begin{equation}
\|\hat{u}^{n+1}\|^2 - \|u^*_n\|^2 + \|\hat{u}^{n+1} - u^*_n\|^2 + 2\eta \delta \|\nabla \hat{u}^{n+1}\|^2 + 2\tau (\nabla p^n, \hat{u}^{n+1}) = 0.
\end{equation}

To deal with the pressure term, we take the inner product of (3.77) with $2\tau \nabla p^n$:

\begin{equation}
\tau^2 (\|\nabla p^{n+1}\|^2 - \|\nabla p^n\|^2 - \|\nabla p^{n+1} - \nabla p^n\|^2) = 2\tau (\hat{u}^{n+1}, \nabla p^n).
\end{equation}

Taking the inner product of (3.77) with $u^{n+1}$, we obtain

\begin{equation}
\|u^{n+1}\|^2 + \|u^{n+1} - \hat{u}^{n+1}\|^2 = \|\hat{u}^{n+1}\|^2.
\end{equation}

It follows from (3.77) that

\begin{equation}
\tau^2 \|\nabla p^{n+1} - \nabla p^n\|^2 = \|\hat{u}^{n+1} - u^{n+1}\|^2.
\end{equation}

Combining (3.90) and (3.91)–(3.94), we have

\begin{equation}
\|u^{n+1}\|^2 - \|\hat{u}^{n+1}\|^2 + \|u^{n+1} - \hat{u}^{n+1}\|^2 + \|\hat{u}^{n+1} - u^*_n\|^2 + \delta^2 (\|\nabla p^{n+1}\|^2 - \|\nabla p^n\|^2) + 2\eta \tau \|\nabla u^*_n\|^2 - C^{n+1}r^4 = 0.
\end{equation}

Finally, adding up (3.95), (3.85) and dividing both sides by 2, we arrive at

\begin{equation}
\frac{1}{2} (\|u^{n+1}\|^2 - \|u^n\|^2 + \|\hat{u}^{n+1} - u^n\|^2 + \|u^*_n - u^n\|^2) + \frac{1}{2} \tau^2 (\|\nabla p^{n+1}\|^2 - \|\nabla p^n\|^2) + \eta \tau \|\nabla \hat{u}^{n+1}\|^2 + \tau M \|h^{n+1}\|^2 - (d^{n+1} - d^n, h^{n+1}) - C^{n+1}r^4 = 0.
\end{equation}

Using Lemma 3.5,

\begin{equation}
-d^{n+1} - d^n, h^{n+1} \geq E^{n+1} - E^n,
\end{equation}

we finally obtain

\begin{equation}
\frac{1}{2} \|u^{n+1}\|^2 + E^{n+1} + \frac{1}{2} \tau^2 (\|\nabla p^{n+1}\|^2 + \tau \|\nabla \hat{u}^{n+1}\|^2 + M \|h^{n+1}\|^2) \leq \frac{1}{2} \|u^n\|^2 + E^n + \frac{1}{2} \tau^2 \|\nabla p^n\|^2 + C^{n+1}r^4.
\end{equation}

Remark 3.6. We note that this scheme is not unconditionally stable since there is an extra $O(\tau^4)$ term in the energy dissipation inequality. However, when $\tau$ is relatively small and $C_{n+1}$ is bounded, this scheme gives a good approximation of the energy dissipation law. We thus refer to this scheme as quasi-energy-stable.

There exists an alternative approach that can overcome this quasi-energy-stability issue, which is stated in the following.
Algorithm 3.4. Set \( d^0 = d_0, u^0 = u_0 \), and \( p^0 = 0 \). Repeat for \( 1 \leq n \leq N \leq T/\tau - 1 \):

1. Step 1: solve for \( d^{n+1} \):

\[
\begin{aligned}
\frac{d^{n+1} - d^n}{\tau} + \nabla d^n - W^*_n \cdot d^n - a D^*_n \cdot d^n &= M h^{n+1}, \\
h^{n+1} &= -C_1 (d^{n+1} - d^n) + \Delta d^{n+1} - g'(d^n), \\
\frac{\partial d^{n+1}}{\partial n}\big|_{\partial \Omega} &= 0, \quad u^n|_{\partial \Omega} = 0,
\end{aligned}
\]  

(3.99)

where

\[
\begin{aligned}
u^n &= u^n - \tau h^{n+1} \nabla d^n + \tau \nabla \left( \frac{1 - a}{2} d^n d^{n+1} - \frac{1 + a}{2} h^{n+1} d^n \right), \\
W^*_n &= \frac{1}{2} (\nabla u^*_n - (\nabla u^*_n)^T), \quad D^*_n = \frac{1}{2} (\nabla u^*_n + (\nabla u^*_n)^T).
\end{aligned}
\]  

(3.100)

2. Step 2: solve for \( u^{n+1} \):

\[
\begin{aligned}
\frac{\hat{u}^{n+1} - u^n}{\tau} + (u^n \cdot \nabla) \hat{u}^{n+1} &= \eta \Delta \hat{u}^{n+1} - \nabla p^n - h^{n+1} \nabla d^n \\
&+ \nabla \left( -\frac{a}{2} (d^n h^{n+1} + h^{n+1} d^n) + \frac{1}{2} (d^n h^{n+1} - h^{n+1} d^n) \right), \\
\hat{u}^{n+1}|_{\partial \Omega} &= 0.
\end{aligned}
\]  

(3.101)

\[
\begin{aligned}
\frac{\hat{u}^{n+1} - u^n}{\tau} + (u^n \cdot \nabla) \hat{u}^{n+1} - \eta \Delta \hat{u}^{n+1} + \nabla p^n &= 0.
\end{aligned}
\]  

(3.102)

Theorem 3.5. If \( C_1 \geq L \), the scheme defined by (3.99)–(3.102) satisfies the following semidiscrete energy dissipation law:

\[
\frac{1}{2} \| u^{n+1} \|^2 + E^{n+1} + \frac{\tau^2}{2} \| \nabla p^{n+1} \|^2 + \tau (\eta \| \nabla \hat{u}^{n+1} \|^2 + M \| h^{n+1} \|^2) \leq \frac{1}{2} \| u^n \|^2 + E^n + \frac{\tau^2}{2} \| \nabla p^n \|^2.
\]  

(3.103)

Proof. Using the definition of \( u^n \) in (3.100), we rewrite the momentum equation as follows:

\[
\frac{\hat{u}^{n+1} - u^n}{\tau} + (u^n \cdot \nabla) \hat{u}^{n+1} - \eta \Delta \hat{u}^{n+1} + \nabla p^n = 0.
\]  

(3.104)

Taking the inner product of (3.104) with \( 2 \tau \hat{u}^{n+1} \), it reads

\[
\| \hat{u}^{n+1} \|^2 - \| u^n \|^2 + \| \hat{u}^{n+1} - u^n \|^2 + 2 \eta \tau \| \nabla \hat{u}^{n+1} \|^2 + 2 \tau (\nabla p^n, \hat{u}^{n+1}) = 0.
\]  

(3.105)

To deal with the pressure term, we take the inner product of (3.102) with \( 2 \tau^2 \nabla p^n \):

\[
\tau^2 (\| \nabla p^{n+1} \|^2 - \| \nabla p^n \|^2 - \| \nabla p^{n+1} - \nabla p^n \|^2) = 2 \tau (\hat{u}^{n+1}, \nabla p^n).
\]  

(3.106)

Taking the inner product of (3.102) with \( 2 \tau u^{n+1} \), we have

\[
\| u^{n+1} \|^2 + \| u^{n+1} - \hat{u}^{n+1} \|^2 = \| \hat{u}^{n+1} \|^2.
\]  

(3.107)
It follows from (3.102) that
\begin{equation}
\tau^2 \|
abla p^{n+1} - \nabla p^n \|^2 = \|	ilde{u}^{n+1} - u^{n+1} \|^2.
\end{equation}
Combining (3.105)–(3.108), we obtain
\begin{equation}
\| u^{n+1} \|^2 - \| u^*_n \|^2 + \| \tilde{u}^{n+1} - u^*_n \|^2 \\
+ \delta t^2 (\| \nabla p^{n+1} \|^2 - \| \nabla p^n \|^2) + 2\eta \tau \| \nabla \tilde{u}^{n+1} \|^2 = 0.
\end{equation}
Taking the inner product of (3.99) with $2\tau h^{n+1}$, we obtain
\begin{equation}
2\tau M \| h^{n+1} \|^2 - 2\tau (h^{n+1}, (u^*_n \cdot \nabla)d^n) - 2(d^{n+1} - d^n, h^{n+1}) \\
+ 2\tau (h^{n+1}, (W^*_n + \alpha D^*_n) \cdot d^n) = 0.
\end{equation}
Taking the inner product of (3.100) with $2\tau u^*_n$, we have
\begin{equation}
\| u^*_n \|^2 - \| u^n \|^2 + \| u^*_n - u^n \|^2 + 2\tau (h^{n+1} \nabla d^n, u^*_n) \\
- \tau \left( \nabla \cdot \left( \frac{1-a}{2} d^n h^{n+1} - \frac{1+a}{2} h^{n+1} d^n \right), u^*_n \right) = 0.
\end{equation}
Adding (3.110) to (3.111) and noticing the fact from Lemma 3.4 that
\begin{equation}
\left( \nabla \cdot \left( \frac{1-a}{2} d^n h^{n+1} - \frac{1+a}{2} h^{n+1} d^n \right), u^*_n \right) = \left( h^{n+1}, (W^*_n + \alpha D^*_n) \cdot d^n \right),
\end{equation}
we conclude that
\begin{equation}
\| u^*_n \|^2 - \| u^n \|^2 + \| u^*_n - u^n \|^2 + 2\tau M \| h^{n+1} \|^2 - 2(d^{n+1} - d^n, h^{n+1}) = 0.
\end{equation}
Finally, adding up (3.109), (3.113) and dividing both sides by 2, we arrive at
\begin{equation}
\frac{1}{2} \left( \| u^{n+1} \|^2 - \| u^n \|^2 + \| \tilde{u}^{n+1} - u^*_n \|^2 + \| u^*_n - u_n \|^2 \right) \\
+ \frac{1}{2} \tau^2 (\| \nabla p^{n+1} \|^2 - \| \nabla p^n \|^2) + \tau \eta \| \nabla \tilde{u}^{n+1} \|^2 \\
+ \tau M \| h^{n+1} \|^2 - (d^{n+1} - d^n, h^{n+1}) = 0.
\end{equation}
Applying Lemma 3.5,
\begin{equation}
- (d^{n+1} - d^n, h^{n+1}) \geq E^{n+1} - E^n,
\end{equation}
we conclude that
\begin{equation}
\frac{1}{2} \| u^{n+1} \|^2 + E^{n+1} + \frac{\tau^2}{2} (\| \nabla p^{n+1} \|^2 + \tau (\eta \| \nabla \tilde{u}^{n+1} \|^2 + M \| h^{n+1} \|^2) \\
\leq \frac{1}{2} \| u^n \|^2 + E^n + \frac{\tau^2}{2} (\| \nabla p^n \|^2). \quad \square
\end{equation}

Remark 3.7. We note that, in (3.99), there exist two boundary conditions. The boundary condition $u^*_n|_{\partial \Omega} = 0$ appears due to the fact that (3.99) is actually a fourth-order equation if we replace $W^*_n$ and $D^*_n$ by (3.100).
4. Numerical results and discussions. In this section, we first conduct the mesh refinement test in time to verify the convergence rate of the first-order and the second-order coupled schemes, respectively. Then, we conduct several numerical simulations of liquid crystal flows in 2-dimensional space focusing on flow-induced defect dynamics. Here, we use $\eta = 1$, $M = 0.01$, $\varepsilon^2 = 10^3$, and $a = 1.5$ and $-1.5$, respectively, which represent the rodlike and disclike nematic liquid crystal system, respectively. We use a square domain, denoted by $[0, Lx] \times [0, Ly]$, in all the simulations below.

4.1. Mesh refinement test. First of all, we conduct the mesh refinement test in time to confirm the order of the coupled schemes. Notice that the schemes are coupled between the velocity field $u$ and nematic field $d$. In the numerical implementation, we employ the extrapolation technique to decouple them, i.e., instead of solving them simultaneously, we solve the equation for $\tilde{u}^{n+1}$ first while extrapolating $d^{n+1}$ by $2d^n - d^{n-1}$ and $d^{n+\frac{1}{2}}$ by $\frac{3}{4}d^n - \frac{1}{4}d^{n-1}$. Then we solve the equation for $d^{n+1}$. This should not lose any temporal accuracy. While solving the equations in model (2.3) via the first-order scheme (3.27)–(3.29), we choose $C_1 = \frac{2}{\tau^2}$.

In order to have a high resolution in space to minimize the influence of the spatial error in the mesh refinement test, we run the code in 2 dimensions with the spatial mesh size: $512 \times 512$ and time step $\tau = 2 \times 10^{-3}, 10^{-3}, 5 \times 10^{-4}, 2.5 \times 10^{-4}$, and $1.25 \times 10^{-4}$, respectively. At $t = 1$, the numerical solutions are compared, where we calculate the error by treating the numerical result with its nearest finer time step as the approximation to the accurate solution. The errors for the first-order scheme in $L_1, L_2$, and $L_{\infty}$ norm for $u$ and $d$ are shown in Figure 1, respectively. From the numerical tests, the first-order scheme is shown to be at least first-order accurate in time. The second-order scheme is also implemented, and the mesh refinement test result is depicted in Figure 2. From the numerical tests, the numerical scheme is shown as second-order accurate. We note that when $\tau = 0.002$, the error of the velocity field is not shown to be second-order. This is due to the explicit extrapolation in our implementation at the coarser grid. However, for the finer time step, the second-order accuracy is reached.

Next, we will compare numerical simulations of liquid crystal flows in a 2-dimensional channel and a cavity flow geometry obtained from model (1.2) with those obtained from model (1.4), respectively.

4.2. Defect dynamics in a channel flow. In this simulation, we set $Lx = Ly = 2$ and use the initial condition

\begin{equation}
\begin{align*}
    u &= 0, \\
    p &= 0, \\
    d &= 0.01 \times (\cos(2\pi y)\cos(2\pi x), \cos(2\pi y)\cos(2\pi x)).
\end{align*}
\end{equation}

Here, we use the periodic boundary condition in the y-direction. In the x-direction, the boundary conditions are given as follows:

\begin{equation}
    u|_{x=0,Lx} = 0, \quad \frac{\partial d}{\partial n}|_{x=0,Lx} = 0.
\end{equation}

The orientational field of liquid crystals is shown in Figure 3. Here, we show three sets of simulations, corresponding to model (1.2) with $a = -1.5, 1.5$ and model (1.4), respectively. Different orientational dynamics of defect annihilations are observed. Defect annihilations are especially dramatic in the first two cases using model (1.2), however, for model (1.4), the defect distribution rarely changes during the course of simulations. The vorticity for the three cases at times $t = 10$ and $t = 50$ are depicted.
Fig. 1. Mesh-refinement test for the first-order coupled scheme. The spatial domain is divided into $512 \times 512$ uniform meshes and the time steps are chosen as $\tau = 2 \times 10^{-3}, 10^{-3}, 5 \times 10^{-4}, 2.5 \times 10^{-4}, 1.25 \times 10^{-4}$, respectively. The $\log_2(L_1, L_2, L_\infty$ norm of the error) for $u$ and $d$ versus $\log_2(\tau)$ are plotted. The slope of the lines is 1, indicating a first-order convergence rate.

In Figure 4, it is apparent that the vorticity predicted by model (1.4) is several orders of magnitude smaller than those by model (1.2). Both the orientational field and the vorticity field predicted by model (1.4) are clearly wrong, an indication for incorrect physics modeled by this reduced model. Although one can prove theorems and design numerical schemes that can be shown to demonstrate good properties in terms of energy stability using the reduced model, it is fundamentally flawed so that
Fig. 2. Mesh-refinement test for the second-order coupled scheme. The spatial domain is divided into $512 \times 512$ uniform meshes and the time steps are chosen as $\tau = 2 \times 10^{-3}, 10^{-3}, 2.5 \times 10^{-4}, 1.25 \times 10^{-4}$, respectively. The $\log_2(L_1, L_2, L_\infty$ norm of the error) for $u$ and $d$ versus $\log_2(\tau)$ are plotted. The slope of the lines is 2, indicating a second-order convergence rate.

the results thereby obtained would have very limited applicability to any real liquid crystal systems.

4.3. Defect dynamics in a cavity flow. In the second numerical example, we simulate liquid crystal dynamics in a cavity with the prescribed physical boundary conditions:

\begin{equation}
\begin{align*}
\mathbf{u}|_{x=0} &= \mathbf{u}|_{y=0, l_y} = 0, & \mathbf{u}|_{x=L_x} &= Pe, & d|_{\partial\Omega} &= (0, 1),
\end{align*}
\end{equation}
where $Pe$ is the moving speed of the top boundary. In the simulations reported below, we choose $Pe = 1$ and the initial conditions as follows:

$$u = 0, \quad p = 0, \quad d = (0, 1).$$

The numerical results are shown in Figure 5. We plot the results of three simulations, where we use model (1.2) in the first two with respect to $a = -1.5$ and 1.5, respectively, and the last one involves model (1.4). As shown in Figure 5, in the first two cases, defects are observed; whereas in the last case using model (1.4), there is little dynamics.
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Fig. 4. Vorticity plots corresponding to the solutions in Figure 3 at times $t = 10, 50$. This figure shows the magnitude of the vorticity at times $t = 10$ and $t = 50$ for model (1.2) with $a = -1.5$ in (a)–(b); model (1.2) with $a = 1.5$ in (c)–(d); model (1.4) in (e)–(f). At the defect cores, the vorticity is zero. Away from the defect cores, the sign of the vorticity in the discotic liquid crystal is exactly opposite to that of the rodlike liquid crystal. The magnitudes of vorticity calculated using model (1.2) are much higher than the one predicted by model (1.4).

observed (i.e., the liquid crystal system is basically in a steady state). This can be seen if we take a look at model (1.4). The only coupling between liquid crystal dynamics and the flow field is through the convective term $\mathbf{u} \cdot \nabla \mathbf{d}$. Since the liquid crystal is already in a nematic steady state, the velocity field would have essentially no effect on liquid crystal dynamics, i.e., the liquid crystal system stays in a nematic steady state. The velocity field for the three cases at time $t = 4$ is also plotted in Figure 6. Once again, orientational dynamics predicted by model (1.4) is nonphysical.

5. Conclusions. In this paper, several energy stable schemes for the modified Ericksen–Leslie model are presented, which can be used to study flow behavior of
Fig. 5. Liquid crystal dynamics in a cavity. The subfigures show liquid crystal dynamics in a cavity with a shearing speed $Pe = 1$ at the top boundary at times $t = 2, 4, 6$, respectively. Here, the first two columns are the results obtained using model (1.2) with $\alpha = -1.5$ and $1.5$, respectively, while the last column shows the result obtained using model (1.4). We observe orientation reversal in the middle of the cavity for both the discotic and rodlike liquid crystal predicted by model (1.2). There is very little orientational dynamics going on in the liquid crystal system described by model (1.4).

Nematic liquid crystals in viscous fluids. In these schemes, we explicitly retain the important invariant derivative terms in the director equation and the correct elastic stress in the momentum equation. These important flow-orientation couplings have been neglected in many previous numerical and theoretical analyses using the reduced model for technical reasons. We demonstrate, using two numerical examples, that the reduced model indeed fails to predict correctly many important orientational dynamics in flows of nematic liquid crystals.

In the first example, we show defect dynamics in a channel flow while in the second one we simulate liquid crystal flows in a cavity. The numerical results demonstrate
that model (1.2) and the reduced model (1.4) are physically distinct, which highlights the novelty of our energy stable schemes and their usefulness in correctly resolving dynamics described by the modified Ericksen–Leslie model.

The schemes developed in this paper lay a solid foundation for pursuing further development of highly efficient numerical methods for solving hydrodynamic liquid crystal models.

REFERENCES


