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ON LIQUID CRYSTAL FLOWS WITH FREE-SLIP BOUNDARY CONDITIONS

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Abstract. In this paper, we study a coupled dynamic system describing nematic liquid crystal flows. The system was motivated by the Ericksen-Leslie equations modeling the flow of nematic liquid crystals. The purpose of studying the simplified system is to understand the flow properties of more complicated materials, the material configurations , as well as the interactions between them. Unlike in the previous studies where the Dirichlet boundary conditions are prescribed, we consider here the free-slip boundary conditions which possess a number of distinct advantages. The results in this paper form the analytical background for the forthcoming numerical simulations of the system.

1. **Introduction.** We are interested in the following system modeling the non-Newtonian flows of liquid crystal materials (cf. [1, 6, 7, 8, 14]):

$$u_t + (u \cdot \nabla)u + \nabla p - \nu \,\mathrm{div} D(u) + \lambda \,\mathrm{div}(\nabla d \odot \nabla d) = 0, \tag{1.1}$$

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

$$d_t + (u \cdot \nabla)d - \gamma(\Delta d - f(d)) = 0, \tag{1.3}$$

with initial conditions

$$u|_{t=0} = u_0, \qquad d|_{t=0} = d_0, \tag{1.4}$$

and appropriate boundary conditions.

In the above system, u represents the velocity vector of the liquid crystal fluid, p is the pressure, and d represents the director of the molecules. $\Omega \subset \Re^n$ is a bounded polygonal domain (unless otherwise stated). $D(u) = \frac{1}{2}(\nabla u + (\nabla u)^T)$ is the stretching tensor, $\sigma = pI + \nu D(u)$ is the fluid viscosity part of the stress tensor, $(\nabla d \odot \nabla d)_{ij} = \sum_{k=1}^{n} (\nabla_i d_k)(\nabla_j d_k)$, and finally, $f(d)$ is a polynomial of d such that $f(d) = F'(d)$ where $F(d)$ is the bulk part of the elastic energy. The choice of $F(d)$ is such that the maximal principle for $|d|$ holds in the equation (1.3), that is, if $|d| \le 1$ on the boundary and in the initial data, then $|d| \le 1$ is true everywhere at any time.

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The nematic liquid crystal is an intermediate state between the isotropic fluids and the crystal solids. The molecules possess certain orientation order, which is characterized by a unit vector field d. The equilibrium configuration of the director field n is determined by the Oseen-Frank elastic free energy:

$$E(d) = k_1(\nabla \cdot d)^2 + k_2|d \times (\nabla \times d)|^2 + k_3(d \cdot (\nabla \times d))^2.$$

with prescribed boundary conditions. The boundary condition can be of Dirichlet type (strong anchoring), natural type (weak anchoring) or mixed type (partial anchoring).

On the other hand, the lack of positional order for the material molecules, unlike those of crystal solids, also makes the flow very relevant, and in many situations, even crucial in describing the physical and mechanical properties. In order to describe the dynamic property of such kind of nematic materials, Ericksen [1] and Leslie [6] established a system consisting the equations for the conservation of the mass, the linear momentum and an extra equation for the conservation of the momentum due to the vector field d. The Ericksen-Leslie system is well suited for describing many special flows for the materials, especially for those with small molecules, and is wildly accepted in the engineering and mathematical communities studying liquid crystals.

The simplified system (1.1) – (1.3) with Dirichlet boundary conditions has been thoroughly studied theoretically in a series of work (cf. [8, 9]), and numerically in [14, 13]. These studies showed that the simplified system avoids many of the complexity of the originally Ericksen-Leslie system, while at the same time maintains most of the essential difficulties. In particular, it retains the energy identity that corresponds to the dissipation of the original system due to the *second law of thermo-dynamics*. The numerical results in [14, 13] also illustrated many interesting flow properties of the system.

In this paper, we consider a *free-slip* boundary condition for the velocity and a Neumann boundary condition for the director:

$$u \cdot n = 0, \qquad (\nabla \times u) \times n = 0, \qquad \frac{\partial d}{\partial n} = 0, \ \text{ on } \partial\Omega, \tag{1.5}$$

where n is the outward normal of $\partial\Omega$.

We want to point out that, in the case of liquid crystal flows, the last relation of (1.5) represents the fact that there is no contribution to the surface forces, $\sigma \cdot n$, from the director field d.

Not only the boundary conditions (1.5) seem to be more appropriate for some types of flow in the bulk of a liquid crystal configuration, but they also allow us to construct more efficient numerical schemes for the numerical simulation of the liquid crystal flows. Furthermore, the influence of the corner singularities is less severe with the free-slip and Neumann boundary conditions than with the Dirichlet boundary conditions. The purpose of this paper is to derive basic theoretical results concerning the liquid crystal flows with the boundary conditions (1.5) and provide an analytical background for the upcoming numerical investigation.

The paper is organized as follows: In the next section, we will introduce some notations and recall some mathematical results which are relevant to the analysis of liquid crystal flows. Then, in Section 3, we study a weak formulation for the liquid crystal flows with the boundary conditions (1.5). we will introduce an iterative Galerkin scheme to prove the global existence of the weak solutions. The crucial step is to maintain the energy law (3.17) for each finite dimensional approximation. In Section 4, we study the regularity and the classical solutions. We then introduce in Section 5 an equivalent formulation which allows us to construct a decoupled time discretization scheme for the liquid crystal flows.

2. **Notations and mathematical preliminaries.**

2.1. **Notations.** We denote by $L^2(\Omega)$ the space of the square integrable functions on Ω equipped with the usual inner product and norm,

$$(u,v)=\int_\Omega u(x)\cdot v(x)\,dx,\qquad \|u(x)\|_{L^2(\Omega)}=(u,u)^{\frac{1}{2}}.$$

For any positive integer m, we denote by $H^m(\Omega)$ the usual Sobolev space of m-th order, and by $H_0^m(\Omega)$ the closure of $C_0^\infty(\Omega)$ functions in $H^m(\Omega)$. We will also adopt the notation (cf. [2]) of $H_n^m(\Omega)$, which denotes the space of vector functions $v\in H^m(\Omega)$ whose normal component on the boundary vanishes, i.e.,

$$H_n^m(\Omega)=\{v\in H^m(\Omega):\ v\cdot n|_{\partial\Omega}=0\}.$$

The spaces $H^m_{\text{div}}(\Omega)$, $H^m_{n\,\text{div}}(\Omega)$ denote the divergence free subspaces of $H^m(\Omega)$ and $H_n^m(\Omega)$, respectively. We also denote by H the closure of $\{v\in C^\infty(\Omega), \nabla\cdot v=0, \text{in}\,\Omega,\ v\cdot n=0\,\text{on}\,\partial\Omega\}$ in $L^2(\Omega)$, and

$$H_c^m(\Omega)=\{v\in H^m(\Omega):\ \int_\Omega v dx=0\}.$$

We recall that $\|\nabla u(x)\|_{L^2(\Omega)}$ is indeed a norm in $H_n^1(\Omega)$ and in $H_c^1(\Omega)$ equivalent to the $H^1(\Omega)$ norm.

2.2. **Interpolating inequalities and compactness lemmas.** We now recall some basic interpolating inequalities that will be used throughout the paper. The first lemma is the Sobolev-Nirenberg inequality [3] and the second lemma contains the Ladyzhenskaya inequalities [5, 10].

Lemma 2.1. *If $\Omega\subset\Re^m$ is a domain with piecewise smooth boundaries, then*

$$\|D^iv\|_{L^r(\Omega)}\le\|v\|^{1-\frac{i}{m}}_{L^q(\Omega)}\|D^mv\|^{\frac{i}{m}}_{L^p(\Omega)},\tag{2.6}$$

where $0\le i\le m$, $\frac{1}{r}=\frac{i}{m}\frac{1}{p}+\left(1-\frac{i}{m}\right)\frac{1}{q}$.

Lemma 2.2. *If $\Omega\subset\Re^m$ is a domain with piecewise smooth boundaries. A $H_0^1(\Omega)$ function v with vanishing boundary value will satisfy the following estimates:*

- *If $m=2$, then $\|v\|^4_{L^4(\Omega)}\le 2\|\nabla v\|^2_{L^2(\Omega)}\|v\|^2_{L^2(\Omega)}$.*
- *If $m=3$, then $\|v\|^4_{L^4(\Omega)}\le 4\|\nabla v\|^3_{L^2(\Omega)}\|v\|_{L^2(\Omega)}$.*

Finally, we will need the following Aubin-Lions compactness lemmas (cf. [15, 11]).

Lemma 2.3. *Let $Y=\{v\in L^{\alpha_0}(0,T;X_0), v_t\in L^{\alpha_1}(0,T;X_1)\}$ with norm $||v||_Y=||v||_{L^{\alpha_0}(0,T;X_0)}+||v_t||_{L^{\alpha_1}(0,T;X_1)}$ where $X_0\subset X\subset X_1$ and injections and continuous. Moreover, $X_0\hookrightarrow X$ is compact. Then $Y\hookrightarrow L^{\alpha_0}(0,T;X)$ is compact.*

Lemma 2.4. *If X is bounded in $L^2(H^1(\Omega))\cap L^\infty(L^2(\Omega))$ and there exists a constant C such that*

$$\int_0^{T-\delta} |v(t+\delta)-v(t)|^2\,dt \le C\delta^{1/2}, \tag{2.7}$$

for any $v\in X$, then X is relatively compact in $L^P(0,T,L^q(\Omega))$ where $\frac{2}{p}+\frac{3}{q}>\frac{3}{2}$.

3. **Weak formulation with the free-slip boundary conditions.**

3.1. **Free-slip boundary conditions.** In the conventional Newtonian fluid, the *free-slip* boundary conditions are

$$(\sigma(u,p)\cdot n)\times n = 0, \qquad \text{on } \partial\Omega, \tag{3.8}$$

together with the *kinetic* boundary condition

$$u\cdot n = 0, \qquad \text{on}\,\partial\Omega. \tag{3.9}$$

Here, the stress tensor $\sigma(u,p) = pI + \nu D(u)$. (3.8) amounts to saying that the surface force is perpendicular to the surface. This is usually the case for the air contacted surfaces.

Lemma 3.1. *Assuming (3.8–3.9) and $\partial\Omega$ is Lipschitz continuous, then*

$$\int_\Omega (\nabla\cdot\sigma)\cdot u\,dx = -\int_\Omega \sigma\cdot\nabla u\,dx. \tag{3.10}$$

If in addition Ω is a polygonal domain, then

$$(\nabla\times u)\times n = 0, \qquad u\cdot n = 0, \qquad \textit{on} \quad \partial\Omega\ (\textit{three dimensional case}), \tag{3.11}$$

$$\nabla\times u = 0, \qquad u\cdot n = 0, \qquad \textit{on} \quad \partial\Omega\ (\textit{two dimension case}). \tag{3.12}$$

Furthermore, if u is sufficiently smooth, we have also

$$n\cdot(\nabla\times(\nabla\times u))|_{\partial\Omega} = 0. \tag{3.13}$$

Proof. We derive from (3.8) and (3.9) that $(\sigma\cdot n)\cdot u|_{\partial\Omega} = 0$. Hence, (3.10) is a direct consequence of the Green's formula.

To fix the idea, we consider the three-dimensional case below. Thanks to (3.8) and (3.9), we have

$$\begin{aligned} 0 &= \int_{\partial\Omega} (\sigma\cdot n)\cdot u\,ds = \int_{\partial\Omega}\sum_{i,j=1}^{3}\sigma_{ij}n_iu_j\,ds \\ &= \int_{\partial\Omega}\frac{1}{2}\sum_{i,j=1}^{3}(\nabla_iu_j+\nabla_ju_i)n_iu_j\,ds \\ &= \int_{\partial\Omega}\frac{1}{2}\sum_{i,j=1}^{3}(\nabla_iu_j-\nabla_ju_i)n_iu_j\,ds + \int_{\partial\Omega}\sum_{i,j=1}^{3}(\nabla_ju_i)n_iu_j\,ds \\ &= \int_{\partial\Omega}\frac{1}{2}((\nabla\times u)\times n)\cdot u\,ds + \int_{\partial\Omega}\sum_{i,j=1}^{3}(\nabla_ju_i)n_iu_j\,ds. \end{aligned} \tag{3.14}$$

Since $u \cdot n|_{\partial\Omega} = 0$, the last term in the above formula can be computed as follows:

$$\begin{aligned}\int_{\partial\Omega} \sum_{i,j=1}^{3} (\nabla_j u_i) n_i u_j \, ds &= \int_{\partial\Omega} \sum_{i=1}^{3} (\sum_{k=1}^{2} (u \cdot \tau_k) \nabla_{\tau_k} u_i) n_i \, ds \\ &= \int_{\partial\Omega} \sum_{i=1}^{3} (\sum_{k=1}^{2} (u \cdot \tau_k) \nabla_{\tau_k} (u_i n_i)) \, ds \\ &\quad - \int_{\partial\Omega} \sum_{i=1}^{3} (\sum_{k=1}^{2} (u \cdot \tau_k) \nabla_{\tau_k} n_i) u_i \, ds \\ &= - \int_{\partial\Omega} \sum_{i=1}^{3} (\sum_{k=1}^{2} (u \cdot \tau_k) \nabla_{\tau_k} n_i) u_i \, ds.\end{aligned}$$

Here, τ_k $(k = 1, 2)$ are the unit tangential vector on the surface. Now, in the case of Ω being a polygonal domain whose boundary consists of flat pieces, the last term in the above formula vanishes since $\nabla_{\tau_k} n_i = 0$. Hence, we derive from (3.14) that

$$\int_{\partial\Omega} \frac{1}{2} ((\nabla \times u) \times n) \cdot u \, ds = 0, \tag{3.15}$$

which implies (in the case of flat boundaries) that

$$((\nabla \times u) \times n) \times n = 0, \qquad \text{on } \partial\Omega. \tag{3.16}$$

In fact, (3.16) can also be viewed as that $(\nabla \times u) \times n$ has to be parallel to n. Therefore, it is also equivalent to (3.11) in the three-dimensional case, and equivalent to (3.12) in the two dimensional case where $\nabla \times u = \partial_{x_1} u_2 - \partial_{x_2} u_1$ is just a scalar function.

Finally, if u is sufficiently smooth, the identity

$$\nabla \cdot (f \times g) = g \cdot (\nabla \times f) - f \cdot (\nabla \times g)$$

implies that

$$\nabla \cdot ((\nabla \times u) \times n) = n \cdot (\nabla \times (\nabla \times u)) - (\nabla \times u) \cdot (\nabla \times n).$$

In the case of flat boundaries, $(\nabla \times u) \cdot (\nabla \times n)|_{\partial\Omega} = 0$. Moreover, if $(\nabla \times u) \times n = 0$ on the boundaries, we have

$$\nabla \cdot ((\nabla \times u) \times n) = \nabla_\tau \cdot ((\nabla \times u) \times n) + \nabla_n (((\nabla \times u) \times n) \cdot n) = 0, \text{ on } \partial\Omega,$$

which implies (3.13). □

3.2. **Energy law.** Previous studies (cf. [8, 9, 14, 13]) on the system (1.1)–(1.3) indicates that it is important to derive an energy law for the system. In fact, such an energy law implies that the system will obey the *second law of thermo-dynamics*, hence, it is dissipative in the isothermal cases.

Under the boundary conditions (1.5), we can formally derive the following energy identity.

Lemma 3.2. *A sufficiently smooth solution (u, d, p) of the system (1.1)–(1.3) under the boundary conditions (1.5) satisfies the following energy identity:*

$$\frac{dE}{dt} = - \left(\nu \|\nabla \times u\|_{L^2(\Omega)}^2 + \lambda\gamma \|\Delta d - f(d)\|_{L^2(\Omega)}^2 \right) \tag{3.17}$$

where $E = \frac{1}{2}\|u\|_{L^2(\Omega)}^2 + \frac{\lambda}{2}\|\nabla d\|_{L^2(\Omega)}^2 + \lambda \int_\Omega F(d)$.

Proof. Because of (1.2), we have the identity

$$\Delta u = \nabla(\nabla \cdot u) - \nabla \times (\nabla \times u) = -\nabla \times (\nabla \times u).$$

Next, we multiply the equation (1.1) by u and the equation (1.3) by $\lambda(\Delta d - f(d))$, integrate by parts and add the two resulting equations. Thanks to Lemma 3.1, all the boundary terms due to the integration by parts vanish under the current boundary conditions. From this, we get (3.17) immediately. □

Remark 3.1. *The procedure of deriving (3.17) is exactly the same as in* [8, 14]*. The key step is to ensure that the boundary terms generated from integration by parts vanish. In fact, it is easy to shown that a sufficiently smooth solution (u, d, p) of the system (1.1)–(1.3) satisfies the energy identity (3.17) with any of the following three boundary conditions:*

- $\nabla \cdot d = 0$, $(\nabla \times d) \times n = 0$; $u \cdot n = 0$, $(\nabla \times u) \times n = 0$,
- $d \cdot n = 0$, $(\nabla \times d) \times n = 0$; $u \cdot n = 0$, $(\nabla \times u) \times n = 0$,
- $d = d_0$; $u \cdot n = 0$, $((\nabla \times u) \times n) \times n = 0$.

3.3. **Existence of weak solutions.** A weak formulation of the system (1.1)–(1.3) under the boundary conditions (1.5) is:
Find $(u, d) \in H^1_{n\text{div}}(\Omega) \times H^1_c(\Omega)$ such that

$$(u_t, v) + \nu(\nabla \times u, \nabla \times v) = -\lambda(\Delta d \nabla d, v), \ \forall\, v \in H^1_{n\text{div}}(\Omega), \tag{3.18}$$

and

$$(d_t, e) + (u \cdot \nabla d, e) = -\gamma(\nabla d, \nabla e) + (f(d), e), \ \forall\, e \in H^1_c(\Omega). \tag{3.19}$$

We recall (cf. [15, 2]) that $\|\nabla \times v\|_{L^2(\Omega)}$ is a norm on the space $H^1_{n\text{div}}(\Omega)$ which is equivalent to the H^1-norm. The bilinear form

$$a(u, v) = \nu(\nabla \times u, \nabla \times v), \quad \text{for any}\, u, v \in H^1_{n\text{div}}(\Omega)$$

defines an isomorphism $A : H^1_{n\text{div}}(\Omega) \to (H^1_{n\text{div}}(\Omega))^*$, such that

$$(Au, v) = a(u, v), \quad \text{for any}\, u, v \in H^1_{n\text{div}}(\Omega).$$

The Rellich's compactness theorem [3] shows that the following inclusions are true and each space is dense in the next one:

$$H^1_{n\text{div}}(\Omega) \subset H \subset (H^1_{n\text{div}}(\Omega))^*.$$

Moreover, the first inclusion is compact.

According to the regularity of the Stokes' operator (cf. [15, 2, 5]),

$$D(A) = \{v \in H^2_{n\text{div}}(\Omega) : v \cdot n = (\nabla \times v) \times n = 0, \text{ on}\, \partial\Omega\},$$

and since $a(u, v)$ is symmetry and positive, A is self-adjoint and positive definite. Moreover, A^{-1} is compact and self-adjoint on H. Accordingly, there exists a sequence of eigenvalues of A, $0 < \lambda_1 \le \lambda_2 \le \ldots \lambda_i \cdots \to +\infty$ as $i \to \infty$, and the corresponding eigenfunction $\phi_1, \phi_2, \ldots$ in $D(A)$ as a basis of H.

Now, we can follow the procedure of [8] to construct a sequence of approximate solutions. For the sake of convenience, we will take $\lambda = \gamma = \nu = 1$ below.

Let $P_m : L^2(\Omega) \to \text{span}\{\phi_1, \ldots, \phi_m\}$ be the orthogonal projector in $L^2(\Omega)$. We consider the following approximate problem:
Find $u_m \in V_m = \text{span}\{\phi_1, \ldots, \phi_m\}$ and $d_m \in H^2_c(\Omega)$ such that

$$u_{mt} + Av_m + P_m((v_m \cdot \nabla)v_m + \nabla \cdot (\nabla d_m \odot \nabla d_m)) = 0, \tag{3.20}$$

and

$$d_{mt} + (u_m \cdot \nabla) d_m - (\Delta d_m - f(d_m)) = 0, \ \frac{\partial d_m}{\partial n}|_{\partial\Omega} = 0, \tag{3.21}$$

with the initial condition:

$$u_m|_{t=0} = P_m u_0, \qquad d_m|_{t=0} = d_0. \tag{3.22}$$

Lemma 3.3. *There exists a constant $T_0 > 0$ such that (3.20)–(3.22) has a unique smooth solution (u_m, d_m) in $\Omega \times [0, T_0]$.*

Proof. The proof of the lemma is standard so we will only sketch the procedure. Given a $u_m \in V_m$, which is a linear combination of $\phi_1, \dots, \phi_m$ with coefficients only depend on time t (hence it is smooth in x), we can substitute it in the equation (3.21). The parabolic equation (3.21) with the initial condition (3.22) admits a unique smooth solution d_m in terms of the given u_m. We can now plug this d_m in the equation (3.20) and solve for $\bar{u}_m$ which is again a linear combination of $\phi_1, \dots, \phi_m$ with coefficients only depend on time t. The equation (3.20) with (3.22) are in fact a nonlinear ordinary differential system in t for the coefficients. The fact that all terms are smooth is enough for this ODE system to have a local solution up to a time T_0. In the case that T_0 is small, the map u_m to $\bar{u}$ is a contraction map. Hence, the Leray-Schauder fixed point theorem [4] gives the desired result. □

Notice that the approximate solutions are in fact all classical solutions. This is due to the smoothness of the basis functions $\{\phi_i\}$, which are eigenfunctions of the Stokes operator A. The energy law (3.23) in the following lemma guarantees that the local solutions from Lemma 3.3 exist for all time.

Lemma 3.4. *The approximate solution (u_m, d_m) of (3.20)–(3.22) satisfies the following energy identity:*

$$\frac{dE_m}{dt} = -\left(\|\nabla \times u_m\|^2_{L^2(\Omega)} + \|\Delta d_m - f(d_m)\|^2_{L^2(\Omega)} \right), \tag{3.23}$$

where $E_m = \frac{1}{2}\|u_m\|^2_{L^2(\Omega)} + \frac{1}{2}\|\nabla d_m\|^2_{L^2(\Omega)} + \int_\Omega F(d_m)$. In particular,

$$\begin{aligned} &\frac{1}{2}\big(\|u_m\|^2_{L^2(\Omega)} + \frac{1}{2}\|\nabla d_m\|^2_{L^2(\Omega)} + \int_\Omega 2F(d_m)\big)(t) \\ &+ \int_0^t \left(\|\nabla \times u_m\|^2_{L^2(\Omega)} + \|\Delta d_m - f(d_m)\|^2_{L^2(\Omega)} \right)(s)\, ds \\ &\le \left(\frac{1}{2}\|u_m\|^2_{L^2(\Omega)} + \frac{1}{2}\|\nabla d_m\|^2_{L^2(\Omega)} + \int_\Omega F(d_m) \right)(0) \le M, \end{aligned} \tag{3.24}$$

for all $t \in (0, T_0)$. Moreover, the system (3.20)–(3.22) admits a global classical solution in $[0, T]$ for any $T < +\infty$.

Now, we can let m go to $+\infty$ and show that the approximate solution (u_m, d_m) convergences to a limit solution (u, d) which is a weak solution of (3.18)–(3.19). Indeed, using the same type of compactness arguments as in [8, 15, 12] enables us to prove the convergence of each terms in the system (3.18)–(3.19), leading to the following theorem:

Theorem 3.1. *Assuming the initial conditions (u_0, d_0) are such that $u_0 \in L^2(\Omega)$, $d_o \in H^1(\Omega)$ and satisfy the boundary conditions (1.5), then, the system (1.1)–(1.3) with* *the boundary conditions (1.5) and the initial condition (1.4) has at least one global weak solution* (u, d) *such that*

$$u \in L^2(0,T;H^1(\Omega)) \cap L^\infty(0,T;L^2(\Omega)),\ d \in L^2(0,T;H^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)),$$

for all $T < +\infty$.

4. **Regularity and uniqueness results.** In order to obtain the global existence of the classical solution for the system (1.1)–(1.4), together with the regularity and the uniqueness of the weak solutions, we need to derive higher-order energy inequalities. Note that the boundary conditions (1.5) played essentially the identical role as the Dirichlet boundary conditions in deriving the energy identity (3.17). However, the role of the boundary conditions will be significantly different for higher-order energy laws. The two-dimensional case and the three-dimensional case share the same treatment while the difference in results is due to the differences in Sobolev embedding theorems (cf. [15, 8]).

Lemma 4.1. *We denote*

$$A = \int_\Omega [\frac{1}{2}|\nabla \times u|^2 + \frac{\lambda}{2}|\Delta d - f(d)|^2]\, dx,$$

$$B = \int_\Omega [-\nu|\nabla \times \nabla \times u|^2 - \gamma\lambda|\nabla(\Delta d - f(d))|^2]\, dx.$$

Then, in the two-dimensional case, the weak solution (u, d) *of the system (1.1)–(1.3) with the free-slip boundary condition (3.12) and the initial conditions (1.4) satisfies the following high-order energy law:*

$$\frac{1}{2}\frac{d}{dt}A + \frac{1}{8}B \le C_1 A^2 + C_2, \tag{4.25}$$

In particular,

$$A(T) + \frac{1}{8}\int_0^T B\, dt \le M(T, u_0, d_0), \quad \text{for any } T < +\infty. \tag{4.26}$$

In the three-dimensional case, any weak solution (u, d) *of the system (1.1)–(1.3) with the boundary conditions (1.5) and the initial conditions (1.4) satisfies the following high-order energy law:*

$$\frac{1}{2}\frac{d}{dt}A + \frac{1}{8}B \le C_1 A^5 + C_2. \tag{4.27}$$

Proof. Thanks to Lemma 3.1, we have formally the following identities:

$$\frac{d}{dt}\int_\Omega \frac{1}{2}|\nabla \times u|^2\, dx = \int_\Omega \nabla \times u \cdot \nabla \times u_t\, dx = \int_\Omega \nabla \times \nabla \times u \cdot u_t\, dx, \tag{4.28}$$

and

$$\frac{d}{dt}\int_\Omega \frac{1}{2}|\Delta d - f(d)|^2\, dx = \int_\Omega (\Delta d - f(d), \Delta d_t - f'(d)d_t)\, dx. \tag{4.29}$$

Note also that the equation (1.1) is equivalent to the following equation under the divergence-free condition (1.2):

$$u_t + (u \cdot \nabla)u + \nabla p - \nu\nabla \times \nabla \times u + \lambda\, \mathrm{div}(\nabla d \odot \nabla d) = 0. \tag{4.30}$$

Hence, we can replace u_t in (4.28) by the above relation to derive

$$\frac{d}{dt}\int_\Omega \frac{1}{2}|\nabla\times u|^2\,dx = \int_\Omega [-\nu|\nabla\times\nabla\times u|^2 + (\nabla\times\nabla\times u, u\cdot\nabla u) + (\nabla\times\nabla\times u, -\lambda\,\mathrm{div}(\nabla d\odot\nabla d))]\,dx.$$

Similarly, we can replace d_t in (4.29) by (1.3) to get

$$\begin{aligned}\frac{d}{dt}\int_\Omega \frac{1}{2}|\Delta d - f(d)|^2\,dx = \int_\Omega &[-\gamma|\nabla(\Delta d - f(d))|^2 \\ &+ (\Delta d - f(d))(-f'(d))(\Delta d - f(d) - u\cdot\nabla d) \\ &+ \nabla(\Delta d - f(d))\nabla((u\cdot\nabla)u)]\,dx.\end{aligned}\tag{4.31}$$

Combining the equations (4.31) and (4.31), we arrive at:

$$\begin{aligned}&\frac{d}{dt}\int_\Omega [\frac{1}{2}|\nabla\times u|^2 + \frac{\lambda}{2}|\Delta d - f(d)|^2]\,dx \\ &= \int_\Omega [-\nu|\nabla\times\nabla\times u|^2 - \gamma\lambda|\nabla(\Delta d - f(d))|^2]\,dx \\ &+ \int_\Omega [(\nabla\times\nabla\times u, u\cdot\nabla u) + \gamma\lambda(\Delta d - f(d))^2(-f'(d)) \\ &+ (\Delta d - f(d))(u\cdot\nabla)f(d) + \nabla(\Delta d - f(d))\nabla((u\cdot\nabla)d))]\,dx.\end{aligned}\tag{4.32}$$

By integration by parts and thanks to $\frac{\partial d}{\partial n}|_{\partial\Omega} = 0$, the last term on the right hand side of the equation (4.32) can be converted into the following combinations:

$$\begin{aligned}&\int_\Omega \nabla(\Delta d - f(d))\nabla((u\cdot\nabla)d))\,dx \\ &= \int_\Omega \nabla(\Delta d - f(d))((u\cdot\nabla)\nabla d + \nabla u\cdot\nabla d)\,dx \\ &= \int_\Omega [-(\Delta d - f(d))(u\cdot\nabla)\Delta d - (\Delta d - f(d))\nabla u\nabla^2 d \\ &\quad + \nabla(\Delta d - f(d))\nabla u\nabla d]\,dx.\end{aligned}\tag{4.33}$$

On the other hand, we derive from $u\cdot n|_{\partial\Omega} = 0$ that

$$\int_\Omega [(\Delta d - f(d))(u\cdot\nabla)f(d) - (\Delta d - f(d))(u\cdot\nabla)\Delta d]\,dx = 0.\tag{4.34}$$

Now, using the fact that $f(d)$ only depends on d which satisfies the maximum principle and hence is bounded, we have

$$\begin{aligned}&\int_\Omega (\Delta d - f(d))\nabla u\nabla^2 d\,dx \\ &\le \|\Delta d - f(d)\|_{L^2(\Omega)}\|\nabla u\|_{L^4(\Omega)}(\|\Delta d - f(d)\|_{L^4(\Omega)} + C.\end{aligned}\tag{4.35}$$

It remains to estimate the right hand side of the last inequality. Now the estimate will depend on the space dimension. In the two dimensional case, we have

$$\begin{aligned}&\|\Delta d - f(d)\|_{L^2(\Omega)}\|\nabla u\|_{L^4(\Omega)}\|\Delta d - f(d)\|_{L^4(\Omega)} \\ \le&\|\Delta d - f(d)\|^{\frac{3}{2}}_{L^2(\Omega)}\|\nabla(\Delta d - f(d))\|^{\frac{1}{2}}_{L^2(\Omega)}\|\Delta u\|^{\frac{1}{2}}_{L^2(\Omega)}\|\nabla u\|^{\frac{1}{2}}_{L^2(\Omega)} \\ \le&\epsilon_1\|\nabla(\Delta d - f(d))\|^2_{L^2(\Omega)} + \epsilon_2\|\Delta u\|^2_{L^2(\Omega)} \\ &+ C_1\|\Delta d - f(d)\|^4_{L^2(\Omega)} + C_2\|\nabla u\|^4_{L^2(\Omega)}.\end{aligned}$$

Combining the above inequalities, we arrive at (4.25).

Finally, we can derive the inequality (4.27) in the same way as the two-dimensional case. The only difference is that instead of the last estimate above, we have

$$\begin{aligned}
&\|\Delta d - f(d)\|_{L^2(\Omega)}\|\nabla u\|_{L^4(\Omega)}\|\Delta d - f(d)\|_{L^4(\Omega)}\\
&\le\|\Delta d - f(d)\|^{\frac{5}{4}}_{L^2(\Omega)}\|\nabla(\Delta d - f(d))\|^{\frac{3}{4}}_{L^2(\Omega)}\|\Delta u\|^{\frac{3}{4}}_{L^2(\Omega)}\|\nabla u\|^{\frac{1}{4}}_{L^2(\Omega)}\\
&\le\epsilon_1\|\nabla(\Delta d - f(d))\|^2_{L^2(\Omega)} + \epsilon_2\|\Delta u\|^2_{L^2(\Omega)}\\
&\quad + C_1\|\Delta d - f(d)\|^{10}_{L^2(\Omega)} + C_2\|\nabla u\|^2_{L^2(\Omega)}.
\end{aligned}$$

Substitute this into the argument for the two-dimensional case, we get the estimate (4.27) for the three-dimensional case. □

The immediate consequences of the above lemma is the following theorem:

Theorem 4.1. *For any $0 < T < +\infty$, there exists $0 < T_1 \le T$ such that the system (1.1)–(1.3) with the boundary conditions (1.5) and the initial conditions (1.4) admits a unique classical solution (u, d, p) in $[0, T_1]$. In particular, $T_1 = T$ in the two-dimensional case.*

5. **A decoupled numerical algorithm.**

5.1. **An equivalent formulation with the boundary conditions (1.5).** The main computational advantage with the boundary conditions (1.5) is that it leads an equivalent formulation which allows the decoupling of the pressure from the velocity in the computation.

Consider the following equation:

$$\begin{aligned}
-\Delta p &= \operatorname{div}\left((u\cdot\nabla)u + \lambda \operatorname{div}(\nabla \mathrm{d}\odot\nabla \mathrm{d})\right),\\
\frac{\partial p}{\partial n}|_{\partial\Omega} &= -\left((u\cdot\nabla)u + \lambda \operatorname{div}(\nabla \mathrm{d}\odot\nabla \mathrm{d})\right)\cdot n|_{\partial\Omega}.
\end{aligned}\tag{5.36}$$

Lemma 5.1. *Given $u_0 \in H$ and $d_0 \in L^2(\Omega)$. The system (5.36), (1.1) and (1.3–1.5) is equivalent to the system (1.1–1.5).*

Proof. Taking the divergence of (1.1), using(1.2) and the fact that $\operatorname{div}D(u) = \Delta u = -\nabla\times(\nabla\times u)$, together with the result (3.13) in Lemma 3.1, we can derive (5.36) easily.

On the other hand, taking the divergence of (1.1) and using (5.36), we find that

$$(\operatorname{div} u)_t - \nu\Delta(\operatorname{div} u) = 0.$$

This relation together with (1.5) and the initial condition $\operatorname{div} u|_{t=0} = \operatorname{div} u_0 = 0$, we derive (1.2). □

A weak formulation of (5.36)–(1.1)–(1.3) is: Find $(u, d, p) \in H^1_n(\Omega)\times H^1_c(\Omega)\times H^1_c(\Omega)$ such that

$$(\nabla p, \nabla q) = -((u\cdot\nabla)u, \nabla q) - \lambda(\operatorname{div}(\nabla \mathrm{d}\odot\nabla \mathrm{d}), \nabla \mathrm{q}),\ \forall \mathrm{q}\in \mathrm{H}^1_\mathrm{c}(\Omega),\tag{5.37}$$

$$\begin{aligned}
(u_t, v) + \mu(\nabla\times u, \nabla\times v) + ((u\cdot\nabla)u, v) + \lambda(\operatorname{div}(\nabla d\odot\nabla d), v)&\\
= -(\nabla p, v),\ \forall v\in H^1_n(\Omega),&
\end{aligned}\tag{5.38}$$

and

$$(d_t, e) + (u\cdot\nabla d, e) = -\gamma(\nabla d, \nabla e) + (f(d), e),\ \forall\, e\in H^1_c(\Omega).\tag{5.39}$$

5.2. **A decoupled numerical scheme.** A main advantage of using the boundary conditions (1.5) is that it allows us to decouple the computations of u and p since the divergent free constraint on u is no longer explicitly enforced but rather a implied consequence. For instance, we can use the following semi-implicit scheme for (5.36)–(1.1)–(1.3):

Let (u^m, d^m, p^m) be an approximation of (u, d, p) at $t = m\,\delta t$, we compute $(u^{m+1}, d^{m+1}, p^{m+1})$, approximation of (u, d, p) at $t = (m+1)\,\delta t$, as follows:

$$\begin{aligned} \frac{u^{m+1}-u^m}{\delta t} - \nu\Delta u^{m+1} &= -(u^m\cdot\nabla)u^m - \nabla p^m \\ &\qquad - \lambda\,\mathrm{div}(\nabla d^m \odot \nabla d^m), \\ u^{m+1}\cdot n = 0, (\nabla\times u^{m+1})\times n &= 0, \quad \text{on } \partial\Omega; \end{aligned} \tag{5.40}$$

$$\begin{aligned} -\Delta p^{m+1} &= \mathrm{div}\left((u^{m+1}\cdot\nabla)u^{m+1} + \lambda\mathrm{div}(\nabla \mathrm{d}^\mathrm{m}\odot\nabla\mathrm{d}^\mathrm{m})\right), \\ \frac{\partial p^{m+1}}{\partial n}|_{\partial\Omega} &= -\left((u^{m+1}\cdot\nabla)u^{m+1} + \lambda\mathrm{div}(\nabla \mathrm{d}^\mathrm{m}\odot\nabla\mathrm{d}^\mathrm{m})\right)\cdot n|_{\partial\Omega}; \end{aligned} \tag{5.41}$$

$$\frac{d^{m+1}-d^m}{\delta t} - \gamma(\Delta d^{m+1} - f(d^{m+1})) = -(u^{m+1}\cdot\nabla)d^m, \ \frac{\partial d^{m+1}}{\partial n}|_{\partial\Omega} = 0. \tag{5.42}$$

For the sake of simplicity, we only wrote a first-order time discretization. However, higher-order (≥ 2) time discretization can be easily adopted and should be used in practice. In a forthcoming paper, we shall analyze and implement such a scheme using a spectral discretization for the spatial variables.

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