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A LINEAR MIXED FINITE ELEMENT SCHEME FOR A NEMATIC ERICKSEN–LESLIE LIQUID CRYSTAL MODEL *

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Abstract. In this work we study a fully discrete mixed scheme, based on continuous finite elements in space and a linear semi-implicit first-order integration in time, approximating an *Ericksen–Leslie* nematic liquid crystal model by means of a *Ginzburg–Landau* penalized problem. Conditional stability of this scheme is proved *via* a discrete version of the energy law satisfied by the continuous problem, and conditional convergence towards generalized Young measure-valued solutions to the *Ericksen–Leslie* problem is showed when the discrete parameters (in time and space) and the penalty parameter go to zero at the same time. Finally, we will show some numerical experiences for a phenomenon of annihilation of singularities.

Mathematics Subject Classification. 35Q35, 65M12, 65M60.

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1. Introduction

1.1. Statement of the problem

Let Ω be a bounded open subset of $\mathbb{R}^d$ ($d = 2$ or 3) with boundary $\partial\Omega$, and $T > 0$ the final time of observation. We will use the notation $Q = \Omega \times (0,T)$, $\Sigma = \partial\Omega \times (0,T)$, and $\boldsymbol{n}$ the unit outwards normal vector on $\partial\Omega$. Boldfaced letters will be used to denote matrix and vector spaces and their elements. The unknowns are $\boldsymbol{u} : Q \to \mathbb{R}^d$, the incompressible velocity field, $p : Q \to \mathbb{R}$, the pressure, and $\boldsymbol{d} : Q \to \mathbb{R}^d$, the orientation vector of liquid crystal molecules. These variables satisfy the following Ericksen–Leslie system:

$$\begin{cases} |\boldsymbol{d}| = 1, \quad \partial_t \boldsymbol{d} + \boldsymbol{u}\cdot\nabla\boldsymbol{d} + \gamma(-\Delta\boldsymbol{d} - |\nabla\boldsymbol{d}|^2\boldsymbol{d}) = \boldsymbol{0} & \text{in } Q, \\ \partial_t \boldsymbol{u} + \boldsymbol{u}\cdot\nabla\boldsymbol{u} - \nu\Delta\boldsymbol{u} + \nabla p + \lambda\nabla\cdot((\nabla\boldsymbol{d})^t\nabla\boldsymbol{d}) = \boldsymbol{0} & \text{in } Q, \\ \nabla\cdot\boldsymbol{u} = 0 & \text{in } Q, \end{cases} \tag{1.1}$$

where $\nu > 0$ is a constant depending on the fluid viscosity, $\lambda > 0$ is an elasticity constant, and $\gamma > 0$ is a relaxation time constant. $(\nabla\boldsymbol{d})^t$ denotes the transposed matrix of $\nabla\boldsymbol{d} = (\partial_j d_i)_{i,j}$, and $|\boldsymbol{d}| = |\boldsymbol{d}(\boldsymbol{x},t)|$ is the Euclidean norm in $\mathbb{R}^d$ (and $|\nabla\boldsymbol{d}| = |\nabla\boldsymbol{d}(\boldsymbol{x},t)|$ is the Euclidean norm in $\mathbb{R}^{d\times d}$).

Keywords and phrases. Liquid crystal, Navier–Stokes, stability, convergence, finite elements, penalization.

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To these equations we will add homogeneous and non-homogeneous boundary conditions for the velocity and orientation vector fields, respectively:

$$\boldsymbol{u}(\boldsymbol{x},t)=0,\quad \boldsymbol{d}(\boldsymbol{x},t)=\boldsymbol{l}(\boldsymbol{x})\quad \text{on } (\boldsymbol{x},t)\in\Sigma, \tag{1.2}$$

and the initial conditions

$$\boldsymbol{d}(\boldsymbol{x},0)=\boldsymbol{d}_0(\boldsymbol{x}),\qquad \boldsymbol{u}(\boldsymbol{x},0)=\boldsymbol{u}_0(\boldsymbol{x}),\quad \boldsymbol{x}\in\Omega. \tag{1.3}$$

Here $\boldsymbol{l}:\partial\Omega\to\mathbb{R}^d$, $\boldsymbol{u}_0:\Omega\to\mathbb{R}^d$, and $\boldsymbol{d}_0:\Omega\to\mathbb{R}^d$ are given functions. Throughout this work, we fix $d=3$ (the results for two-dimensional domains are easier) and the boundary datum $\boldsymbol{l}$ is assumed to be time-independent. In fact, the compatibility condition $\boldsymbol{l}=\boldsymbol{d}_0|_{\partial\Omega}$ must be satisfied. The case of time-dependent boundary conditions is more technical (see [8]).

Model (1.1) was introduced by *Lin* [13] as a simplification of an Ericksen–Leslie-type model related to the dynamic behavior of nematic liquid crystal flows.

To construct approximations of (1.1), it is usual to use the penalty Ginzburg–Landau model

$$\begin{cases} |\boldsymbol{d}|\le 1,\quad \partial_t\boldsymbol{d}+\boldsymbol{u}\cdot\nabla\boldsymbol{d}+\gamma(-\Delta\boldsymbol{d}+\boldsymbol{f}_\varepsilon(\boldsymbol{d}))=\boldsymbol{0} & \text{in } Q,\\ \partial_t\boldsymbol{u}+\boldsymbol{u}\cdot\nabla\boldsymbol{u}-\nu\Delta\boldsymbol{u}+\nabla p+\lambda\nabla\cdot((\nabla\boldsymbol{d})^t\nabla\boldsymbol{d})=\boldsymbol{0} & \text{in } Q,\\ \nabla\cdot\boldsymbol{u}=0 & \text{in } Q, \end{cases} \tag{1.4}$$

where

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

is the penalty function related to the constraint $|\boldsymbol{d}|=1$, and $\varepsilon>0$ is the penalty parameter. It is important to observe that $\boldsymbol{f}_\varepsilon$ is the gradient of the Ginzburg–Landau potential

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

that is, $\boldsymbol{f}_\varepsilon(\boldsymbol{d})=\nabla_{\boldsymbol{d}}F_\varepsilon(\boldsymbol{d})$ for all $\boldsymbol{d}\in\mathbb{R}^d$.

Problem (1.4) has two important properties for sufficiently regular solutions [14]:

1. The following *energy law* holds:

$$\frac{\mathrm{d}}{\mathrm{d}t}E(\boldsymbol{u}(t),\boldsymbol{d}(t))+D(\boldsymbol{u}(t),\boldsymbol{w}(t))=0,\quad \forall\, t\in[0,T], \tag{1.5}$$

depending on the *free energy*

$$E(\boldsymbol{u},\boldsymbol{d}):=\frac12\int_\Omega|\boldsymbol{u}|^2+\frac{\lambda}{2}\int_\Omega|\nabla\boldsymbol{d}|^2+\lambda\int_\Omega F_\varepsilon(\boldsymbol{d}), \tag{1.6}$$

and the *physical dissipation*

$$D(\boldsymbol{u},\boldsymbol{w}):=\nu\int_\Omega|\nabla\boldsymbol{u}|^2d\boldsymbol{x}+\lambda\gamma\int_\Omega|\boldsymbol{w}|^2\mathrm{d}\boldsymbol{x}, \tag{1.7}$$

where

$$\boldsymbol{w}:=-\Delta\boldsymbol{d}+\boldsymbol{f}_\varepsilon(\boldsymbol{d}) \tag{1.8}$$

is the Euler–Lagrange equation associated with the elastic energy functional $\int_\Omega\left(\frac12|\nabla\boldsymbol{d}|^2+F_\varepsilon(\boldsymbol{d})\right)$.

Energy equality (1.5) is obtained by testing $(1.4)_a$, $(1.4)_b$ and $(1.4)_c$ by $\lambda\boldsymbol{w}$, $\boldsymbol{u}$ and p, respectively, and using the fact that the elastic tensor $\lambda\nabla\cdot((\nabla\boldsymbol{d})^t\nabla\boldsymbol{d})$ of $(1.4)_b$ can be written in terms of $\boldsymbol{w}=-\Delta\boldsymbol{d}+\boldsymbol{f}_\varepsilon(\boldsymbol{d})$ as:

$$\lambda\nabla\cdot((\nabla\boldsymbol{d})^t\nabla\boldsymbol{d})=\lambda\nabla\left(\frac12|\nabla\boldsymbol{d}|^2+F_\varepsilon(\boldsymbol{d})\right)-\lambda(\nabla\boldsymbol{d})^t(-\Delta\boldsymbol{d}+\boldsymbol{f}_\varepsilon(\boldsymbol{d})). \tag{1.9}$$

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2. The following maximum principle holds:

"If $|\boldsymbol{d}_0| \leq 1$ in $\overline{\Omega}$ then $|\boldsymbol{d}(t)| \leq 1$ in $\overline{\Omega}$ for each $t \in [0,T]$".

This result is based on the following time-differential inequality satisfied by $|\boldsymbol{d}|^2$ [4]:

$$\frac{1}{2}\partial_t|\boldsymbol{d}|^2 + \boldsymbol{u}\cdot\nabla|\boldsymbol{d}|^2 - \Delta|\boldsymbol{d}|^2 + \boldsymbol{f}_\varepsilon(\boldsymbol{d})\cdot\boldsymbol{d} \leq 0 \quad \text{in } Q$$

(which is obtained by making the scalar product of $(1.4)_a$ by $\boldsymbol{d}$) jointly with the property

$$\boldsymbol{f}_\varepsilon(\boldsymbol{d})\cdot\boldsymbol{d} \geq 0 \quad \text{if } |\boldsymbol{d}| \geq 1. \tag{1.10}$$

Remark 1.1. As a consequence of this maximum principle, problem (1.4) can be equivalently written with $F_\varepsilon(\boldsymbol{d})$ and $\boldsymbol{f}_\varepsilon(\boldsymbol{d}) = \nabla_{\boldsymbol{d}}F_\varepsilon(\boldsymbol{d})$ replaced by $\widetilde{F}_\varepsilon(\boldsymbol{d})$ and $\widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d}) = \nabla_{\boldsymbol{d}}\widetilde{F}_\varepsilon(\boldsymbol{d})$ such that

$$\widetilde{F}_\varepsilon(\boldsymbol{d}) = F_\varepsilon(\boldsymbol{d}) \quad \text{if } |\boldsymbol{d}| \leq 1 \quad \text{and} \quad \widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d})\cdot\boldsymbol{d} \geq 0 \quad \text{if } |\boldsymbol{d}| \geq 1, \tag{1.11}$$

where $\widetilde{F}_\varepsilon(\boldsymbol{d})$ is a regular extension outside the unit sphere $|\boldsymbol{d}| \leq 1$ of $F_\varepsilon(\boldsymbol{d})$. It is remarkable that the energy law (1.5) holds as well, where the following free energy which appears is

$$\widetilde{E}(\boldsymbol{u},\boldsymbol{d}) := \frac{1}{2}\int_\Omega |\boldsymbol{u}|^2 + \frac{\lambda}{2}\int_\Omega |\nabla\boldsymbol{d}|^2 + \lambda\int_\Omega \widetilde{F}_\varepsilon(\boldsymbol{d}),$$

and the equilibrium variable turns out to be $\boldsymbol{w} = -\Delta\boldsymbol{d} + \widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d})$.

From (1.9) and using the fact that $\boldsymbol{w} = -\Delta\boldsymbol{d} + \boldsymbol{f}_\varepsilon(\boldsymbol{d})$, model (1.4) can then be reformulated as [3]:

$$\begin{cases} |\boldsymbol{d}| \leq 1, \quad \partial_t\boldsymbol{d} + \boldsymbol{u}\cdot\nabla\boldsymbol{d} + \gamma\,\boldsymbol{w} = \boldsymbol{0} & \text{in } Q, \\ -\Delta\boldsymbol{d} + \boldsymbol{f}_\varepsilon(\boldsymbol{d}) - \boldsymbol{w} = \boldsymbol{0} & \text{in } Q, \\ \partial_t\boldsymbol{u} + \boldsymbol{u}\cdot\nabla\boldsymbol{u} - \nu\Delta\boldsymbol{u} + \nabla p - \lambda(\nabla\boldsymbol{d})^t\boldsymbol{w} = \boldsymbol{0} & \text{in } Q, \\ \nabla\cdot\,\boldsymbol{u} = 0 & \text{in } Q, \end{cases} \tag{1.12}$$

where the pressure p in (1.4) is replaced by the potential function $p + \frac{\lambda}{2}|\nabla\boldsymbol{d}|^2 + \lambda F_\varepsilon(\boldsymbol{d})$ in (1.12) (which is called again p for simplicity). This differential reformulation will lead us to a finite-element time-stepping scheme which will be stable in the sense that it reproduces a discrete version of the continuous energy law (1.5) (see (2.2) below).

This type of reformulation is also possible for the Ericksen–Leslie problem (1.1). Indeed, the stress tensor of (1.1) reads

$$\lambda\nabla\cdot((\nabla\boldsymbol{d})^t\nabla\boldsymbol{d}) = \lambda\nabla\left(\frac{1}{2}|\nabla\boldsymbol{d}|^2\right) - \lambda(\nabla\boldsymbol{d})^t(-\Delta\boldsymbol{d} - |\nabla\boldsymbol{d}|^2\boldsymbol{d}), \tag{1.13}$$

from $\lambda(\nabla\boldsymbol{d})^t(|\nabla\boldsymbol{d}|^2\boldsymbol{d}) = \frac{1}{2}|\nabla\boldsymbol{d}|^2\nabla(|\boldsymbol{d}|^2) = 0$ (because of $|\boldsymbol{d}| = 1$). Therefore, system (1.1) can be rewritten as (1.12) but $\boldsymbol{w}$ is now replaced by $-\Delta\boldsymbol{d} - |\nabla\boldsymbol{d}|^2\boldsymbol{d}$ (the Euler–Lagrange equation related to the elastic energy functional $\int_\Omega \frac{1}{2}|\nabla\boldsymbol{d}|^2$ subject to $|\boldsymbol{d}| = 1$) and the potential function p is replaced by $p + \frac{\lambda}{2}|\nabla\boldsymbol{d}|^2$.

1.2. Notations and definition of solutions

We will assume the following notation throughout this paper. As usual $L^p(\Omega)$ denotes the space of functions defined and pth-summable in Ω, and $\|\cdot\|_{L^p(\Omega)}$ its norm. If $p = 2$ we denote the inner-product in $L^2(\Omega)$ by $\left(\cdot,\cdot\right)$, and the $L^2(\Omega)$-norm by $\|\cdot\|$. By $W^{p,s}(\Omega)$ with $s \geq 0$ and $p \geq 1$ (or $H^s(\Omega)$ for $p = 2$), we denote the classical Sobolev spaces. Let $\mathcal{C}_c^\infty(\Omega)$ be the space of infinitely differentiable functions with compact support in

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Ω. Then $W_0^{m,p}(\Omega)$ is introduced as the closure of $\mathcal{C}_c^\infty(\Omega)$ in $W^{m,p}(\Omega)$ (and $H_0^m(\Omega) = W_0^{m,p}(\Omega)$). The dual spaces of $H^s(\Omega)$ and $H_0^s(\Omega)$ will be represented by $(H^s(\Omega))'$ and $H^{-s}(\Omega)$, respectively. For a real Banach space X, $L^p(0,T;X)$ denotes the space of Bochner-measurable, X-valued functions f defined on $(0,T)$ such that $\|f\|_{L^p(0,T;X)} := (\int_0^T \|f(t)\|_X^p \,\mathrm{d}t)^{1/p} < \infty$. Moreover, $\mathcal{C}_c^\infty([0,T);X)$ is the space of infinitely differentiable, X-valued functions with compact support in $[0,T)$. Boldfaced letters will be related to vectro spaces, for instance $\boldsymbol{L}^p$ denotes a vectorial L^p space.

On the other hand, let $\mathcal{C}_0(A)$ with $A \subset \mathbb{R}^M$ be the closure of $\mathcal{C}_c^\infty(A)$ in the $\|\cdot\|_{L^\infty(A)}$-norm and let $\mathcal{M}(A)$ be the space of real-valued Radon measures with finite total variation, *i.e.*,

$$\|\mu\|_{\mathcal{M}(A)} = \sup_{\phi\in\mathcal{C}_0(A)\setminus\{0\}} \frac{|\int_A \phi \mathrm{d}\mu|}{\|\phi\|_{L^\infty(A)}}.$$

One version of the Riesz representation theorem states that the dual space of $\mathcal{C}_0(A)$ can be identified with $\mathcal{M}(A)$ *via* the duality

$$\langle \mu, \phi\rangle = \int_A \phi \mathrm{d}\mu, \quad \forall\, \mu \in \mathcal{M}(A), \quad \forall\, \phi \in \mathcal{C}_0(A).$$

Let $\mathrm{Prob}(\mathbb{R}^{d\times d})$ be the space of probability measures, *i.e.* $\mu \in \mathcal{M}(\mathbb{R}^{d\times d})$ such that $\mu > 0$ and $\mu(\mathbb{R}^{d\times d}) = 1$.

We will now introduce the function spaces in the context of the Navier–Stokes equations. Firstly, we define

$$L_0^2(\Omega) = \left\{ p : p \in L^2(\Omega), \int_\Omega p(\boldsymbol{x})\mathrm{d}\boldsymbol{x} = 0 \right\},$$
$$\boldsymbol{\mathcal{V}} = \left\{ \boldsymbol{v} \in \boldsymbol{\mathcal{C}}_c^\infty(\Omega); \nabla\cdot\boldsymbol{v} = 0 \right\}.$$

Then, let $\boldsymbol{H}$ and $\boldsymbol{V}$ be the closure of $\boldsymbol{\mathcal{V}}$ in $\boldsymbol{L}^2(\Omega)$ and $\boldsymbol{H}_0^1(\Omega)$, respectively, characterized by

$$\boldsymbol{H} = \left\{ \boldsymbol{u} \in \boldsymbol{L}^2(\Omega); \nabla\cdot\boldsymbol{u} = 0, \boldsymbol{u}\cdot\boldsymbol{n} = 0 \text{ on } \partial\Omega \right\},$$
$$\boldsymbol{V} = \left\{ \boldsymbol{u} \in \boldsymbol{H}^1(\Omega); \nabla\cdot\boldsymbol{u} = 0, \boldsymbol{u} = \boldsymbol{0} \text{ on } \partial\Omega \right\}.$$

Next, let us introduce the concept of generalized Young measure-valued solutions of (1.1) (as in [20]) and the concept of weak solutions for the penalized problem (1.4).

Definition 1.2. A 4-tuple $(\boldsymbol{u}, \boldsymbol{d}, \mu, \boldsymbol{M})$ is called a generalized Young measure-valued solution of (1.1)–(1.3) in $(0,T)$ if:

a) $\boldsymbol{u} \in L^\infty(0,T;\boldsymbol{H}) \cap L^2(0,T;\boldsymbol{V})$, $\quad \boldsymbol{d} \in L^\infty(0,T;\boldsymbol{H}^1(\Omega))$,
$|\boldsymbol{d}(\boldsymbol{x},t)| = 1$ for a.e. $(\boldsymbol{x},t) \in Q$, $\quad \boldsymbol{d}(\boldsymbol{x},t) = \boldsymbol{l}(\boldsymbol{x})$ for a.e. $(\boldsymbol{x},t) \in \Sigma$,
$\mu \in \mathcal{M}(Q)$, $\quad (\boldsymbol{x},t) \in Q \to \boldsymbol{M}_{\boldsymbol{x},t} \in \mathrm{Prob}(\mathbb{R}^{d\times d})$ is a weak-$\star$ μ-measurable map.

b) For all $\boldsymbol{\phi} \in \mathcal{C}_c^\infty([0,T);\boldsymbol{\mathcal{V}})$,

$$\int_0^T \left\{ -\Big(\boldsymbol{u}, \partial_t\boldsymbol{\phi}\Big) + \Big((\boldsymbol{u}\cdot\nabla)\boldsymbol{u}, \boldsymbol{\phi}\Big) + \nu\Big(\nabla\boldsymbol{u}, \nabla\boldsymbol{\phi}\Big) \right\} \mathrm{d}t - \lambda \int_Q \Big(\int_{\mathbb{R}^{d\times d}} \frac{\boldsymbol{y}^t\boldsymbol{y}}{|\boldsymbol{y}|^2} \mathrm{d}\boldsymbol{M}_{\boldsymbol{x},t}(\boldsymbol{y}) \Big) : \nabla\boldsymbol{\phi}\, \mathrm{d}\mu(\boldsymbol{x},t) = \Big(\boldsymbol{u}_0, \boldsymbol{\phi}(0)\Big).$$

c) For all $\boldsymbol{\psi} \in \mathcal{C}_c^\infty([0,T);\boldsymbol{\mathcal{C}}_c^\infty(\Omega))$,

$$\int_0^T \left\{ -\Big(\boldsymbol{d}, \partial_t\boldsymbol{\psi}\Big) + \Big(\boldsymbol{u}\cdot\nabla\boldsymbol{d}, \boldsymbol{\psi}\Big) + \gamma\Big(\nabla\boldsymbol{d}, \nabla\boldsymbol{\psi}\Big) - \gamma\Big(|\nabla\boldsymbol{d}|^2\boldsymbol{d}, \boldsymbol{\psi}\Big) \right\} \mathrm{d}t = \Big(\boldsymbol{d}_0, \boldsymbol{\psi}(0)\Big).$$

Definition 1.3. A pair $(\boldsymbol{d}, \boldsymbol{u})$ is called a weak solution of (1.4) and (1.2)–(1.3) in $(0,T)$ if:

a) $\boldsymbol{u} \in L^\infty(0,T;\boldsymbol{H}) \cap L^2(0,T;\boldsymbol{V})$, $\quad \boldsymbol{d} \in L^\infty(0,T;\boldsymbol{H}^1(\Omega)) \cap L^2(0,T;\boldsymbol{H}^2(\Omega))$,
$|\boldsymbol{d}(\boldsymbol{x},t)| \le 1$ a.e. $(\boldsymbol{x},t) \in Q$, $\quad \boldsymbol{d}(\boldsymbol{x},t) = \boldsymbol{l}(\boldsymbol{x})$ a.e. $(\boldsymbol{x},t) \in \Sigma$.

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b) For all $\boldsymbol{\phi} \in \mathcal{C}_c^\infty([0,T);\boldsymbol{\mathcal{V}})$,

$$\int_0^T \Big\{ -\Big(\boldsymbol{u}, \partial_t \boldsymbol{\phi}\Big) + \Big((\boldsymbol{u}\cdot\nabla)\boldsymbol{u}, \boldsymbol{\phi}\Big) + \Big(\nu\nabla\boldsymbol{u} - \lambda(\nabla\boldsymbol{d})^t\nabla\boldsymbol{d}, \nabla\boldsymbol{\phi}\Big)\Big\}\, \mathrm{d}t = \Big(\boldsymbol{u}_0, \boldsymbol{\phi}(0)\Big).$$

c) $\partial_t \boldsymbol{d} + \boldsymbol{u}\cdot\nabla\boldsymbol{d} + \gamma(-\Delta\boldsymbol{d} + \boldsymbol{f}_\varepsilon(\boldsymbol{d})) = \boldsymbol{0}$ a.e. in Q, $\quad \boldsymbol{d}(0) = \boldsymbol{d}_0$ a.e. in Ω.

1.3. Known results for systems (1.1) and (1.4)

Considering the boundary condition for the director vector $\boldsymbol{d}$ to be time-independent and for any fixed ε, Lin and Liu proved [14] the local existence of classical solutions and the global existence of weak solutions to problem (1.4) by means of a semi-Galerkin method (where the $\boldsymbol{d}$-system is not discretized in space in order to preserve the energy equality (1.5) and the maximum principle).

In [4], the existence of weak time-periodic solutions was proved by using a (fully) Galerkin method for which the maximum principle does not hold; therefore, a truncated potential had to be used.

The first finite element schemes for problem (1.4) were proposed by *Liu* and *Walkington* [18,19], obtaining error estimates. In the first work [18], they proposed a scheme requiring globally C^1-finite elements for approximating the director vector $\boldsymbol{d}$. Later, in the second work [19], a C^0-approximation is only used by introducing the auxiliary variable $\nabla\boldsymbol{d}$. In both works the resulting schemes are totally coupled and nonlinear. In order to avoid the large degrees of freedom and the nonlinearity of these schemes, *Girault* and *Guillén–González* [8] considered the auxiliary variable $-\Delta\boldsymbol{d}$ constructing a fully discrete mixed scheme for (1.4) (that is, for $\varepsilon > 0$ fixed) which is coupled but linear, unconditionally stable and convergent towards weak solutions to (1.4). Also, optimal error estimates for $(\boldsymbol{u}, \boldsymbol{d})$ and convergence of iterative methods (decoupling the fluids variables $(\boldsymbol{u}, p)$ from the elastic one $\boldsymbol{d}$) were obtained. In [16], *Lin* and *Liu* presented two linear numerical algorithms by using C^0-finite elements. The first of them uses an explicit-implicit backward Euler approximation in time and the second one uses a characteristic method. Although stability properties of these schemes are not provided, some numerical experiments show that both schemes recover the numerical results obtained in [18].

In [3], *Becker, Feng* and *Prohl* considered two nonlinear fully discrete methods based on C^0-finite elements. The first scheme is defined by considering the auxiliary variable $\boldsymbol{w} = -\Delta\boldsymbol{d} + \boldsymbol{f}_\varepsilon(\boldsymbol{d})$ and it is unconditionally stable and convergent to problem (1.1). This convergence is attained in two steps; firstly when the time and space discretization parameters go to zero (*i.e.* $(k,h) \to 0$), the convergence towards a weak solution to the penalized problem (1.12) is proved, and afterwards when the penalty parameter ε goes to zero, one obtains a measure-valued solution to problem (1.1), where the elastic tensor $(\nabla\boldsymbol{d})^t\nabla\boldsymbol{d}$ tends to a certain measure (see [15]). It should be noted that the proof of the compactness for the discrete velocity in $L^2(0,T;\boldsymbol{L}^2(\Omega))$ done in [3] does not seem to be clear because the discrete velocity is bounded in $L^\infty(0,T;\boldsymbol{L}^2(\Omega)) \cap L^2(0,T;\boldsymbol{H}_0^1(\Omega))$ while the time derivative is bounded in the dual space of $\boldsymbol{V} \cap \boldsymbol{H}^2(\Omega)$. However, in order to apply an Aubin–Lions compactness argument, one would need the continuous embeddings $\boldsymbol{H}_0^1(\Omega) \hookrightarrow \boldsymbol{L}^2(\Omega) \hookrightarrow (\boldsymbol{V} \cap \boldsymbol{H}^2(\Omega))'$ (with the former being compact), but the embedding from $\boldsymbol{L}^2(\Omega)$ into $(\boldsymbol{V} \cap \boldsymbol{H}^2(\Omega))'$ is not injective.

The second algorithm in [3] discretizes directly problem (1.1) being conditionally stable, but the convergence when the discrete parameters go to zero remains as an open problem.

Approximating model (1.1) directly could be much more adequate for regular initial data without defects (that is, with a unit vector in the whole domain), since we would avoid the problem of balancing the penalty parameter with the discretization parameters. Otherwise, we have to face the problem of dealing with the sphere constraint. One way to solve such a difficulty numerically is to use *Alouges'* technique [1] for imposing the sphere constraint at every nodes.

In [17], Lin *et al.* introduced an unconditionally stable, nonlinear scheme for the penalized Ginzburg–Landau associated to a nematic liquid crystal model which is a slightly modified version of (1.4), where stretching terms appear in the $\boldsymbol{d}$-system. In this scheme, a mid-point approximation of the Ginzburg–Landau potential is considered preserving the energy law at the discrete level, and the use of an auxiliary variable like $\boldsymbol{w}$ is avoided.

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In the light of the previous works, our task in this paper is to design a linear and C^0-finite element scheme based on reformulation (1.12), *i.e.*, using the auxiliary variable $\boldsymbol{w} = -\Delta \boldsymbol{d} + \boldsymbol{f}_\varepsilon(\boldsymbol{d})$) as in [3]. For this scheme, the following two properties will be discussed:

1. Conditional *a priori* energy estimates independent of (h, k, ε) provided that an explicit constraint with respect to the numerical parameters (k, h) and ε (see (S) below). Moreover, such a constraint will be to able to be weakened (see (S′) below) when $\widetilde{F}_\varepsilon(\boldsymbol{d})$ is considered instead of $F_\varepsilon(\boldsymbol{d})$.
2. Convergence (as $(h, k, \varepsilon) \to 0$) towards a measure-valued solution of (1.1). For this, the compactness for the velocity in $L^2(0, T; \boldsymbol{L}^2(\Omega))$ will be proved. The elastic tensor $(\nabla \boldsymbol{d})^t \boldsymbol{w}$ is responsible for not obtaining the convergence towards weak solutions of (1.1). Thus the concept of measure-valued solutions is introduced to identify the limit of such an elastic tensor. It will be only possible when the truncating potential $\widetilde{F}_\varepsilon(\boldsymbol{d})$ is considered instead of $F_\varepsilon(\boldsymbol{d})$.

The idea of using a truncated potential in Nematic Liquid crystals was introduced in [14] in order to deduce analytical results. Recently, it has been used for numerical purposes in the context of Allen–Cahn and Cahn–Hilliard phase-field models in [22].

Note that, for the unconditional stable nonlinear schemes given in [3, 17], an iterative process has to be implemented to approach the nonlinear scheme, where some constraints on the numerical parameters will appear to assure its convergence. For instance, in [17], a Picard linearization is considered, where following the proof of the conditional stability given in our paper (see Lem. 2.1 below), a constraint like (S) appears in order to assure convergence.

Finally, it is not clear how to extend the convergence result (as $(h, k, \varepsilon) \to 0$) obtained in this paper to other types of stable approximations such as [3,17], where there is not truncation of the potential term. On the other hand, from a numerical point of view it is not possible to take a truncated potential in an implicit manner (since $\widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d}_h^{n+1})$ is defined by parts when $|\boldsymbol{d}_h^{n+1}| \leq 1$ or $|\boldsymbol{d}_h^{n+1}| \geq 1$, but $\boldsymbol{d}_h^{n+1}$ is an unknown).

1.4. Numerical scheme

The numerical scheme will be based on the following mixed weak formulation of problem (1.12). Find $(\boldsymbol{u}(t), p(t), \boldsymbol{d}(t), \boldsymbol{w}(t)) \in \boldsymbol{H}_0^1(\Omega) \times L_0^2(\Omega) \times \boldsymbol{H}^1(\Omega) \times \boldsymbol{L}^2(\Omega)$ with $\boldsymbol{d}(t) = \boldsymbol{l}$ on $\partial\Omega$ such that

$$\begin{aligned}
\Big(\partial_t \boldsymbol{u}, \bar{\boldsymbol{u}}\Big) + \nu\Big(\nabla \boldsymbol{u}, \nabla \bar{\boldsymbol{u}}\Big) + \Big((\boldsymbol{u}\cdot\nabla)\boldsymbol{u}, \bar{\boldsymbol{u}}\Big) \\
-\lambda\Big((\nabla \boldsymbol{d})^t \boldsymbol{w}, \bar{\boldsymbol{u}}\Big) - \Big(p, \nabla\cdot\bar{\boldsymbol{u}}\Big) = 0 \;\forall\, \bar{\boldsymbol{u}} \in \boldsymbol{H}_0^1(\Omega), \\
\Big(\nabla\cdot\boldsymbol{u}, \bar{p}\Big) = 0 \;\forall\, \bar{p} \in L_0^2(\Omega), \\
\Big(\partial_t \boldsymbol{d}, \bar{\boldsymbol{w}}\Big) + \Big((\boldsymbol{u}\cdot\nabla)\boldsymbol{d}, \bar{\boldsymbol{w}}\Big) + \gamma\Big(\boldsymbol{w}, \bar{\boldsymbol{w}}\Big) = 0 \;\forall\, \bar{\boldsymbol{w}} \in \boldsymbol{L}^2(\Omega), \\
\Big(\nabla \boldsymbol{d}, \nabla \bar{\boldsymbol{d}}\Big) + \Big(\boldsymbol{f}_\varepsilon(\boldsymbol{d}), \bar{\boldsymbol{d}}\Big) - \Big(\boldsymbol{w}, \bar{\boldsymbol{d}}\Big) = 0 \;\forall\, \bar{\boldsymbol{d}} \in \boldsymbol{H}_0^1(\Omega).
\end{aligned} \tag{1.14}$$

Roughly speaking, velocity, pressure, orientation vector, and the Euler–Lagrange equation $\boldsymbol{w} = -\Delta \boldsymbol{d} + \boldsymbol{f}_\varepsilon(\boldsymbol{d})$ will be approximated in the finite element spaces

$$(\boldsymbol{X}_h, Q_h, \boldsymbol{D}_h, \boldsymbol{W}_h) \subset (\boldsymbol{H}_0^1(\Omega), L_0^2(\Omega), \boldsymbol{H}^1(\Omega), \boldsymbol{L}^2(\Omega)), \quad \boldsymbol{D}_{0h} \subset \boldsymbol{H}_0^1(\Omega).$$

The algorithm that we present consists of:

Initialization: Let $(\boldsymbol{u}_h^0, \boldsymbol{d}_h^0) \in (\boldsymbol{X}_h, \boldsymbol{D}_h)$ be a suitable approximation of $(\boldsymbol{u}_0, \boldsymbol{d}_0)$.

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Step $(n+1)$**:** Given $(\boldsymbol{u}_h^n, \boldsymbol{d}_h^n) \in (\boldsymbol{X}_h, \boldsymbol{D}_h)$, find $(\boldsymbol{u}_h^{n+1}, p_h^{n+1}, \boldsymbol{d}_h^{n+1}, \boldsymbol{w}_h^{n+1}) \in \boldsymbol{X}_h \times Q_h \times \boldsymbol{D}_h \times \boldsymbol{W}_h$ with $\boldsymbol{d}_h^{n+1} = \boldsymbol{l}_h$ on $\partial\Omega$, where $\boldsymbol{l}_h$ is an approximation of $\boldsymbol{l}$, solving the algebraic linear system:

$$\begin{aligned}&\left(\frac{\boldsymbol{u}_h^{n+1}-\boldsymbol{u}_h^n}{k}, \bar{\boldsymbol{u}}_h\right) + c\left(\boldsymbol{u}_h^n, \boldsymbol{u}_h^{n+1}, \bar{\boldsymbol{u}}_h\right) + \nu\left(\nabla \boldsymbol{u}_h^{n+1}, \nabla \bar{\boldsymbol{u}}_h\right)\\ &-\lambda\left((\nabla \boldsymbol{d}_h^n)^t \boldsymbol{w}_h^{n+1}, \bar{\boldsymbol{u}}_h\right) - \left(p_h^{n+1}, \nabla \cdot \bar{\boldsymbol{u}}_h\right) = 0,\end{aligned} \tag{1.15}$$

$$\left(\nabla \cdot \boldsymbol{u}_h^{n+1}, \bar{p}_h\right) = 0, \tag{1.16}$$

$$\left(\frac{\boldsymbol{d}_h^{n+1}-\boldsymbol{d}_h^n}{k}, \bar{\boldsymbol{w}}_h\right) + \left((\boldsymbol{u}_h^{n+1} \cdot \nabla)\boldsymbol{d}_h^n, \bar{\boldsymbol{w}}_h\right) + \gamma\left(\boldsymbol{w}_h^{n+1}, \bar{\boldsymbol{w}}_h\right) = 0, \tag{1.17}$$

$$\left(\nabla \boldsymbol{d}_h^{n+1}, \nabla \bar{\boldsymbol{d}}_h\right) - \left(\boldsymbol{w}_h^{n+1}, \bar{\boldsymbol{d}}_h\right) = -\left(\boldsymbol{f}_\varepsilon(\boldsymbol{d}_h^n), \bar{\boldsymbol{d}}_h\right), \tag{1.18}$$

for all $(\bar{\boldsymbol{u}}_h, \bar{p}_h, \bar{\boldsymbol{d}}_h, \bar{\boldsymbol{w}}_h) \in \boldsymbol{X}_h \times Q_h \times \boldsymbol{D}_{0h} \times \boldsymbol{W}_h$, where we have considered the trilinear form $c(\cdot,\cdot,\cdot)$ defined by

$$c\left(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}\right) = \left((\boldsymbol{u} \cdot \nabla)\boldsymbol{v}, \boldsymbol{w}\right) + \frac{1}{2}\left((\nabla \cdot \boldsymbol{u})\,\boldsymbol{v}, \boldsymbol{w}\right) \quad \forall\, \boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w} \in \boldsymbol{H}_0^1(\Omega),$$

which displays the skew-symmetry $c(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{v}) = 0$, although $\boldsymbol{u}$ does not satisfy the incompressibility condition pointwisely. The scheme introduced in [3] is very similar, except for the approximation of the potential function $\boldsymbol{f}_\varepsilon(\boldsymbol{d}(t_{n+1}))$. Here this approximation is explicit (resulting in a linear scheme) and in [3] is semi-implicit (and nonlinear with respect to $\boldsymbol{d}_h^{n+1}$)

Throughtout this paper, $C > 0$ will denote different constants always independent of k, h and ε.

1.5. Hypotheses

Hereafter, we will assume that $\Omega \subset \mathbb{R}^3$ is a bounded domain with polyhedral boundary, and there exists a family of regular triangulations $\{\mathcal{T}_h\}_{h>0}$ of Ω made up of tetrahedrons, where h is the maximum diameter of the elements of $\{\mathcal{T}_h\}_{h>0}$.

The following hypotheses will be required:

(H0) Hypotheses for the data:

$$\boldsymbol{u}_0 \in \boldsymbol{H}, \quad \boldsymbol{d}_0 \in \boldsymbol{H}^1(\Omega) \text{ with } |\boldsymbol{d}_0| = 1 \text{ in } \Omega, \quad \boldsymbol{l} \in \boldsymbol{H}^{3/2}(\partial\Omega) \text{ with } |\boldsymbol{l}| = 1 \text{ on } \partial\Omega \times (0,T).$$

(H1) The boundary of Ω is assumed to be such that the $\boldsymbol{H}^2(\Omega) \times H^1(\Omega)$-regularity property of the *Stokes* problem and the $H^2(\Omega)$-regularity property of the *Poisson* problem hold.

(H2) The triangulation of Ω and the discrete spaces satisfy:

(a) The inverse inequalities:

(i) $\|\bar{\boldsymbol{d}}_h\|_{L^\infty(\Omega)} \le C\, h^{-1/2} \|\bar{\boldsymbol{d}}_h\|_{H^1(\Omega)} \quad \forall\, \bar{\boldsymbol{d}}_h \in \boldsymbol{D}_h,$

(ii) $\|\bar{\boldsymbol{d}}_h\| \le C\, h^{-1/2} \|\bar{\boldsymbol{d}}_h\|_{L^{3/2}(\Omega)} \quad \forall\, \bar{\boldsymbol{d}}_h \in \boldsymbol{D}_h.$

(b) The approximation properties:

(i) $\|\boldsymbol{d} - I_h \boldsymbol{d}\| \le C\, h \|\boldsymbol{d}\|_{H^1(\Omega)} \quad \forall\, \boldsymbol{d} \in \boldsymbol{H}^1(\Omega),$

(ii) $\|p - K_h p\| \le C\, h \|p\|_{H^1(\Omega)} \quad \forall\, p \in H^1(\Omega) \cap L_0^2(\Omega),$

(iii) $\|\boldsymbol{u} - J_h \boldsymbol{u}\|_{H^1(\Omega)} \le C\, h \|\boldsymbol{u}\|_{H^2(\Omega)} \quad \forall\, \boldsymbol{u} \in \boldsymbol{H}^2(\Omega) \cap \boldsymbol{H}_0^1(\Omega),$

(iv) $\|\boldsymbol{d} - I_h \boldsymbol{d}\|_{H^1(\Omega)} \le C\, h \|\boldsymbol{d}\|_{H^2(\Omega)} \quad \forall\, \boldsymbol{d} \in \boldsymbol{H}^2(\Omega),$

(v) $\|\boldsymbol{d} - I_h \boldsymbol{d}\|_{W^{1,3}} \le C\, h \|\boldsymbol{d}\|_{W^{2,3}(\Omega)} \quad \forall\, \boldsymbol{d} \in \boldsymbol{W}^{2,3}(\Omega),$

(vi) $\|\boldsymbol{d} - I_h \boldsymbol{d}\|_{L^\infty} \le C\, h \|\boldsymbol{d}\|_{W^{1,\infty}(\Omega)} \quad \forall\, \boldsymbol{d} \in \boldsymbol{W}^{1,\infty}(\Omega),$

where I_h, J_h and K_h are interpolation operators into $\boldsymbol{D}_h$, $\boldsymbol{X}_h$ and Q_h, respectively.

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(c) The stability properties:
  (i) $\|J_h \boldsymbol{u}\| \leq C\|\boldsymbol{u}\| \quad \forall\, \boldsymbol{u} \in \boldsymbol{L}^2(\Omega)$,
  (ii) $\|I_h \boldsymbol{d}\|_{H^1(\Omega)} \leq C\|\boldsymbol{d}\|_{H^1(\Omega)} \quad \forall\, \boldsymbol{d} \in \boldsymbol{H}^1(\Omega)$,
  (iii) $\|I_h \boldsymbol{d}\|_{L^\infty(\Omega)} \leq C\|\boldsymbol{d}\|_{L^\infty(\Omega)} \quad \forall\, \boldsymbol{d} \in \boldsymbol{L}^\infty(\Omega)$,
  (iv) $\|I_h \boldsymbol{d}\|_{W^{1,3}(\Omega)} \leq C\|\boldsymbol{d}\|_{W^{1,3}(\Omega)} \quad \forall\, \boldsymbol{d} \in \boldsymbol{W}^{1,3}(\Omega)$.

(H3) *Inf-Sup condition* (Compatibility condition between $\boldsymbol{X}_h$ and Q_h): there exists $\beta > 0$ (independent of h) such that

$$\|q_h\|_{L^2_0(\Omega)} \leq \beta \sup_{\boldsymbol{v} \in \boldsymbol{X}_h \setminus \{0\}} \frac{\left(q_h, \nabla \cdot \boldsymbol{v}\right)}{\|\boldsymbol{v}\|_{H^1(\Omega)}}, \qquad \forall\, q_h \in Q_h.$$

(H4) Compatibility condition between $\boldsymbol{W}_h$ and $\boldsymbol{D}_h$: $\boldsymbol{D}_h \subset \boldsymbol{W}_h$.

Now, we are going to set up a concrete finite element spaces and interpolation operators satisfying the foregoing hypotheses:

$$\begin{aligned}
\boldsymbol{X}_h &= \left\{ \bar{\boldsymbol{u}}_h \in \mathcal{C}^0(\overline{\Omega})^3 \cap \boldsymbol{H}^1_0(\Omega) \,:\, \forall\, T \in \mathcal{T}_h, \bar{\boldsymbol{u}}_h|_T \in (\mathbb{P}_1 + bubble)^3 \right\}, \\
P_h &= \left\{ \bar{p}_h \in \mathcal{C}^0(\overline{\Omega}) \cap L^2_0(\Omega) \,:\, \forall\, T \in \mathcal{T}_h, \bar{p}_h|_T \in \mathbb{P}_1 \right\}, \\
\boldsymbol{W}_h &= \left\{ \bar{\boldsymbol{w}}_h \in \mathcal{C}^0(\overline{\Omega})^3 \,:\, \forall\, T \in \mathcal{T}_h, \bar{\boldsymbol{w}}_h|_T \in \mathbb{P}^3_1 \right\}, \\
\boldsymbol{D}_h &= \left\{ \bar{\boldsymbol{d}}_h \in \mathcal{C}^0(\overline{\Omega})^3 \,:\, \forall\, T \in \mathcal{T}_h, \bar{\boldsymbol{d}}_h|_T \in \mathbb{P}^3_1 \right\} \,,\ \boldsymbol{D}_{0h} = \boldsymbol{D}_h \cap \boldsymbol{H}^1_0(\Omega).
\end{aligned}$$

Another possibility is to construct $\boldsymbol{X}_h$ and/or $\boldsymbol{W}_h$ and $\boldsymbol{D}_h$ by using $\mathbb{P}_2$ approximation.

To define I_h, J_h and K_h, we may choice average interpolators of Scott–Zhang type [21]. For instance, we can choose the interpolator defined in [10] (see also [8]), in order to get stability properties in L^2 and L^∞ imposed in (H2).(c).(i) and (H2).(c).(iii). Finally, the discrete lifting $\boldsymbol{l}_h$ of the boundary datum $\boldsymbol{l}$ can also be constructed with a Scott–Zhang interpolator (that we denote SZ_h) as follows. Let $\widetilde{\boldsymbol{d}} \in \boldsymbol{H}^2(\Omega)$ the solution of

$$-\Delta \widetilde{\boldsymbol{d}} = 0 \quad \text{in } \Omega, \quad \widetilde{\boldsymbol{d}}|_{\partial\Omega} = \boldsymbol{l}, \tag{1.19}$$

and define $\boldsymbol{l}_h = SZ_h(\widetilde{\boldsymbol{d}})|_{\partial\Omega}$.

1.6. Main results of the paper

Although in general the maximum principle $|\boldsymbol{d}| \leq 1$ is not assured for the numerical approximations, we will get the following stability and convergence results.

Theorem 1.4 (Stability for non-truncated potential)**.** *Assume that hypotheses* (H0)–(H4) *hold. Further suppose that* (h, k, ε) *are chosen to satisfy the "initial estimate" constraint*

$$\frac{h}{\varepsilon} \leq C \tag{IE}$$

and the "stability" constraint

$$\lim_{(h,k,\varepsilon)\to 0} \frac{k}{h^2\varepsilon^2} = 0. \tag{S}$$

Then the solution of scheme (1.15)-(1.18) satisfies the "global energy inequality":

$$\begin{cases} E(\boldsymbol{u}_h^{r+1}, \boldsymbol{d}_h^{r+1}) + \dfrac{k}{2} \displaystyle\sum_{n=0}^{r} D(\boldsymbol{u}_h^{n+1}, \boldsymbol{w}_h^{n+1}) \\ + \dfrac{1}{2} \displaystyle\sum_{n=0}^{r} \left(\|\boldsymbol{u}_h^{n+1} - \boldsymbol{u}_h^n\|^2 + \|\nabla(\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n)\|^2 \right) \leq E(\boldsymbol{u}_h^0, \boldsymbol{d}_h^0), \end{cases} \tag{1.20}$$

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for each $r = 0, \cdots, N-1$. *In particular, one has the estimates (independent of* (h, k, ε)*):*

$$\text{i)} \max_{0\le n\le N} \|\boldsymbol{u}_h^n\| \le C, \qquad \text{ii)}\ k\sum_{n=0}^{N-1} \|\nabla \boldsymbol{u}_h^{n+1}\|^2 \le C, \ \text{iii)}\ \sum_{n=0}^{N-1} \|\boldsymbol{u}_h^{n+1} - \boldsymbol{u}_h^n\|^2 \le C,$$

$$\text{iv)} \max_{0\le n\le N} \|\boldsymbol{d}_h^n\|_{H^1(\Omega)} \le C, \ \text{v)}\ k\sum_{n=0}^{N-1} \|\boldsymbol{w}_h^{n+1}\|^2 \le C \quad \text{vi)}\ \sum_{n=0}^{N-1} \|\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n\|_{H^1(\Omega)}^2 \le C,$$

$$\text{vii)} \max_{0\le n\le N} \int_\Omega F_\varepsilon(\boldsymbol{d}_h^n) \le C.$$

Remark 1.5. Hypothesis (IE) will be applied to get the initial estimate $E(\boldsymbol{u}_h^0, \boldsymbol{d}_h^0) \le C$.

Corollary 1.6 (Stability for truncated potential)**.** *Assume that hypotheses* (H0)–(H4) *hold. Consider scheme (1.15)–(1.18) with* $\widetilde{F}_\varepsilon(\boldsymbol{d})$ *a truncated potential, as in Remark 1.1, satisfying (1.11) and such that*

$$\widetilde{F}_\varepsilon(\boldsymbol{d}) \in \mathcal{C}^2(\mathbb{R}^3; \mathbb{R}) \quad \textit{and} \quad \max_{\boldsymbol{d}\in\mathbb{R}^3} |D^2\widetilde{F}_\varepsilon(\boldsymbol{d})| \le \frac{C}{\varepsilon^2} \tag{1.21}$$

(here $|\cdot|$ *denotes the Euclidean norm of the Hessian matrix* $D^2\widetilde{F}_\varepsilon$*). Further suppose* (IE) *and*

$$\text{(S}')\qquad \lim_{(h,k,\varepsilon)\to 0} \frac{k}{h\,\varepsilon^2} = 0.$$

Then the statements of Theorem 1.4 remain true.

Note that (S′) is weakener than (S).

Theorem 1.7 (Convergence for truncated potential)**.** *Assume hypotheses* (H0)–(H4) *together with* (S′) *and the "convergence" constraint*

$$\text{(C)}\qquad \lim_{(h,\varepsilon)\to 0} \frac{h}{\varepsilon^2} = 0,$$

(which implies in particular that (IE) *holds). Consider scheme (1.15)–(1.18) with* $\widetilde{F}_\varepsilon(\boldsymbol{d})$ *as in Corollary 1.6 such that, for any* $\boldsymbol{d} \in \mathbb{R}^3$,

$$\widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d}) \wedge \boldsymbol{d} = 0, \tag{1.22}$$

where the symbol $\wedge$ *denotes the vectorial product, and*

$$\|\widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d})\|^2 \le \frac{C}{\varepsilon^2}\int_\Omega \widetilde{F}_\varepsilon(\boldsymbol{d}). \tag{1.23}$$

Then there exists a subsequence of solutions given by scheme (1.15)–(1.18) convergent, as $(h, k, \varepsilon) \to 0$*, towards a generalized Young measure-valued solution of the Ericksen–Leslie problem (1.1)–(1.3).*

Remark 1.8. An example of a truncated potential $\widetilde{F}_\varepsilon$, which satisfies all the previous hypotheses, is:

$$\widetilde{F}_\varepsilon(\boldsymbol{d}) := \begin{cases} \dfrac{1}{4\varepsilon^2}(|\boldsymbol{d}|^2 - 1)^2 = F_\varepsilon(\boldsymbol{d}) & \text{if } |\boldsymbol{d}| \le 1, \\ \dfrac{1}{\varepsilon^2}(|\boldsymbol{d}| - 1)^2 & \text{if } |\boldsymbol{d}| > 1, \end{cases}$$

whose gradient is

$$\widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d}) := \nabla_{\boldsymbol{d}}\widetilde{F}(\boldsymbol{d}) = \begin{cases} \dfrac{1}{\varepsilon^2}(|\boldsymbol{d}|^2 - 1)\boldsymbol{d} = \boldsymbol{f}_\varepsilon(\boldsymbol{d}) & \text{if } |\boldsymbol{d}| \le 1, \\ \dfrac{2}{\varepsilon^2}(|\boldsymbol{d}| - 1)\dfrac{\boldsymbol{d}}{|\boldsymbol{d}|} & \text{if } |\boldsymbol{d}| > 1. \end{cases}$$

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Then (1.11), (1.22) and (1.23) hold. Moreover, using the relations

$$\nabla|\boldsymbol{d}| = \frac{\boldsymbol{d}}{|\boldsymbol{d}|}, \quad \nabla(\frac{\boldsymbol{d}}{|\boldsymbol{d}|}) = \frac{1}{|\boldsymbol{d}|}Id - \frac{1}{|\boldsymbol{d}|^3}\boldsymbol{d}\otimes\boldsymbol{d},$$

one has

$$\nabla^2_{\boldsymbol{d}}\widetilde{F}(\boldsymbol{d}) = \begin{cases} \frac{1}{\varepsilon^2}\Big[(|\boldsymbol{d}|^2-1)Id + 2\boldsymbol{d}\otimes\boldsymbol{d}\Big] & \text{if } |\boldsymbol{d}|\le 1, \\ \frac{2}{\varepsilon^2}\Big(1-\frac{1}{|\boldsymbol{d}|}\Big)Id + \frac{2}{\varepsilon^2}\frac{1}{|\boldsymbol{d}|^3}\boldsymbol{d}\otimes\boldsymbol{d} & \text{if } |\boldsymbol{d}|>1, \end{cases}$$

hence (1.21) is deduced.

The rest of this work is organized as follows. In Section 2, we derive *a priori* energy estimates for scheme (1.15)–(1.18) from a discrete version of the energy law (1.5) by means of a recursive process with respect to the time step. Section 3 is devoted to the compactness results in $\boldsymbol{L}^2(Q)$ for the director vector and for the velocity (the latter result will be based on an estimate by perturbation of a fractional-time derivative). In Section 4 we guarantee that the limit orientation vector satisfies the pointwise constraint $|\boldsymbol{d}| = 1$ and we pass to the limit in an adequate reformulation of the $\boldsymbol{d}$-system. Then, we establish the convergence for the momentum equation in Section 5, obtaining a generalized Young measure related to the elastic tensor. Finally, in Section 6, some numerical computations are shown, demonstrating its stability at least numerically.

2. *A priori* estimates and weak convergence

2.1. Existence and uniqueness of the scheme

Since scheme (1.15)–(1.18) is an algebraic linear system, existence and uniqueness are equivalent. The uniqueness of a solution to scheme (1.15)–(1.18) follows along the same line of arguments as in obtaining *a priori* energy estimates. It is worth mentioning that we need not impose any additional constraint to prove the well-posedness of scheme (1.15)–(1.18). This is due to the fact that the potential term, which is explicitly treated, vanishes when comparing to different solutions.

2.2. A local discrete energy inequality

Now, we are going to obtain a "discrete local energy inequality", that will be essential for the *a priori* estimates of scheme (1.15)–(1.18). Recall the notation of the free energy

$$E(\boldsymbol{u},\boldsymbol{d}) = \frac{1}{2}\|\boldsymbol{u}\|^2 + \frac{\lambda}{2}\|\nabla\boldsymbol{d}\|^2 + \lambda\int_\Omega F_\varepsilon(\boldsymbol{d}),$$

and the physcial dissipation

$$D(\boldsymbol{u},\boldsymbol{w}) = \nu\|\nabla\boldsymbol{u}\|^2 + \lambda\gamma\,\|\boldsymbol{w}\|^2.$$

Lemma 2.1. *Assume that hypotheses* (H0)-(H4) *and constraint* (S) *hold. Suppose that there exists a constant* $C_0 > 0$*, independent of* h*,* k *and* ε*, such that*

$$E(\boldsymbol{u}_h^n, \boldsymbol{d}_h^n) \le C_0. \tag{2.1}$$

Then, there exists $\delta_0 > 0$ *small enough (depending only on* C_0*, but otherwise independent of* (h,k,ε) *and* n*) such that for all* (h,k,ε) *satisfying* $k/(h^2\varepsilon^2) \le \delta_0$ *(that is possible owing to constraint* (S)*), the corresponding solution* $(\boldsymbol{u}_h^{n+1}, \boldsymbol{d}_h^{n+1}, \boldsymbol{w}_h^{n+1})$ *of scheme (1.15)–(1.18) satisfies the following inequality:*

$$\begin{cases} E\left(\boldsymbol{u}_h^{n+1}, \boldsymbol{d}_h^{n+1}\right) - E\left(\boldsymbol{u}_h^n, \boldsymbol{d}_h^n\right) + \dfrac{k}{2}D\left(\boldsymbol{u}_h^{n+1}, \boldsymbol{w}_h^{n+1}\right) \\ +\dfrac{1}{2}\left(\|\boldsymbol{u}_h^{n+1} - \boldsymbol{u}_h^n\|^2 + \lambda\|\nabla\left(\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n\right)\|^2\right) \le 0. \end{cases} \tag{2.2}$$

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Corollary 2.2. *Assume that hypotheses (H0)–(H4) and constraint (S′) hold. Consider scheme (1.15)–(1.18) with $\widetilde{F}_\varepsilon(\boldsymbol{d})$ satisfying (1.11) and (1.21). Then the statements of Lemma 2.1 remain true if one assumes that $\widetilde{E}(\boldsymbol{u}_h^n, \boldsymbol{d}_h^n) \le C_0$ and $k/(h\varepsilon^2) \le \delta_0$ are satisfied.*

Proof of Lemma 2.1. Take $\bar{\boldsymbol{u}}_h = k\,\boldsymbol{u}_h^{n+1}$ in (1.15) and $\bar{p}_h = p_h^{n+1}$ in (1.16). Then the term $\Big(p_h^{n+1}, \nabla\cdot \boldsymbol{u}_h^{n+1}\Big)$ vanishes, and the identity $(a-b, 2a) = |a|^2 - |b|^2 + |a-b|^2$ leads to

$$\frac{1}{2}\Big(\|\boldsymbol{u}_h^{n+1}\|^2 - \|\boldsymbol{u}_h^n\|^2 + \|\boldsymbol{u}_h^{n+1} - \boldsymbol{u}_h^n\|^2\Big) + \nu\, k\|\nabla \boldsymbol{u}_h^{n+1}\|^2 - \lambda\, k\Big((\nabla \boldsymbol{d}_h^n)^t \boldsymbol{w}_h^{n+1}, \boldsymbol{u}_h^{n+1}\Big) = 0. \tag{2.3}$$

Next, consider $\bar{\boldsymbol{w}}_h = \lambda\, k \boldsymbol{w}_h^{n+1}$ in (1.17) jointly with $\bar{\boldsymbol{d}}_h = \boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n \in \boldsymbol{D}_{0h}$ in (1.18) to get

$$\begin{aligned}&\frac{\lambda}{2}\Big(\|\nabla \boldsymbol{d}_h^{n+1}\|^2 - \|\nabla \boldsymbol{d}_h^n\|^2 + \|\nabla(\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n)\|^2\Big) + \lambda\Big(\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n, \boldsymbol{f}_\varepsilon(\boldsymbol{d}_h^n)\Big)\\ &+\lambda\, k\Big(\boldsymbol{u}_h^{n+1}\cdot\nabla \boldsymbol{d}_h^n, \boldsymbol{w}_h^{n+1}\Big) + \lambda\,\gamma\, k\|\boldsymbol{w}_h^{n+1}\|^2 = 0.\end{aligned} \tag{2.4}$$

Now, we add (2.3) and (2.4) and use the identity

$$-\Big((\nabla \boldsymbol{d}_h^n)^t \boldsymbol{w}_h^{n+1}, \boldsymbol{u}_h^{n+1}\Big) + \Big(\boldsymbol{u}_h^{n+1}\cdot\nabla \boldsymbol{d}_h^n, \boldsymbol{w}_h^{n+1}\Big) = 0$$

to get

$$\begin{aligned}&\frac{1}{2}\Big(\|\boldsymbol{u}_h^{n+1}\|^2 + \lambda\|\nabla \boldsymbol{d}_h^{n+1}\|^2\Big) - \frac{1}{2}\Big(\|\boldsymbol{u}_h^n\|^2 + \lambda\|\nabla \boldsymbol{d}_h^n\|^2\Big) + \frac{1}{2}\Big(\|\boldsymbol{u}_h^{n+1} - \boldsymbol{u}_h^n\|^2 + \lambda\|\nabla(\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n)\|^2\Big)\\ &\qquad + k\, D(\boldsymbol{u}_h^{n+1}, \boldsymbol{w}_h^{n+1}) + \lambda\Big(\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n, \boldsymbol{f}_\varepsilon(\boldsymbol{d}_h^n)\Big) = 0.\end{aligned} \tag{2.5}$$

Next, we decompose the last term of (2.5) as follows:

$$\begin{aligned}\lambda\Big(\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n, \boldsymbol{f}_\varepsilon(\boldsymbol{d}_h^n)\Big) &= \frac{\lambda}{\varepsilon^2}\Big(\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n, (|\boldsymbol{d}_h^{n+1}|^2 - 1)\boldsymbol{d}_h^n\Big)\\ &\quad + \frac{\lambda}{\varepsilon^2}\Big(\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n, (|\boldsymbol{d}_h^n|^2 - |\boldsymbol{d}_h^{n+1}|^2)\boldsymbol{d}_h^n\Big) := I_1 - I_2.\end{aligned}$$

Rewriting I_1 as

$$\begin{aligned}I_1 &= \frac{\lambda}{2\varepsilon^2}\int_\Omega (|\boldsymbol{d}_h^{n+1}|^2 - 1)(|\boldsymbol{d}_h^{n+1}|^2 - |\boldsymbol{d}_h^n|^2 - |\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n|^2)\\ &= \frac{\lambda}{4\varepsilon^2}\int_\Omega \Big((|\boldsymbol{d}_h^{n+1}|^2 - 1)^2 - (|\boldsymbol{d}_h^n|^2 - 1)^2 + (|\boldsymbol{d}_h^{n+1}|^2 - |\boldsymbol{d}_h^n|^2)^2\Big)\frac{\lambda}{2\varepsilon^2}\int_\Omega (1 - |\boldsymbol{d}_h^{n+1}|^2)|\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n|^2\end{aligned}$$

and bounding I_2 as

$$I_2 \le \frac{C}{\varepsilon^2}\|\boldsymbol{d}_h^n\|^2_{L^\infty(\Omega)}\|\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n\|^2 + \frac{\lambda}{8\varepsilon^2}\int_\Omega (|\boldsymbol{d}_h^{n+1}|^2 - |\boldsymbol{d}_h^n|^2)^2,$$

we arrive at the inequality

$$\begin{aligned}\lambda\Big(\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n, \boldsymbol{f}_\varepsilon(\boldsymbol{d}_h^n)\Big) &\ge \lambda\int_\Omega F_\varepsilon(\boldsymbol{d}_h^{n+1}) - \lambda\int_\Omega F_\varepsilon(\boldsymbol{d}_h^n)\\ &\quad + \frac{\lambda}{2\varepsilon^2}\int_\Omega\left(\frac{1}{4}(|\boldsymbol{d}_h^{n+1}|^2 - |\boldsymbol{d}_h^n|^2)^2 + |\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n|^2\right)\\ &\quad - \frac{C}{\varepsilon^2}\Big(\|\boldsymbol{d}_h^n\|^2_{L^\infty(\Omega)} + \|\boldsymbol{d}_h^{n+1}\|^2_{L^\infty(\Omega)}\Big)\|\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n\|^2.\end{aligned} \tag{2.6}$$

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Therefore, (2.5) and (2.6) yield

$$\begin{cases} E(\boldsymbol{u}_h^{n+1},\boldsymbol{d}_h^{n+1}) - E(\boldsymbol{u}_h^{n},\boldsymbol{d}_h^{n}) + k\,D(\boldsymbol{u}_h^{n+1},\boldsymbol{w}_h^{n+1}) \\ +\dfrac{1}{2}\Big(\|\boldsymbol{u}_h^{n+1}-\boldsymbol{u}_h^{n}\|^2 + \lambda\|\nabla(\boldsymbol{d}_h^{n+1}-\boldsymbol{d}_h^{n})\|^2\Big) \\ \le \dfrac{C}{\varepsilon^2}\Big(\|\boldsymbol{d}_h^{n}\|^2_{L^\infty(\Omega)} + \|\boldsymbol{d}_h^{n+1}\|^2_{L^\infty(\Omega)}\Big)\|\boldsymbol{d}_h^{n+1}-\boldsymbol{d}_h^{n}\|^2 := I_3. \end{cases} \tag{2.7}$$

The main idea now is to absorb the term I_3 with the physical dissipation $k\,D(\boldsymbol{u}_h^{n+1},\boldsymbol{w}_h^{n+1})$, with the help of (S).

In order to bound the term $\|\boldsymbol{d}_h^{n+1}-\boldsymbol{d}_h^{n}\|^2$ of I_3, we take $\bar{\boldsymbol{w}}_h = P_h^0(\bar{\boldsymbol{w}})$, for any $\bar{\boldsymbol{w}}\in \boldsymbol{L}^3(\Omega)$, as test functions into (1.17), where P_h^0 is the L^2-projector onto $\boldsymbol{W}_h$, to obtain

$$\Big(\frac{\boldsymbol{d}_h^{n+1}-\boldsymbol{d}_h^{n}}{k},\bar{\boldsymbol{w}}\Big) = -\Big((\boldsymbol{u}_h^{n+1}\cdot\nabla)\boldsymbol{d}_h^{n}, P_h^0(\bar{\boldsymbol{w}})\Big) - \gamma\Big(\boldsymbol{w}_h^{n+1},\bar{\boldsymbol{w}}\Big),$$

where hypothesis (H4) allows us to neglect P_h^0 in the discrete time derivative term. Then, a standard duality argument using the fact that $L^{3/2}(\Omega) = L^3(\Omega)'$ jointly to the stability property $\|P_h^0\bar{w}\|_{L^3} \le C\,\|\bar{w}\|_{L^3}$ [7]) and (2.1) (which in particular implies that $\lambda\|\nabla\boldsymbol{d}_h^n\|^2 \le 2\,C_0$) yields

$$\left\|\frac{\boldsymbol{d}_h^{n+1}-\boldsymbol{d}_h^{n}}{k}\right\|^2_{L^{3/2}(\Omega)} \le C\Big(\|\boldsymbol{u}_h^{n+1}\|^2_{L^6}\|\nabla\boldsymbol{d}_h^{n}\|^2 + \|\boldsymbol{w}_h^{n+1}\|^2\Big) \le C\,D(\boldsymbol{u}_h^{n+1},\boldsymbol{w}_h^{n+1}). \tag{2.8}$$

Next, the term I_3 can be handled, using inverse inequalities $(H2).(a).(\boldsymbol{i})$ and (H2).(a).(ii), as

$$\begin{aligned} I_3 &= C\frac{k^2}{\varepsilon^2}\Big(\|\boldsymbol{d}_h^{n}\|^2_{L^\infty(\Omega)} + \|\boldsymbol{d}_h^{n+1}\|^2_{L^\infty(\Omega)}\Big)\left\|\frac{\boldsymbol{d}_h^{n+1}-\boldsymbol{d}_h^{n}}{k}\right\|^2 \\ &\le C\frac{k^2}{h^2\varepsilon^2}\Big(\|\boldsymbol{d}_h^{n}\|^2_{H^1(\Omega)} + \|\boldsymbol{d}_h^{n+1}\|^2_{H^1(\Omega)}\Big)\left\|\frac{\boldsymbol{d}_h^{n+1}-\boldsymbol{d}_h^{n}}{k}\right\|^2_{L^{3/2}(\Omega)}. \end{aligned}$$

Therefore, by using (2.8) the bound of I_3 remains as

$$I_3 \le C\frac{k}{h^2\varepsilon^2}\Big(\|\boldsymbol{d}_h^{n+1}\|^2_{H^1(\Omega)} + \|\boldsymbol{d}_h^{n}\|^2_{H^1(\Omega)}\Big)k\,D(\boldsymbol{u}_h^{n+1},\boldsymbol{w}_h^{n+1}). \tag{2.9}$$

Our next goal is to bound $\|\boldsymbol{d}_h^{n+1}\|_{H^1(\Omega)}$ in terms of $E(\boldsymbol{d}_h^n,\boldsymbol{u}_h^n)$. Recall that $\|\boldsymbol{d}_h^n\|_{H^1(\Omega)} \le C$, because of (2.1). Consider (2.5) rewritten as

$$\begin{aligned} \frac{1}{2}\Big(\|\boldsymbol{u}_h^{n+1}\|^2 + \lambda\|\nabla\boldsymbol{d}_h^{n+1}\|^2\Big) + \frac{1}{2}\Big(\|\boldsymbol{u}_h^{n+1}-\boldsymbol{u}_h^{n}\|^2 + \lambda\|\nabla(\boldsymbol{d}_h^{n+1}-\boldsymbol{d}_h^{n})\|^2\Big) \\ + k\,D(\boldsymbol{u}_h^{n+1},\boldsymbol{w}_h^{n+1}) = \frac{1}{2}\Big(\|\boldsymbol{u}_h^{n}\|^2 + \lambda\|\nabla\boldsymbol{d}_h^{n}\|^2\Big) - \lambda\Big(\boldsymbol{d}_h^{n+1}-\boldsymbol{d}_h^{n},\boldsymbol{f}_\varepsilon(\boldsymbol{d}_h^{n})\Big) \end{aligned} \tag{2.10}$$

and bound the last term, using (2.8), the inequality

$$\|\boldsymbol{f}_\varepsilon(\boldsymbol{d})\|^2 \le \frac{4}{\varepsilon^2}\|\boldsymbol{d}\|^2_{L^\infty}\int_\Omega F_\varepsilon(\boldsymbol{d}) \tag{2.11}$$

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and the estimates $\int_\Omega F_\varepsilon(\boldsymbol{d}_h^n) \le C$ and $\|\boldsymbol{d}_h^n\|^2_{H^1(\Omega)} \le C$, from (2.1), as follows:

$$\begin{aligned}\lambda\Big(\boldsymbol{d}_h^{n+1}-\boldsymbol{d}_h^n, \boldsymbol{f}_\varepsilon(\boldsymbol{d}_h^n)\Big) &\le C\,k\left\|\frac{\boldsymbol{d}_h^{n+1}-\boldsymbol{d}_h^n}{k}\right\|\|\boldsymbol{f}_\varepsilon(\boldsymbol{d}_h^n)\|\\ &\le \delta\,k\left\|\frac{\boldsymbol{d}_h^{n+1}-\boldsymbol{d}_h^n}{k}\right\|^2_{L^{3/2}(\Omega)} + C_\delta\frac{k}{h\varepsilon^2}\|\boldsymbol{d}_h^n\|^2_{L^\infty(\Omega)}\int_\Omega F_\varepsilon(\boldsymbol{d}_h^n)\\ &\le C\,\delta\,k\,D(\boldsymbol{u}_h^{n+1},\boldsymbol{w}_h^{n+1}) + C_\delta\frac{k}{h^2\varepsilon^2}\|\boldsymbol{d}_h^n\|^2_{H^1(\Omega)},\\ &\le C\,\delta\,k\,D(\boldsymbol{u}_h^{n+1},\boldsymbol{w}_h^{n+1}) + C_\delta\frac{k}{h^2\varepsilon^2}.\end{aligned}$$

Here, $\delta>0$ is arbitrary, and thus $C_\delta = C/\delta$. Then, from (2.10), we can get, for $\delta>0$ small enough,

$$\begin{aligned}\frac{1}{2}\Big(\|\boldsymbol{u}_h^{n+1}\|^2+\lambda\|\nabla\boldsymbol{d}_h^{n+1}\|^2\Big)+\frac{1}{2}\Big(\|\boldsymbol{u}_h^{n+1}-\boldsymbol{u}_h^n\|^2+\lambda\|\nabla(\boldsymbol{d}_h^{n+1}-\boldsymbol{d}_h^n)\|^2\Big)\\ +\frac{k}{2}D(\boldsymbol{u}_h^{n+1},\boldsymbol{w}_h^{n+1}) \le \frac{1}{2}\Big(\|\boldsymbol{u}_h^n\|^2+\lambda\|\nabla\boldsymbol{d}_h^n\|^2\Big)+C\frac{k}{h^2\varepsilon^2}.\end{aligned}$$

In particular, one obtains

$$\frac{\lambda}{2}\|\nabla\boldsymbol{d}_h^{n+1}\|^2 \le E(\boldsymbol{u}_h^n,\boldsymbol{d}_h^n)+C\frac{k}{h^2\varepsilon^2}.$$

Consequently, from (2.1) and (S), for each (k,h,ε) such that $k/(h^2\varepsilon^2)\le\delta_0$, with δ_0 small enough, we get the bound

$$\|\nabla\boldsymbol{d}_h^{n+1}\|^2 \le \frac{2}{\lambda}\left(C_0+C\frac{k}{h^2\varepsilon^2},\right)\le\frac{4C_0}{\lambda}.$$

Next, the discrete lifting $SZ_h(\widetilde{\boldsymbol{d}})$ of the boundary datum $\boldsymbol{l}_h$ (which is stable in the $\boldsymbol{H}^1$-norm) allows us to complete up to the $H^1(\Omega)$-norm and hence

$$\|\boldsymbol{d}_h^n\|^2_{H^1(\Omega)}\le C,\quad \|\boldsymbol{d}_h^{n+1}\|^2_{H^1(\Omega)}\le C, \tag{2.12}$$

with C depending on C_0. Finally, using (2.12) in (2.9), I_3 remains bounded as

$$I_3 \le C\frac{k}{h^2\varepsilon^2}k\,D(\boldsymbol{u}_h^{n+1},\boldsymbol{w}_h^{n+1}).$$

By hypothesis (S), we may choice δ_0 such that

$$C\frac{k}{h^2\,\varepsilon^2}\le\frac{1}{2}$$

arriving at

$$I_3\le\frac{k}{2}\,D(\boldsymbol{u}_h^{n+1},\boldsymbol{w}_h^{n+1}).$$

Finally, we obtain inequality (2.2) by absorbing the above estimate of I_3 is absorbed by the physical dissipation $k\,D(\boldsymbol{u}_h^{n+1},\boldsymbol{w}_h^{n+1})$ in (2.7). □

Remark 2.3. Following the proof of Lemma 2.1 for two-dimensional ($2D$) domains, the stability constraint (S) could be weakened to

$$\lim_{(h,k,\varepsilon)\to 0}\frac{k}{h^\alpha\varepsilon^2}=0$$

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for any $\alpha > 0$ small enough. This is possible because the inverse inequality $\|\bar{\boldsymbol{d}}_h\|_{L^\infty(\Omega)} \leq C\, h^{-\alpha}\|\bar{\boldsymbol{d}}_h\|_{H^1(\Omega)}$ can be used instead of (H2).(a).(***i***) and estimate (2.8) in $\boldsymbol{L}^{2-\alpha}(\Omega)$ instead of $\boldsymbol{L}^{3/2}(\Omega)$ owing to the Sobolev embedding $H^1(\Omega) \hookrightarrow L^\beta(\Omega)$ for all $\beta > 0$ (valid only in $2D$ domains). It means that the dependence of constraint (S) on h is very weak. In fact, for the numerical simulations in Section 6, we will take $k = \mathcal{O}(\varepsilon^2)$, showing (at least numerically), that scheme (1.15)–(1.18) is stable in the sense that a decreasing energy is obtained.

Proof of Corollary 2.2. Recall that we are now considering the truncated potential function $\widetilde{F}_\varepsilon(\boldsymbol{d})$. Thus we have the following inequality (instead of (2.6))

$$\lambda\Big(\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n, \widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d}_h^n)\Big) \geq \lambda \int_\Omega \widetilde{F}_\varepsilon(\boldsymbol{d}_h^{n+1}) - \lambda \int_\Omega \widetilde{F}_\varepsilon(\boldsymbol{d}_h^n) - \frac{C}{\varepsilon^2}\|\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n\|^2,$$

which can be deduced from the Taylor expansion up to order 2 of $\widetilde{F}_\varepsilon(\boldsymbol{d}_h^{n+1})$ with center at $\boldsymbol{d}_h^n$. Moreover, one must use (1.21) to bound the second-order remainder term.

Then (2.7) is now changed by:

$$\begin{cases} \widetilde{E}\left(\boldsymbol{u}_h^{n+1}, \boldsymbol{d}_h^{n+1}\right) - \widetilde{E}\left(\boldsymbol{u}_h^n, \boldsymbol{d}_h^n\right) + k\, D\left(\boldsymbol{u}_h^{n+1}, \boldsymbol{w}_h^{n+1}\right) \\ +\dfrac{1}{2}\Big(\|\boldsymbol{u}_h^{n+1} - \boldsymbol{u}_h^n\|^2 + \lambda\|\nabla\left(\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n\right)\|^2\Big) \\ \leq \dfrac{C}{\varepsilon^2}\|\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n\|^2 := \widetilde{I}_3 \leq C\dfrac{k}{h\varepsilon^2} k\, D\left(\boldsymbol{u}_h^{n+1}, \boldsymbol{w}_h^{n+1}\right), \end{cases} \tag{2.13}$$

where the right hand-side of (2.13) can be absorbed by the physical dissipation $k\, D(\boldsymbol{u}_h^{n+1}, \boldsymbol{w}_h^{n+1})$ provided that $Ck/(h\varepsilon^2) \leq 1/2$ holds (which is possible owing to (S')). Again, as in Remark 2.3, the term h in (S') can be changed by h^α $(\alpha > 0)$ in $2D$ domains. □

Remark 2.4. Following in the case of using $\widetilde{F}_\varepsilon(\boldsymbol{d})$ instead of $F_\varepsilon(\boldsymbol{d})$, if hypothesis $(H4)$ is not imposed, then we can only control the projection part $\frac{C}{\varepsilon^2}\|P_h^0(\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n)\|^2$ of $\widetilde{I}_3$ from the arguments shown in the proof of Lemma 2.1. Instead, the orthogonal part is estimated as

$$\frac{C}{\varepsilon^2}\|(I - P_h^0)(\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n)\|^2 \leq C\,\frac{h^2}{\varepsilon^2}\|\nabla(\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n)\|^2.$$

This bound can be absorbed by the numerical dissipation term $\lambda\|\nabla(\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n)\|^2/2$ of (2.13), imposing h/ε small enough. Therefore, the *a priori* energy estimates proved in Corollary 2.2 also holds by replacing hypothesis (H4) by h/ε small enough. This fact will be noted in the numerical computations of Section 6.

2.3. Initial estimates

In order to get global stability estimates for scheme (1.15)–(1.18), we will need an initial estimate.

Lemma 2.5. *Assume that hypotheses* (H0) *and* (H2) *together with* (IE) *hold. Then there exists a constant* $C_0 > 0$ *independent of* h k, *and* ε *such that*

$$E(\boldsymbol{u}_h^0, \boldsymbol{d}_h^0) \leq C_0 \quad \textit{and} \quad \widetilde{E}(\boldsymbol{u}_h^0, \boldsymbol{d}_h^0) \leq C_0. \tag{2.14}$$

Proof. For instance, (2.14) can be guaranteed defining $\boldsymbol{d}_h^0 = I_h\boldsymbol{d}_0$ and $\boldsymbol{u}_h^0 = J_h\boldsymbol{u}_0$. Indeed, in view of the stability of the interpolation operators J_h and I_h given in (H2).(c).(i)–(ii), there exist $K_1 > 0$ and $K_2 > 0$ such

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that $\lambda\|\nabla \boldsymbol{d}_h^0\|^2/2 \le K_1$ and $\|\boldsymbol{u}_h^0\|^2/2 \le K_2$. Then, it suffices to bound $\lambda\int_\Omega F_\varepsilon(\boldsymbol{d}_h^0) \le K_3$ and $\lambda\int_\Omega \widetilde{F}_\varepsilon(\boldsymbol{d}_h^0) \le K_3$, because then (2.14) holds defining $C_0 = K_1 + K_2 + K_3$. Since $|\boldsymbol{d}_0| = 1$ in Ω, we have

$$\int_\Omega F_\varepsilon(\boldsymbol{d}_h^0) = \frac{1}{4\varepsilon^2}\int_\Omega \left(|\boldsymbol{d}_h^0|^2 - |\boldsymbol{d}_0|^2\right)^2 = \frac{1}{4\varepsilon^2}\int_\Omega \left((\boldsymbol{d}_0 + \boldsymbol{d}_h^0)\cdot(\boldsymbol{d}_0 - \boldsymbol{d}_h^0)\right)^2$$
$$\le \frac{1}{4\varepsilon^2}\|\boldsymbol{d}_0 + \boldsymbol{d}_h^0\|^2_{L^\infty(\Omega)}\|\boldsymbol{d}_0 - \boldsymbol{d}_h^0\|^2.$$

Now, using the approximation property (H2).(b).(***i***), the stability condition (H2).(c).(iii) and the constraint (IE), we can find a positive constant K_3 such that

$$\lambda\int_\Omega F_\varepsilon(\boldsymbol{d}_h^0) \le C\frac{h^2}{\varepsilon^2}\|\boldsymbol{d}_0\|^2_{H^1} \le K_3.$$

The bound for $\lambda\int_\Omega \widetilde{F}_\varepsilon(\boldsymbol{d}_h^0)$ is similar. □

Remark 2.6. Notice that the initial estimate for the energy (2.14) has been possible because the vector $\boldsymbol{d}$ has a vector with two or three components, hence there exists non-constant initial conditions $\boldsymbol{d}_0 \in \boldsymbol{H}^1(\Omega)$ such that $|\boldsymbol{d}_0| = 1$ in Ω. For instance, in $2D$ domains, it suffices to define $\boldsymbol{d}_0(\boldsymbol{x}) = (sin(\theta(\boldsymbol{x})), cos(\theta(\boldsymbol{x})))$ with $\theta(\boldsymbol{x})$ a regular function.

2.4. Conditional stability (Proofs of Thm. 1.4 and Cor. 1.6)

It suffices to prove the local energy inequality (2.2) for all $n = 0, \dots, N-1$ because in this case the global energy inequality (1.20) and estimates (i)–(vii) can be deduced by adding (2.2) with respect to n and using the bound for the initial data (2.14).

To prove (2.2) we argue by induction on n. Clearly, $(\boldsymbol{u}_h^0, \boldsymbol{d}_h^0)$ satisfies the hypotheses of Lemma 2.1 (or Cor. 2.2) for $n = 0$: $E(\boldsymbol{u}_h^0, \boldsymbol{d}_h^0) \le C_0$ (or $\widetilde{E}(\boldsymbol{u}_h^0, \boldsymbol{d}_h^0) \le C_0$), then (2.2) holds for $n = 0$. In particular,

$$E\left(\boldsymbol{u}_h^1, \boldsymbol{d}_h^1\right) \le E\left(\boldsymbol{u}_h^0, \boldsymbol{d}_h^0\right) \le C_0 \quad \left(\text{or } \widetilde{E}\left(\boldsymbol{u}_h^1, \boldsymbol{d}_h^1\right) \le \widetilde{E}\left(\boldsymbol{u}_h^0, \boldsymbol{d}_h^0\right) \le C_0\right).$$

Now, we assume that $(\boldsymbol{u}_h^s, \boldsymbol{d}_h^s)$ satisfies (2.2) for $s = 1, ..., n-1$. Adding (2.2) for $s = 1, ..., n-1$,

$$E\left(\boldsymbol{u}_h^n, \boldsymbol{d}_h^n\right) \le E\left(\boldsymbol{u}_h^0, \boldsymbol{d}_h^0\right) \le C_0 \quad \left(\text{or } \widetilde{E}\left(\boldsymbol{u}_h^n, \boldsymbol{d}_h^n\right) \le \widetilde{E}\left(\boldsymbol{u}_h^0, \boldsymbol{d}_h^0\right) \le C_0\right),$$

which implies from Lemma 2.1 (or Cor. 2.2) that (2.2) holds for n.

2.5. Global estimates and weak convergence

Definition 2.7. Let $\boldsymbol{u}_{h,k,\varepsilon}$ (respectively $\boldsymbol{u}^0_{h,k,\varepsilon}$) be the piecewise constant function taking the value $\boldsymbol{u}_h^{n+1}$ on $(t_n, t_{n+1}]$ (respectively $\boldsymbol{u}_h^n$). Analogously, we define $p_{h,k,\varepsilon}$, $\boldsymbol{w}_{h,k,\varepsilon}$, $\boldsymbol{d}_{h,k,\varepsilon}$ and $\boldsymbol{d}^0_{h,k,\varepsilon}$. Moreover, let $\boldsymbol{u}^l_{h,k,\varepsilon} \in C^0([0,T];\boldsymbol{V}_h)$ and $\boldsymbol{d}^l_{h,k,\varepsilon} \in C^0([0,T];\boldsymbol{D}_h)$ be the piecewise linear functions such that $\boldsymbol{u}^l_{h,k,\varepsilon}(t_n) = \boldsymbol{u}_h^n$ and $\boldsymbol{d}^l_{h,k,\varepsilon}(t_n) = \boldsymbol{d}_h^n$, respectively.

With the previous notations, Theorem 1.4 (or Cor. 1.6) yields to the following stability estimates (independent of (h,k,ε)):

$$\begin{aligned}
\boldsymbol{u}_{h,k,\varepsilon} \quad &\text{is bounded in} \quad L^\infty(0,T;\boldsymbol{L}^2(\Omega)) \cap L^2(0,T,\boldsymbol{H}^1_0(\Omega)),\\
\boldsymbol{u}^l_{h,k,\varepsilon}, \boldsymbol{u}^0_{h,k,\varepsilon}, \quad &\text{are bounded in} \quad L^\infty(0,T;\boldsymbol{L}^2(\Omega)),\\
\boldsymbol{d}^l_{h,k,\varepsilon}, \boldsymbol{d}^0_{h,k,\varepsilon}, \boldsymbol{d}_{h,k,\varepsilon} \quad &\text{are bounded in} \quad L^\infty(0,T;\boldsymbol{H}^1(\Omega)), \qquad (2.15)\\
\boldsymbol{w}_{h,k,\varepsilon} \quad &\text{is bounded in} \quad L^2(0,T;\boldsymbol{L}^2(\Omega)). \qquad (2.16)
\end{aligned}$$

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Moreover, from estimates (iii) and (vi) of Theorem 1.4,

$$\boldsymbol{u}^0_{h,k,\varepsilon} - \boldsymbol{u}_{h,k,\varepsilon} \to 0 \quad \text{and} \quad \boldsymbol{u}^l_{h,k,\varepsilon} - \boldsymbol{u}_{h,k,\varepsilon} \to 0 \quad \text{in } L^2(0,T;\boldsymbol{L}^2(\Omega)),$$

with the same convergences for $\boldsymbol{d}^l_{h,k,\varepsilon}, \boldsymbol{d}^0_{h,k,\varepsilon}, \boldsymbol{d}_{h,k,\varepsilon}$ in $L^2(0,T;\boldsymbol{H}^1(\Omega))$.

By weak compactness results, there exist subsequences (denoted in the same way) of $\{\boldsymbol{u}^l_{h,k,\varepsilon}\}_{h,k,\varepsilon}$, $\{\boldsymbol{u}_{h,k,\varepsilon}\}_{h,k,\varepsilon}$, $\{\boldsymbol{u}^0_{h,k,\varepsilon}\}_{h,k,\varepsilon}$, $\{\boldsymbol{d}^l_{h,k,\varepsilon}\}_{h,k,\varepsilon}$, $\{\boldsymbol{d}^0_{h,k,\varepsilon}\}_{h,k,\varepsilon}$, $\{\boldsymbol{d}_{h,k,\varepsilon}\}_{h,k,\varepsilon}$, and $\{\boldsymbol{w}_{h,k,\varepsilon}\}_{h,k,\varepsilon}$, and limit functions $\boldsymbol{u}$, $\boldsymbol{d}$, and $\boldsymbol{w}$ satisfying the following weak convergences as $(h,k,\varepsilon) \to 0$:

$$\begin{gathered}\boldsymbol{u}_{h,k,\varepsilon} \to \boldsymbol{u} \text{ in } L^2\left(0,T;\boldsymbol{H}^1_0(\Omega)\right)\text{-weak and } L^\infty\left(0,T;\boldsymbol{L}^2(\Omega)\right)\text{-weak}*,\\ \boldsymbol{u}^l_{h,k,\varepsilon} \to \boldsymbol{u}, \quad \boldsymbol{u}^0_{h,k,\varepsilon} \to \boldsymbol{u}, \text{ in } L^\infty\left(0,T;\boldsymbol{L}^2(\Omega)\right)\text{-weak}*,\end{gathered}$$

$$\boldsymbol{d}^l_{h,k,\varepsilon} \to \boldsymbol{d}, \quad \boldsymbol{d}^0_{h,k,\varepsilon} \to \boldsymbol{d}, \quad \boldsymbol{d}_{h,k,\varepsilon} \to \boldsymbol{d} \text{ in } L^\infty\left(0,T;H^1(\Omega)\right)\text{-weak}*, \tag{2.17}$$

$$\boldsymbol{w}_{h,k,\varepsilon} \to \boldsymbol{w} \text{ in } L^2(0,T;\boldsymbol{L}^2(\Omega))\text{-weak}. \tag{2.18}$$

3. Compactness for $\boldsymbol{d}$ and $\boldsymbol{u}$

3.1. Strong convergence for the director vector

By using the dual estimate (2.8) for the time discrete derivative of the director, we arrive at the following

Lemma 3.1. *Under the assumptions of Theorem 1.4 (or Cor. 1.6), there exists $C > 0$ independent of (h,k,ε) such that*

$$k \sum_{n=0}^{N-1} \left\| \frac{\boldsymbol{d}^{n+1}_h - \boldsymbol{d}^n_h}{k} \right\|^2_{L^{3/2}(\Omega)} \le C. \tag{3.1}$$

Note that (3.1) can be expressed as

$$\partial_t \boldsymbol{d}^l_{h,k,\varepsilon} \quad \text{is bounded in } L^2\left(0,T;\boldsymbol{L}^{3/2}(\Omega)\right).$$

Therefore, from (2.15) and (3.1), a compactness result of Aubin–Lions type implies that there exists a subsequence of $\boldsymbol{d}^l_{h,k,\varepsilon}$ (denoted in the same way) such that

$$\boldsymbol{d}^l_{h,k,\varepsilon} \to \boldsymbol{d} \quad \text{in } C([0,T];\boldsymbol{L}^r(\Omega)) \text{ as } (k,h,\varepsilon) \to 0 \text{ for any } r : 1 \le r < 6.$$

As a consequence of estimate (vi) in Theorem 1.4 and (2.15), one obtains

$$\boldsymbol{d}^0_{h,k,\varepsilon}, \boldsymbol{d}_{h,k,\varepsilon} \to \boldsymbol{d} \quad \text{in } L^q\left(0,T;\boldsymbol{L}^r(\Omega)\right) \text{ as } (h,k,\varepsilon) \to 0, \tag{3.2}$$

with $1 \le r < 6$ and $1 \le q < \infty$.

3.2. Strong convergence for the velocity

This section is devoted to obtaining the following compactness result for the discrete velocity

$$\boldsymbol{u}_{h,k,\varepsilon} \to \boldsymbol{u} \quad \text{in } L^2\left(0,T;\boldsymbol{L}^2(\Omega)\right)\text{-strong as } (k,h,\varepsilon) \to 0. \tag{3.3}$$

Let

$$\boldsymbol{V}_h = \left\{ \boldsymbol{v}_h \in \boldsymbol{X}_h : \left(\nabla \cdot \boldsymbol{v}_h, q_h\right) = 0 \ \forall\, q_h \in Q_h \right\}$$

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and consider $A_h^{-1} : \boldsymbol{V}_h \to \boldsymbol{V}_h$ the discrete inverse Stokes operator defined as

$$\left(\nabla A_h^{-1}\boldsymbol{u}_h, \nabla \boldsymbol{v}_h\right) = \left(\boldsymbol{u}_h, \boldsymbol{v}_h\right) \quad \forall\, \boldsymbol{v}_h \in \boldsymbol{V}_h. \tag{3.4}$$

Notice that (3.4) is well-defined thanks to the Inf-Sup condition $(H3)$.

Observe that $\|\nabla A_h^{-1}\boldsymbol{u}_h\|$ and $\|\boldsymbol{u}_h\|_{\boldsymbol{V}_h'}$ are equivalent norms in $\boldsymbol{V}_h'$ (the dual space of $\boldsymbol{V}_h$). Indeed, we take $\boldsymbol{v}_h = A_h^{-1}\boldsymbol{u}_h$ in (3.4), then

$$\|\nabla A_h^{-1}\boldsymbol{u}_h\|^2 = \left(\boldsymbol{u}_h, A_h^{-1}\boldsymbol{u}_h\right) \leq C\|\boldsymbol{u}_h\|_{\boldsymbol{V}_h'}\|\nabla A_h^{-1}\boldsymbol{u}_h\|,$$

whence

$$\|\nabla A_h^{-1}\boldsymbol{u}_h\| \leq C\|\boldsymbol{u}_h\|_{\boldsymbol{V}_h'}.$$

Conversely, we take any $\boldsymbol{v}_h \in \boldsymbol{V}_h$ in (3.4), then

$$\left(\boldsymbol{u}_h, \boldsymbol{v}_h\right) = \left(\nabla A_h^{-1}\boldsymbol{u}_h, \nabla \boldsymbol{v}_h\right) \leq \|\nabla A_h^{-1}\boldsymbol{u}_h\|\,\|\nabla \boldsymbol{v}_h\| \quad \forall\, \boldsymbol{v}_h \in \boldsymbol{V}_h.$$

The dual definition of $\boldsymbol{V}_h'$ provides $\|\boldsymbol{u}_h\|_{\boldsymbol{V}_h'} \leq \|\nabla A_h^{-1}\boldsymbol{u}_h\|$.

Lemma 3.2. *Under the conditions of Theorem 1.4 or Corollary 1.6, it follows that*

$$\int_0^{T-\delta} \|\boldsymbol{u}_{h,k,\varepsilon}(t+\delta) - \boldsymbol{u}_{h,k,\varepsilon}(t)\|_{\boldsymbol{V}_h'}^2 \,\mathrm{d}t \leq C\,\delta^{1/2} \quad \forall\, \delta : 0 < \delta < T, \tag{3.5}$$

where $C > 0$ is independent of (h, k, ε).

Proof. Since $\boldsymbol{u}_{h,k,\varepsilon}$ is a piecewise constant function, it suffices to suppose that δ is proportional to the time step k, *i.e.*, $\delta = r\,k$ for any $r = 0, ..., N$. Then, to obtain (3.5) it suffices to prove

$$k \sum_{m=0}^{N-r} \|\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m\|_{\boldsymbol{V}_h'}^2 \leq C\,(r\,k)^{1/2}, \quad \forall\, r : 0 < r < N. \tag{3.6}$$

Multiplying (1.15) by k and summing for $n = m, \ldots, m-1+r$, we have

$$\begin{aligned}\left(\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m, \bar{\boldsymbol{u}}_h\right) = -k \sum_{n=m}^{m-1+r} c\left(\boldsymbol{u}_h^n, \boldsymbol{u}_h^{n+1}, \bar{\boldsymbol{u}}_h\right) - \nu\, k \sum_{n=m}^{m-1+r} \left(\nabla \boldsymbol{u}^{n+1}, \nabla \bar{\boldsymbol{u}}_h\right) \\ + \lambda\, k \sum_{n=m}^{m-1+r} \left((\nabla \boldsymbol{d}_h^n)^t\, \boldsymbol{w}_h^{n+1}, \bar{\boldsymbol{u}}_h\right) + k \sum_{n=m}^{m-1+r} \left(p_h^{n+1}, \nabla \cdot \bar{\boldsymbol{u}}_h\right).\end{aligned} \tag{3.7}$$

Setting $\bar{\boldsymbol{u}}_h = A_h^{-1}(\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m)$ as a test function in (3.7), observing that

$$\left(\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m, A_h^{-1}(\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m)\right) = \|\nabla A_h^{-1}(\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m)\|^2$$

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(which is easily seen by taking $\boldsymbol{u}_h = \boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m$ and $\bar{\boldsymbol{u}}_h = A_h^{-1}(\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m)$ in (3.4)), multiplying by k, and summing for $m = 0, ..., N-r$, we get

$$\begin{aligned} k \sum_{m=0}^{N-r} \|\nabla A_h^{-1}(\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m)\|^2 = & -k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} c\Big(\boldsymbol{u}_h^n, \boldsymbol{u}_h^{n+1}, A_h^{-1}\left(\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m\right)\Big) \\ & + \nu\, k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \Big(\nabla \boldsymbol{u}^{n+1}, \nabla A_h^{-1}(\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m)\Big) \\ & + \lambda\, k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \Big((\nabla \boldsymbol{d}_h^n)^t\, \boldsymbol{w}_h^{n+1}, A_h^{-1}\left(\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m\right)\Big) \\ := & J_1 + J_2 + J_3. \end{aligned} \tag{3.8}$$

The right-hand side of (3.8) can be estimated as follows:

$$J_1 \le C\, k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \|\boldsymbol{u}_h^n\|_{H^1} \|\boldsymbol{u}_h^{n+1}\|_{H^1} \|A_h^{-1}\left(\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m\right)\|_{H^1}.$$

Applying Fubini's discrete rule, we infer that

$$J_1 \le C\, k^2 \sum_{n=0}^{N-1} \|\boldsymbol{u}_h^n\|_{H^1} \|\boldsymbol{u}_h^{n+1}\|_{H^1} \sum_{m=\overline{n-r+1}}^{\overline{n}} \|A_h^{-1}\left(\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m\right)\|_{H^1},$$

where

$$\overline{n} = \begin{cases} 0 & \text{if } n < 0, \\ n & \text{if } 0 \le n \le N-r, \\ N-r & \text{if } n > N-r. \end{cases}$$

Finally, using the fact that $\|A_h^{-1}(\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m)\|_{H^1} \le \|\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m\|$, Theorem 1.4, Hölder's inequality, and that $|\overline{n} - \overline{n-r+1}| \le r$, we bound

$$\begin{aligned} k \sum_{m=\overline{n-r+1}}^{\overline{n}} \|A_h^{-1}(\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m)\|_{H^1} & \le C \left(k \sum_{m=\overline{n-r+1}}^{\overline{n}} \|A_h^{-1}(\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m)\|_{H^1}^2 \right)^{1/2} \left(k \sum_{m=\overline{n-r+1}}^{\overline{n}} 1^2 \right)^{1/2} \\ & \le C\,(r\,k)^{1/2}; \end{aligned}$$

hence

$$J_1 \le C(r\,k)^{1/2} k \sum_{n=0}^{N-1} \|\boldsymbol{u}_h^n\|_{H^1} \|\boldsymbol{u}_h^{n+1}\|_{H^1} \le C(r\,k)^{1/2}.$$

Once J_1 has been bounded, there are no additional difficulties in checking that $J_2 \le C\,(r\,k)^{1/2}$.

From estimate (iv) of Theorem 1.4, J_3 can be estimated as

$$\begin{aligned} J_3 & \le C\, k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \|\nabla \boldsymbol{d}_h^n\|\, \|\boldsymbol{w}_h^{n+1}\|\, \|A_h^{-1}(\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m)\|_{L^\infty(\Omega)} \\ & \le C\, k^2 \sum_{m=0}^{N-r} \sum_{n=m}^{m-1+r} \|\boldsymbol{w}_h^{n+1}\|\, \|A_h^{-1}(\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m)\|_{L^\infty(\Omega)}. \end{aligned}$$

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Sobolev's inequality shows that

$$\|A_h^{-1}(\boldsymbol{u}_h^{m+r}-\boldsymbol{u}_h^m)\|_{L^\infty(\Omega)} \le C\,\|A^{-1}(\boldsymbol{u}_h^{m+r}-\boldsymbol{u}_h^m)\|_{W^{1,r}(\Omega)}$$

with $r>d$, d being the dimension of Ω. It is proven in [9], the following bound

$$\|A_h^{-1}(\boldsymbol{u}_h^{m+r}-\boldsymbol{u}_h^m)\|_{W^{1,r}(\Omega)} \le C\,\|A^{-1}(\boldsymbol{u}_h^{m+r}-\boldsymbol{u}_h^m)\|_{W^{1,r}(\Omega)},$$

where A^{-1} is the continuous Stokes resolvent. Thus, Sobolev's inequality, $H^2(\Omega)\hookrightarrow W^{1,r}(\Omega)$, with $r\le 6$, and hypothesis $(H1)$ guarantee

$$\|A^{-1}(\boldsymbol{u}_h^{m+r}-\boldsymbol{u}_h^m)\|_{L^\infty(\Omega)} \le C\|A^{-1}(\boldsymbol{u}_h^{m+r}-\boldsymbol{u}_h^m)\|_{H^2(\Omega)} \le C\|\boldsymbol{u}_h^{m+r}-\boldsymbol{u}_h^m\|. \tag{3.9}$$

Therefore,

$$\begin{aligned} J_3 &\le C\,k^2\sum_{m=0}^{N-r}\sum_{n=m}^{m-1+r}\|\boldsymbol{w}_h^{n+1}\|\,\|\boldsymbol{u}_h^{m+r}-\boldsymbol{u}_h^m\| \\ &\le k\sum_{m=0}^{N-r}\|\boldsymbol{u}_h^{m+r}-\boldsymbol{u}_h^m\|\left(k\sum_{n=m}^{m-1+r}\|\boldsymbol{w}_h^{n+1}\|^2\right)^{1/2}(r\,k)^{1/2} \le C(r\,k)^{1/2}. \end{aligned}$$

Finally, we conclude that

$$k\sum_{m=0}^{N-r}\|\nabla A_h^{-1}(\boldsymbol{u}_h^{m+r}-\boldsymbol{u}_h^m)\|^2 \le C\,(r\,k)^{1/2},$$

which is equivalent to (3.6), due to the fact that $\|\nabla A_h^{-1}\boldsymbol{u}_h\|$ and $\|\boldsymbol{u}_h\|_{\boldsymbol{V}_h'}$ are equivalent norms. Then, the proof of Lemma 3.2 is finished. □

The first idea to obtain compactness of the discrete velocities $\{\boldsymbol{u}_{h,k,\varepsilon}\}_{h,k,\varepsilon}$ is to use the following compactness result (due to Simon [23]):

Lemma 3.3. *Let $X\mapsto B\hookrightarrow Y$ be three Banach spaces with continuous imbeddings, with the imbedding $X\mapsto B$ compact. Then the following imbedding is compact*

$$L^q(0,T;X)\cap\left\{\phi\in L^q(0,T;Y):\|\phi(t+\delta)-\phi(t)\|_{L^q(0,T-\delta;Y)}\le C\,\delta^\alpha\right\}\longmapsto L^q(0,T;B), \tag{3.10}$$

for $1\le q\le\infty$ and $0<\alpha<1$.

But one observes that the fractional time derivative estimate for the discrete velocities (3.5) has been done in the norm $\boldsymbol{V}_h'$ which moves with respect to the space parameter h. In these conditions, the previous result does not work.

The following idea is to find a fixed norm where the fractional time derivative can be bounded. For this, we consider the orthogonal Stokes projector $R_h:\boldsymbol{V}_h\to\boldsymbol{V}$ defined as

$$\Big(\nabla(R_h\boldsymbol{u}_h-\boldsymbol{u}_h),\nabla\boldsymbol{v}\Big)=0,\quad\forall\,\boldsymbol{v}\in\boldsymbol{V}.$$

We will use here the following properties of R_h:

- $H^1(\Omega)$-stability : $\|R_h\boldsymbol{u}_h\|_{H^1(\Omega)}\le\|\boldsymbol{u}_h\|_{H^1(\Omega)}$.
- $L^2(\Omega)$-error estimate : $\|R_h\boldsymbol{u}_h-\boldsymbol{u}_h\|_{L^2(\Omega)}\le C\,h\|\nabla\cdot\boldsymbol{u}_h\|_{L^2(\Omega)}$.

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Indeed, setting $\boldsymbol{v} = R_h\boldsymbol{u}_h$ as a test function, the estimate $\|R_h\boldsymbol{u}_h\|_{H^1(\Omega)} \le \|\boldsymbol{u}_h\|_{H^1(\Omega)}$ is easily obtained. To prove the $L^2(\Omega)$-error estimate, we consider the following Stokes problem: find $(\varphi,\chi) \in (\boldsymbol{V}\cap\boldsymbol{H}^2(\Omega))\times(L^2_0(\Omega)\cap H^1(\Omega))$ such that

$$\begin{cases} -\Delta\varphi + \nabla\chi = R_h\boldsymbol{u}_h - \boldsymbol{u}_h \ \text{ in } \Omega, \\ \nabla\cdot\varphi = 0 \text{ in } \Omega, \quad \varphi = 0 \ \text{ on } \partial\Omega. \end{cases} \tag{3.11}$$

Multiplying (3.11) by $R_h\boldsymbol{u}_h - \boldsymbol{u}_h$ and making use of the definition of R_h gives

$$\|R_h\boldsymbol{u}_h - \boldsymbol{u}_h\|^2 = \Big(\chi, \nabla\cdot(R_h\boldsymbol{u}_h - \boldsymbol{u}_h)\Big).$$

In view of $\boldsymbol{u}_h \in \boldsymbol{V}_h$ and $R_h\boldsymbol{u}_h \in \boldsymbol{V}$, the previous equality becames

$$\|R_h\boldsymbol{u}_h - \boldsymbol{u}_h\|^2 = -\Big(\chi - K_h\chi, \nabla\cdot\boldsymbol{u}_h\Big),$$

where $K_h\chi \in Q_h$ is the interpolation operator defined in hypothesis (H2). Thus, using the approximation property (H2).(b).(ii) and the H^2-continuity of the Stokes problem (3.11) given in (H1), $\|\varphi\|_{H^2(\Omega)} + \|\chi\|_{H^1(\Omega)} \le C\|R_h\boldsymbol{u}_h - \boldsymbol{u}_h\|$, one has

$$\|R_h\boldsymbol{u}_h - \boldsymbol{u}_h\|^2 \le \|\chi - K_h\chi\|\,\|\nabla\cdot\boldsymbol{u}_h\| \le C\,h\,\|\chi\|_{H^1(\Omega)}\|\nabla\cdot\boldsymbol{u}_h\| \le C\,h\,\|R_h\boldsymbol{u}_h - \boldsymbol{u}_h\|\,\|\nabla\cdot\boldsymbol{u}_h\|;$$

hence the error estimate $\|R_h\boldsymbol{u}_h - \boldsymbol{u}_h\| \le C\,h\,\|\nabla\cdot\boldsymbol{u}_h\|$ holds.

Next, we will prove that $\|R_h\boldsymbol{u}_h\|_{\boldsymbol{V}'} \le C\Big(\|\boldsymbol{u}_h\|_{\boldsymbol{V}_h'} + h\,\|\nabla\cdot\boldsymbol{u}_h\|\Big)$. For this, we define the orthogonal L^2 projector $\widetilde{P}_h^0 : \boldsymbol{V} \to \boldsymbol{V}_h$ defined as $\Big(\widetilde{P}_h^0\boldsymbol{v} - \boldsymbol{v}, \boldsymbol{v}_h\Big) = 0$ for all $\boldsymbol{v}_h \in \boldsymbol{V}_h$. Indeed, for any $\boldsymbol{v} \in \boldsymbol{V}$:

$$\Big(R_h\boldsymbol{u}_h, \boldsymbol{v}\Big) = \Big(R_h\boldsymbol{u}_h - \boldsymbol{u}_h, \boldsymbol{v}\Big) + \Big(\boldsymbol{u}_h, \widetilde{P}_h^0\boldsymbol{v}\Big) \le C\,h\,\|\nabla\cdot\boldsymbol{u}_h\|\,\|\boldsymbol{v}\| + \Big(\boldsymbol{u}_h, \widetilde{P}_h^0\boldsymbol{v}\Big).$$

The definition of dual norms in $\boldsymbol{V}'$ and $\boldsymbol{V}_h'$, jointly to the stability property $\|\widetilde{P}_h^0\boldsymbol{v}\| \le \|\boldsymbol{v}\|$, gives

$$\|R_h\boldsymbol{u}_h\|_{\boldsymbol{V}'} \le C\,h\ \|\nabla\cdot\boldsymbol{u}_h\| + \sup_{\boldsymbol{v}\in\boldsymbol{V}} \frac{\Big(\boldsymbol{u}_h, \widetilde{P}_h^0\boldsymbol{v}\Big)}{\|\boldsymbol{v}\|_{H^1}} \le C\,h\,\|\nabla\cdot\boldsymbol{u}_h\| + C \sup_{\boldsymbol{v}_h\in\boldsymbol{V}_h} \frac{\Big(\boldsymbol{u}_h, \boldsymbol{v}_h\Big)}{\|\boldsymbol{v}_h\|};$$

hence,

$$\|R_h\boldsymbol{u}_h\|_{\boldsymbol{V}'} \le C\,\Big(h\|\nabla\cdot\boldsymbol{u}_h\| + \|\boldsymbol{u}_h\|_{\boldsymbol{V}_h'}\Big).$$

Taking $\boldsymbol{u}_h = \boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m$ and using (3.6), it follows that

$$k\sum_{m=0}^{N-r}\|R_h(\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m)\|^2_{\boldsymbol{V}'} \le C\,k\sum_{m=0}^{N-r}\|\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m\|^2_{\boldsymbol{V}_h'} + C\,h^2 k\sum_{m=0}^{N-r}\|\nabla\cdot(\boldsymbol{u}_h^{m+r} - \boldsymbol{u}_h^m)\|^2$$

$$\le C\,(r\,k)^{1/2} + C\,h^2.$$

This inequality can be written as

$$\int_0^{T-\delta}\|R_h\boldsymbol{u}_{h,k,\varepsilon}(t+\delta) - R_h\boldsymbol{u}_{h,k,\varepsilon}(t)\|^2_{\boldsymbol{V}'}\,\mathrm{d}t \le C\,\delta^{1/2} + C\,h^2.$$

We observe that the previous fractional time derivative does not satisfy the hypotheses of compactness of Lemma 3.3, because of the additional term $C\,h^2$ on the right-hand side of the previous bound. For this reason,

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we use the following "compactness by perturbation" result due to Azérad and Guillén [2]:

Lemma 3.4. *Let $X \hookrightarrow B \hookrightarrow Y$ be three Banach spaces with continuous imbeddings, with the imbedding from X to B being compact. Let $\{f_\epsilon\}_{\epsilon>0}$ be a family of functions of $L^p(0,T;X), 1 \le p \le \infty$, with the extra condition $\{f_\epsilon\}_{\epsilon>0} \subset C(0,T;Y)$ if $p=\infty$ such that*

(C1) $\{f_\epsilon\}_{\epsilon>0}$ is bounded in $L^p(0,T;X)$,
(C2) $\|f_\epsilon(\cdot+\delta)-f_\epsilon(\cdot)\|_{L^p(0,T;Y)} \le \varphi(\delta)+\psi(\epsilon)$ with

$$\lim_{\delta\to 0}\varphi(\delta)=0, \quad \lim_{\epsilon\to 0}\psi(\epsilon)=0.$$

Then, the family $\{f_\epsilon\}_{\epsilon>0}$ possesses a cluster point in $L^p(0,T;B)$ as $\epsilon\to 0$.

Therefore, if we select $X=\boldsymbol{V}$, $B=\boldsymbol{H}$ and $Y=\boldsymbol{V}'$, then there exists $\boldsymbol{u}\in\boldsymbol{V}$ such that $R_h\boldsymbol{u}_{k,h,\varepsilon}\to\boldsymbol{u}$ in $L^2(0,T;\boldsymbol{L}^2(\Omega))$-strong as $(k,h,\varepsilon)\to 0$. To conclude, we prove (3.3). Indeed,

$$\begin{aligned}\|\boldsymbol{u}_{h,k,\varepsilon}-\boldsymbol{u}\|_{L^2(0,T;\boldsymbol{L}^2(\Omega))} &\le \|\boldsymbol{u}_{h,k,\varepsilon}-R_h\boldsymbol{u}_{h,k,\varepsilon}\|_{L^2(0,T;\boldsymbol{L}^2(\Omega))}+\|R_h\boldsymbol{u}_{h,k,\varepsilon}-\boldsymbol{u}\|_{L^2(0,T;\boldsymbol{L}^2(\Omega))}\\ &\le C\,h+\|R_h\boldsymbol{u}_{h,k,\varepsilon}-\boldsymbol{u}\|_{L^2(0,T;\boldsymbol{L}^2(\Omega))}\to 0 \text{ as } (h,k,\varepsilon)\to 0.\end{aligned}$$

Remark 3.5 (Convergence to the Ginzburg–Landau model)**.** Fixed $\varepsilon>0$, the convergence of scheme (1.15)–(1.18) to weak solutions of the penalized problem (1.4) (as in Def. 1.3) could be proved by using the compactness of $\{\boldsymbol{d}_{h,k}\}_{h,k}$ in $L^2(0,T;\boldsymbol{H}^1(\Omega))$ (see [3,8] for the convergence as $(h,k)\to 0$ for other semi-implicit schemes). To prove this compactness, we observe that

$$\|\Delta_h\boldsymbol{d}_h^{n+1}\|^2 \le \|\boldsymbol{w}_h^{n+1}\|^2+\frac{C}{\varepsilon^4}\Big(\|\boldsymbol{d}_h^n\|_{H^1(\Omega)}^6+\|\boldsymbol{d}_h^n\|^2\Big),$$

where Δ_h is the discrete Laplacian operator. Multiplying by k and summing up over n, using estimates (2.15) and (2.16), it yields

$$k\sum_{n=0}^{N-1}\|\Delta_h\boldsymbol{d}^{n+1}\|^2\le\frac{C}{\varepsilon^4}.$$

Finally, we can use a compactness result established in [3], Lemma 2.4 in order to deduce

$$\boldsymbol{d}_{h,k,\varepsilon}\to\boldsymbol{d}_\varepsilon \quad \text{in } L^2(0,T;\boldsymbol{H}^1(\Omega)) \text{ as } (h,k)\to 0,$$

where $\boldsymbol{d}_\varepsilon$ will be, jointly to $\boldsymbol{u}_\varepsilon$ (a limit of $\{\boldsymbol{u}_{h,k}\}_{h,k}$ as $(h,k)\to 0$), a weak solution of the penalized problem (1.4). It is clear that this argument is not useful to pass to the limit as (h,k,ε) go to zero.

4. Convergence towards the director system $(1.1)_a$

From now on, we will consider the truncated potential $\widetilde{F}_\varepsilon$ and its corresponding functional $\widetilde{\boldsymbol{f}}_\varepsilon$ defined in Remark 1.8 instead of F_ε and $\boldsymbol{f}_\varepsilon$, respectively. The reason for this modification will be explained later on, see Remark 5.3.

The convergence for (1.17)–(1.18) is based on the following result, whose proof can be found in [5], Lemma 2.2 without the convective term (see also [15], Lem. 7.1).

Lemma 4.1. *The next two systems are equivalent at least in a weak sense:*

$$\partial_t\boldsymbol{d}+(\boldsymbol{u}\cdot\nabla)\boldsymbol{d}-\gamma\Delta\boldsymbol{d}-\gamma|\nabla\boldsymbol{d}|^2\boldsymbol{d}=\boldsymbol{0} \quad \text{in } Q, \tag{4.1}$$

and

$$|\boldsymbol{d}|=1, \quad \partial_t\boldsymbol{d}\wedge\boldsymbol{d}+(\boldsymbol{u}\cdot\nabla)\boldsymbol{d}\wedge\boldsymbol{d}-\gamma\nabla\cdot(\nabla\boldsymbol{d}\wedge\boldsymbol{d})=\boldsymbol{0} \quad \text{in } Q, \tag{4.2}$$

where $(\nabla\boldsymbol{d}\wedge\boldsymbol{d})_{ij}=(\partial_i\boldsymbol{d}\wedge\boldsymbol{d})_j$.

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4.1. Checking $(4.2)_a$: $|\boldsymbol{d}| = 1$

Since

$$\min\left\{(|\boldsymbol{d}|^2-1)^2,(|\boldsymbol{d}|-1)^2\right\} = (|\boldsymbol{d}|-1)^2, \quad \forall\, \boldsymbol{d}\in\mathbb{R}^d,$$

then

$$\max_{t\in[0,T]}\int_\Omega (|\boldsymbol{d}_{h,k,\varepsilon}(t)|-1)^2 d\boldsymbol{x} \le 4\varepsilon^2 \max_n \int_\Omega \widetilde{F}_\varepsilon(\boldsymbol{d}_h^{n+1}) \le C\varepsilon^2 \to 0,$$

as $(h,k,\varepsilon)\to 0$, *i.e.*

$$|\boldsymbol{d}_{h,k,\varepsilon}(t,\boldsymbol{x})| \to 1 \quad \text{in } L^\infty(0,T;L^2(\Omega)).$$

On the other hand, from (3.2) for $q=r=2$,

$$|\boldsymbol{d}_{h,k,\varepsilon}| \to |\boldsymbol{d}| \quad \text{in } L^2(Q).$$

From these last two convergences, $|\boldsymbol{d}|=1$ is deduced.

4.2. Checking $(4.2)_b$

Next, we would like to write the discrete weak formulation of equation $(4.2)_b$ starting from (1.17) and (1.18). Indeed, we consider $\bar{\boldsymbol{w}}_h = P_h^0\bar{\boldsymbol{w}}$ into (1.17) for any $\bar{\boldsymbol{w}}\in \boldsymbol{L}^2(\Omega)$, with P_h^0 being the $\boldsymbol{L}^2(\Omega)$-projector onto $\boldsymbol{W}_h$, and use that $\boldsymbol{d}_h^{n+1}-\boldsymbol{d}_h^n \in \boldsymbol{D}_h \subset \boldsymbol{W}_h$ (due to hypothesis $(H4)$) to obtain

$$\frac{\boldsymbol{d}_h^{n+1}-\boldsymbol{d}_h^n}{k} + P_h^0((\boldsymbol{u}_h^{n+1}\cdot\nabla)\boldsymbol{d}_h^n) + \gamma\,\boldsymbol{w}_h^{n+1} = 0 \quad \text{in } \Omega. \tag{4.3}$$

Taking the vectorial product of (4.3) by $\boldsymbol{d}_h^{n+1}$,

$$\frac{\boldsymbol{d}_h^{n+1}-\boldsymbol{d}_h^n}{k}\wedge\boldsymbol{d}_h^{n+1} + P_h^0((\boldsymbol{u}_h^{n+1}\cdot\nabla)\boldsymbol{d}_h^n)\wedge\boldsymbol{d}_h^{n+1} + \gamma\,\boldsymbol{w}_h^{n+1}\wedge\boldsymbol{d}_h^{n+1} = 0 \quad \text{in } \Omega.$$

Next, multiplying by any test function $\bar{\boldsymbol{d}}_h\in\boldsymbol{D}_{0h}$, we infer the discrete weak formulation

$$\left(\frac{\boldsymbol{d}_h^{n+1}-\boldsymbol{d}_h^n}{k}\wedge\boldsymbol{d}_h^{n+1},\bar{\boldsymbol{d}}_h\right) + \left(P_h^0((\boldsymbol{u}_h^{n+1}\cdot\nabla)\boldsymbol{d}_h^n)\wedge\boldsymbol{d}_h^{n+1},\bar{\boldsymbol{d}}_h\right) + \gamma\left(\boldsymbol{w}_h^{n+1}\wedge\boldsymbol{d}_h^{n+1},\bar{\boldsymbol{d}}_h\right) = 0, \tag{4.4}$$

on which we will pass to the limit once the last two terms have been rewritten. For this, let us consider the equality

$$\left(\boldsymbol{w}\wedge\boldsymbol{d},\bar{\boldsymbol{d}}\right) = \left(\boldsymbol{w},\boldsymbol{d}\wedge\bar{\boldsymbol{d}}\right) \quad \forall\,\boldsymbol{w},\boldsymbol{d},\bar{\boldsymbol{d}}\in\mathbb{R}^d.$$

To start with, we treat the last term in (4.4). To fix ideas, we want to obtain a discrete version of the continuous identity

$$\left(\boldsymbol{w}\wedge\boldsymbol{d},\bar{\boldsymbol{d}}\right) = -(\Delta\boldsymbol{d}\wedge\boldsymbol{d},\bar{\boldsymbol{d}}) = -(\Delta\boldsymbol{d},\boldsymbol{d}\wedge\bar{\boldsymbol{d}}) = (\nabla\boldsymbol{d},\nabla(\boldsymbol{d}\wedge\bar{\boldsymbol{d}})) = (\nabla\boldsymbol{d}\wedge\boldsymbol{d},\nabla\bar{\boldsymbol{d}}), \tag{4.5}$$

where the hypothesis $\widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d})\wedge\boldsymbol{d}=0$ given in (1.22) has been used.

Taking $Q_h^1(\boldsymbol{d}_h^{n+1}\wedge\bar{\boldsymbol{d}}_h)\in\boldsymbol{D}_{0h}$ as a test function in (1.18), with Q_h^1 being the orthogonal $\boldsymbol{H}_0^1(\Omega)$-projector onto $\boldsymbol{D}_{0h}$, one has

$$\left(\nabla\boldsymbol{d}_h^{n+1},\nabla Q_h^1(\boldsymbol{d}_h^{n+1}\wedge\bar{\boldsymbol{d}}_h)\right) + \left(\widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d}_h^n),Q_h^1(\boldsymbol{d}_h^{n+1}\wedge\bar{\boldsymbol{d}}_h)\right) = \left(\boldsymbol{w}_h^{n+1},Q_h^1(\boldsymbol{d}_h^{n+1}\wedge\bar{\boldsymbol{d}}_h)\right). \tag{4.6}$$

Using the discrete lifting function $\widetilde{\boldsymbol{d}}_h\in\boldsymbol{D}_h$ with $\widetilde{\boldsymbol{d}}_h|_{\partial\Omega}=\boldsymbol{l}_h$ defined as

$$\left(\nabla\widetilde{\boldsymbol{d}}_h,\nabla\bar{\boldsymbol{d}}_h\right) = 0 \quad \forall\,\bar{\boldsymbol{d}}_h\in\boldsymbol{D}_{0h}$$

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and the equality $\left(\nabla \boldsymbol{d}_h^{n+1}, \nabla(\boldsymbol{d}_h^{n+1} \wedge \bar{\boldsymbol{d}}_h)\right) = \left(\nabla \boldsymbol{d}_h^{n+1} \wedge \boldsymbol{d}_h^{n+1}, \nabla \bar{\boldsymbol{d}}_h\right)$, the first term on the right-hand side of (4.6) is written as

$$\begin{aligned}\left(\nabla \boldsymbol{d}_h^{n+1}, \nabla Q_h^1(\boldsymbol{d}_h^{n+1} \wedge \bar{\boldsymbol{d}}_h)\right) &= \left(\nabla(\boldsymbol{d}_h^{n+1} - \widetilde{\boldsymbol{d}}_h), \nabla Q_h^1(\boldsymbol{d}_h^{n+1} \wedge \bar{\boldsymbol{d}}_h)\right) + \left(\nabla \widetilde{\boldsymbol{d}}_h, \nabla Q_h^1(\boldsymbol{d}_h^{n+1} \wedge \bar{\boldsymbol{d}}_h)\right) \\ &= \left(\nabla(\boldsymbol{d}_h^{n+1} - \widetilde{\boldsymbol{d}}_h), \nabla(\boldsymbol{d}_h^{n+1} \wedge \bar{\boldsymbol{d}}_h)\right) \\ &= \left(\nabla \boldsymbol{d}_h^{n+1} \wedge \boldsymbol{d}_h^{n+1}, \nabla \bar{\boldsymbol{d}}_h\right) - R_0^{n+1} \end{aligned} \tag{4.7}$$

where

$$R_0^{n+1} = \left(\nabla \widetilde{\boldsymbol{d}}_h, \nabla\left(\boldsymbol{d}_h^{n+1} \wedge \bar{\boldsymbol{d}}_h\right)\right) = \left(\nabla\left(\widetilde{\boldsymbol{d}}_h - \widetilde{\boldsymbol{d}}\right), \nabla\left(\boldsymbol{d}_h^{n+1} \wedge \bar{\boldsymbol{d}}_h\right)\right)$$

with $\widetilde{\boldsymbol{d}}$ the (continuous) lifting function defined in (1.19).

From (4.6) and (4.7), we obtain the following discrete version of (4.5):

$$\left(\nabla \boldsymbol{d}_h^{n+1} \wedge \boldsymbol{d}_h^{n+1}, \nabla \bar{\boldsymbol{d}}_h\right) = \left(\boldsymbol{w}_h^{n+1} \wedge \boldsymbol{d}_h^{n+1}, \bar{\boldsymbol{d}}_h\right) + R_0^{n+1} + R_1^{n+1} + R_2^{n+1} + R_3^{n+1}, \tag{4.8}$$

where

$$\begin{aligned} R_1^{n+1} &= \left(\boldsymbol{w}_h^{n+1}, Q_h^1\left(\boldsymbol{d}_h^{n+1} \wedge \bar{\boldsymbol{d}}_h\right) - \left(\boldsymbol{d}_h^{n+1} \wedge \bar{\boldsymbol{d}}_h\right)\right), \\ R_2^{n+1} &= -\left(\widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d}_h^n), Q_h^1\left(\boldsymbol{d}_h^{n+1} \wedge \bar{\boldsymbol{d}}_h\right) - \boldsymbol{d}_h^{n+1} \wedge \bar{\boldsymbol{d}}_h\right) \end{aligned}$$

and

$$R_3^{n+1} = -\left(\widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d}_h^n), \boldsymbol{d}_h^{n+1} \wedge \bar{\boldsymbol{d}}_h\right) = -\left(\widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d}_h^n), (\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n) \wedge \bar{\boldsymbol{d}}_h\right)$$

owing to $\widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d}_h^n) \wedge \boldsymbol{d}_h^n = 0$. Now, we write

$$\left(P_h^0\left(\left(\boldsymbol{u}_h^{n+1} \cdot \nabla\right) \boldsymbol{d}_h^n\right) \wedge \boldsymbol{d}_h^{n+1}, \left(\left(\boldsymbol{u}_h^{n+1} \cdot \nabla\right) \boldsymbol{d}_h^n\right) \wedge \boldsymbol{d}_h^{n+1}, \bar{\boldsymbol{d}}_h\right) - R_4^{n+1} \tag{4.9}$$

where

$$R_4^{n+1} = \left(((\boldsymbol{u}_h^{n+1} \cdot \nabla)\boldsymbol{d}_h^n - P_h^0((\boldsymbol{u}_h^{n+1} \cdot \nabla)\boldsymbol{d}_h^n)) \wedge \boldsymbol{d}_h^{n+1}, \bar{\boldsymbol{d}}_h\right) = \left((\boldsymbol{u}_h^{n+1} \cdot \nabla)\boldsymbol{d}_h^n, \boldsymbol{d}_h^{n+1} \wedge \bar{\boldsymbol{d}}_h - P_h^0(\boldsymbol{d}_h^{n+1} \wedge \bar{\boldsymbol{d}}_h)\right).$$

Then, applying (4.8) and (4.9) in (4.4), we have

$$\begin{aligned} k \sum_{n=0}^{N-1} \left\{ \left(\left[\frac{\boldsymbol{d}_h^{n+1} - \boldsymbol{d}_h^n}{k} + \left(\boldsymbol{u}_h^{n+1} \cdot \nabla\right) \boldsymbol{d}_h^n \right] \wedge \boldsymbol{d}_h^{n+1}, \bar{\boldsymbol{d}}_h \right) + \gamma \left(\nabla \boldsymbol{d}_h^{n+1} \wedge \boldsymbol{d}_h^{n+1}, \nabla \bar{\boldsymbol{d}}_h \right) \right\} \\ = k \sum_{n=0}^{N-1} \gamma \left(R_0^{n+1} + R_1^{n+1} + R_2^{n+1} + R_3^{n+1} \right) + R_4^{n+1} := R_{h,k,\varepsilon} \end{aligned} \tag{4.10}$$

which is a discrete weak formulation of $(4.2)_b$.

As mentioned, our intention is to pass to the limit in (4.10) to obtain $(4.2)_b$. For this, we are going to rewrite (4.10) with global time-space functions. Let $\bar{\boldsymbol{d}} \in C^0([0,T]; \boldsymbol{H}_0^1(\Omega) \cap \boldsymbol{W}^{2,3}(\Omega) \cap \boldsymbol{W}^{1,\infty}(\Omega))$ and consider $\bar{\boldsymbol{d}}_h^n = I_h(\bar{\boldsymbol{d}}(t_n))$. Then, by (H2).(b).(v) and (H2).(b).(vi), we define $\bar{\boldsymbol{d}}_{h,k}(t) = \bar{\boldsymbol{d}}_h^{n+1}$ for all $t \in (t_n, t_{n+1}]$ to obtain

$$\bar{\boldsymbol{d}}_{h,k} \to \bar{\boldsymbol{d}} \quad \text{in } L^\infty(0,T; \boldsymbol{W}^{1,3}(\Omega) \cap \boldsymbol{L}^\infty(\Omega)) \text{ strongly.}$$

This test function $\bar{\boldsymbol{d}}_{h,k}$ and Definition 2.7 allow to rewrite (4.10) as:

$$\int_0^T \left(\left[\partial_t \boldsymbol{d}_{h,k,\varepsilon} + (\boldsymbol{u}_{h,k,\varepsilon} \cdot \nabla)\boldsymbol{d}_{h,k,\varepsilon}^0\right] \wedge \boldsymbol{d}_{h,k,\varepsilon}, \bar{\boldsymbol{d}}_{h,k} \right) + \gamma \left(\nabla \boldsymbol{d}_{h,k,\varepsilon} \wedge \boldsymbol{d}_{h,k,\varepsilon}, \nabla \bar{\boldsymbol{d}}_{h,k} \right) = R_{h,k,\varepsilon}$$

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where the reminder terms are collected in the term $R_{h,k,\varepsilon}$. Since the left hand-side passes to the limit as $(h,k,\varepsilon)\to 0$ in a standard manner from the weak and strong convergences already obtained, we just analyze that the residual term $R_{h,k,\varepsilon}$ goes to zero as (h,k,ε) go to zero.

In order to bound R_0^{n+1}, we consider the following error estimate [6]:

$$\|\nabla(\widetilde{\boldsymbol{d}}-\widetilde{\boldsymbol{d}}_h)\|\le C\|\nabla(\widetilde{\boldsymbol{d}}-SZ_h(\widetilde{\boldsymbol{d}}))\|\le C\,h\|\widetilde{\boldsymbol{d}}\|_{H^2(\Omega)};$$

hence $R_0^{n+1}\le C\,h$. On the other hand, we can bound R_4^{n+1} as

$$R_4^{n+1}\le C\,\|\boldsymbol{u}_h^{n+1}\|_{L^\infty}\|\nabla\boldsymbol{d}_h^n\|\,h\,\|\boldsymbol{d}_h^{n+1}\wedge\bar{\boldsymbol{d}}_h\|_{H^1}\le C\,h^{1/2}\|\boldsymbol{u}_h^{n+1}\|_{H^1}.$$

From the approximation inequality $\|\bar{\boldsymbol{d}}-Q_h^1\bar{\boldsymbol{d}}\|\le C\,h\,\|\bar{\boldsymbol{d}}\|_{H^1}$ for all $\bar{\boldsymbol{d}}\in\boldsymbol{H}_0^1(\Omega)$ (which can be obtained by a duality argument by using the approximation inequality (H2).(b).(iv) and the stability property (H2).(c).(ii)), one has

$$\|\boldsymbol{d}_h^{n+1}\wedge\bar{\boldsymbol{d}}_h-Q_h^1[\boldsymbol{d}_h^{n+1}\wedge\bar{\boldsymbol{d}}_h]\|\le C\,h\,\|\boldsymbol{d}_h^{n+1}\|_{H^1(\Omega)}\|\bar{\boldsymbol{d}}_h\|_{W^{1,3}(\Omega)\cap L^\infty(\Omega)}\le C\,h.$$

Then, from $\|\widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d}_h^n)\|\le C\,\varepsilon^{-1}(\int_\Omega F_\varepsilon(\boldsymbol{d}_h^n))^{1/2}\le C\,\varepsilon^{-1}$ in $R_2^{n+1}+R_3^{n+1}$, it is easy to prove the bounds

$$R_1^{n+1}\le C\,h\,\|\boldsymbol{w}_h^{n+1}\|,\quad R_2^{n+1}\le C\frac{h}{\varepsilon}\quad\text{and}\quad R_3^{n+1}\le C\,\frac{\|\boldsymbol{d}_h^{n+1}-\boldsymbol{d}_h^n\|}{\varepsilon}.$$

Therefore, from the above bounds jointly with the energy estimates $k\sum_{n=0}^{N-1}\left(\|\boldsymbol{u}_h^{n+1}\|_{H^1}^2+\|\boldsymbol{w}_h^{n+1}\|^2\right)\le C$ and the numerical dissipation estimate $\sum_{n=0}^{N-1}\|\boldsymbol{d}_h^{n+1}-\boldsymbol{d}_h^n\|^2\le C$, one has

$$R_{h,k,\varepsilon}\le C\,h+C\frac{h+k^{1/2}}{\varepsilon}+C\,h^{1/2}\to 0\quad\text{as }(h,k,\varepsilon)\to 0,$$

due to hypothesis (S) and (C).

In conclusion, we get that the limit function $(\boldsymbol{u},\boldsymbol{d})$ satisfy $(4.2)_b$. Therefore, (4.1) holds.

5. On the convergence of the momentum system

Since we do not have any estimate for the discrete pressure p_h^{n+1}, we must choose a discrete test function which eliminates the pressure term.

Lemma 5.1. *Let $\boldsymbol{v}\in\boldsymbol{C}_c^\infty(\Omega)$. Then there exists $\boldsymbol{v}_h\in\boldsymbol{X}_h$ such that*

$$\boldsymbol{v}_h\to\boldsymbol{v}\quad\textit{in }\boldsymbol{W}_0^{1,\infty}(\Omega)\quad\textit{and}\quad\Big(\nabla\cdot\boldsymbol{v}_h,q_h\Big)=\Big(\nabla\cdot\boldsymbol{v},q_h\Big)\ \forall\,q_h\in Q_h.$$

A proof of this lemma can be seen in [8] when the $\mathbb{P}_1$-bubble approximation for the velocity is considered. In [12] the same type of result is proved for a generic "inf-sup" stable approximation but for a convergence in the $\boldsymbol{H}^1(\Omega)$-norm. Some minor changes can be introduced in order to get the convergence in the $\boldsymbol{W}^{1,\infty}(\Omega)$-norm when the $\mathbb{P}_2$ approximation is considered, by using the inverse inequality $\|\nabla\bar{\boldsymbol{u}}_h\|_{L^\infty(\Omega)}\le C\,h^{-3/2}\|\nabla\bar{\boldsymbol{u}}_h\|$ for all $\bar{\boldsymbol{u}}_h\in\boldsymbol{X}_h$, and the approximation properties $\|\bar{\boldsymbol{u}}-J_h\bar{\boldsymbol{u}}\|_{W^{1,\infty}(\Omega)}\le C\,h^{1/2}\|\bar{\boldsymbol{u}}\|_{H^3(\Omega)}$ and $\|\bar{\boldsymbol{u}}-J_h\bar{\boldsymbol{u}}\|_{H^1(\Omega)}\le C\,h^2\|\bar{\boldsymbol{u}}\|_{H^3(\Omega)}$ for all $\forall\,\bar{\boldsymbol{u}}\in\boldsymbol{H}^3(\Omega)$.

We consider $\boldsymbol{v}\in\mathcal{C}_c^\infty([0,T);\boldsymbol{\mathcal{V}})$. Let $\boldsymbol{v}_h^n$ be the projection of $\boldsymbol{v}(t^n)$ furnished by Lemma 5.1. We define $\boldsymbol{v}_{h,k}\in L^\infty(0,T;\boldsymbol{V}_h)$ as the piecewise constant functions taking values $\boldsymbol{v}_h^{n+1}$ on $(t_n,t_{n+1}]$ and $\boldsymbol{v}_{h,k}^l\in C^0([0,T];\boldsymbol{V}_h)$ as the piecewise linear, globally continuous functions such that $\boldsymbol{v}_{h,k}^l(t_n)=\boldsymbol{v}_h^n$. It is known that, as $(h,k)\to 0$,

$$\boldsymbol{v}_{h,k}\to\boldsymbol{v}\text{ in }L^\infty(0,T;\boldsymbol{W}_0^{1,\infty}(\Omega)),\quad\boldsymbol{v}_{h,k}^l\to\boldsymbol{v}\text{ in }W^{1,\infty}(0,T;\boldsymbol{W}_0^{1,\infty}(\Omega)).$$

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Taking $\bar{\boldsymbol{u}}_h = \boldsymbol{v}_h^{n+1}$ as a test function in (1.15), multiplying by k, summing over n and using the equality (which is a discrete integration by parts in time)

$$\sum_{n=0}^{N-1}\left(\boldsymbol{u}_h^{n+1}-\boldsymbol{u}_h^n,\boldsymbol{v}_h^{n+1}\right)=\left(\boldsymbol{u}_h^N,\boldsymbol{v}_h^N\right)-\sum_{n=0}^{N-1}\left(\boldsymbol{u}_h^n,\boldsymbol{v}_h^{n+1}-\boldsymbol{v}_h^n\right)-\left(\boldsymbol{u}_h^0,\boldsymbol{v}_h^0\right)$$

and the fact that $\boldsymbol{v}_h^N = 0$ (since $\boldsymbol{v}(T) = 0$), the following formulation holds:

$$\begin{cases} -k\displaystyle\sum_{n=0}^{N-1}\left(\boldsymbol{u}_h^n,\frac{\boldsymbol{v}_h^{n+1}-\boldsymbol{v}_h^n}{k}\right)+\nu\,k\displaystyle\sum_{n=0}^{N-1}\left(\nabla\boldsymbol{u}_h^{n+1},\nabla\boldsymbol{v}_h^{n+1}\right) \\ +k\displaystyle\sum_{n=0}^{N-1}\left\{c\left(\boldsymbol{u}_h^n,\boldsymbol{u}_h^{n+1},\boldsymbol{v}_h^{n+1}\right)-\lambda\left((\nabla\boldsymbol{d}_h^n)^t\,\boldsymbol{w}_h^{n+1},\boldsymbol{v}_h^{n+1}\right)\right\}=\left(\boldsymbol{u}_h^0,\boldsymbol{v}_h^0\right). \end{cases}$$

Next, taking into account Definition 2.7, the above equality reads

$$\begin{cases} -\displaystyle\int_0^T\left(\boldsymbol{u}_{h,k,\varepsilon}^0(t),\partial_t\boldsymbol{v}_{h,k}^l(t)\right)\mathrm{d}t+\nu\int_0^T\left(\nabla\boldsymbol{u}_{h,k,\varepsilon}(t),\nabla\boldsymbol{v}_{h,k}(t)\right)\mathrm{d}t \\ +\displaystyle\int_0^T\left\{c\Big(\boldsymbol{u}_{h,k,\varepsilon}^0(t),\boldsymbol{u}_{h,k,\varepsilon}(t),\boldsymbol{v}_{h,k}(t)\Big)-\lambda\Big((\nabla\boldsymbol{d}_{h,k,\varepsilon}^0(t))^t\boldsymbol{w}_{h,k,\varepsilon}(t),\boldsymbol{v}_{h,k}(t)\Big)\right\}\mathrm{d}t=\Big(\boldsymbol{u}_h^0,\boldsymbol{v}_h^0\Big). \end{cases}$$

At this point, we will only pass to the limit in the more conflictive term

$$-\int_0^T\left((\nabla\boldsymbol{d}_{h,k,\varepsilon}^0(t))^t\boldsymbol{w}_{h,k,\varepsilon}(t),\boldsymbol{v}_{h,k}(t)\right)\mathrm{d}t=-k\sum_{n=0}^{N-1}\left((\nabla\boldsymbol{d}_h^n)^t\boldsymbol{w}_h^{n+1},\bar{\boldsymbol{u}}_h\right),\tag{5.1}$$

where, for simplicity, we denote $\bar{\boldsymbol{u}}_h = \boldsymbol{v}_h^{n+1}$. The treatment of the rest of the terms are rather standard in the Navier–Stokes framework.

Let $\boldsymbol{z}_h^{n+1} = \boldsymbol{w}_h^{n+1} - \widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d}_h^n)$. Then, scheme (1.18) is rewritten as $\left(\nabla\boldsymbol{d}_h^{n+1},\nabla\bar{\boldsymbol{d}}_h\right)=\left(\boldsymbol{z}_h^{n+1},\bar{\boldsymbol{d}}_h\right)$ for each $\bar{\boldsymbol{d}}_h\in\boldsymbol{D}_{0h}$. That is, $\boldsymbol{d}_h^{n+1}\in\boldsymbol{D}_h$ is the solution of the problem

$$-\Delta_h\boldsymbol{d}_h^{n+1}=Q_h^0(\boldsymbol{z}_h^{n+1})\quad\text{in }\Omega,\qquad\boldsymbol{d}_h^{n+1}=\boldsymbol{l}_h\quad\text{on }\partial\Omega,\tag{5.2}$$

where Δ_h is the discrete Laplacian operator and Q_h^0 is the L^2-projector onto $\boldsymbol{D}_{0h}$. This problem induces to define $\boldsymbol{d}^{n+1}(h)\in\boldsymbol{H}^2(\Omega)$ as the solution of the non-homogeneous Dirichlet problem

$$-\Delta\boldsymbol{d}^{n+1}(h)=\boldsymbol{z}_h^{n+1}\quad\text{in }\Omega,\qquad\boldsymbol{d}^{n+1}(h)=\boldsymbol{l}\quad\text{on }\partial\Omega.\tag{5.3}$$

Comparing problems (5.2) and (5.3), the following error estimate holds [6]:

$$\|\nabla\boldsymbol{d}^{n+1}(h)-\nabla\boldsymbol{d}_h^{n+1}\|\le C\,h\,\left(\|\boldsymbol{z}_h^{n+1}\|+\|\boldsymbol{l}\|_{H^{3/2}(\partial\Omega)}\right).\tag{5.4}$$

Recall that we have that $\|\widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d}_h^n)\|\le\dfrac{C}{\varepsilon}\|\widetilde{F}_\varepsilon(\boldsymbol{d}_h^n)\|_{L^1(\Omega)}^{1/2}$ holds from (1.23). Then, by the definition of $\boldsymbol{z}_h^{n+1}=\boldsymbol{w}_h^{n+1}-\widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d}_h^n)$ and from estimate (vii) of Theorem 1.4, we obtain

$$\|\boldsymbol{z}_h^{n+1}\|\le\|\boldsymbol{w}_h^{n+1}\|+C\,\frac{1}{\varepsilon}.\tag{5.5}$$

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From inequalities (5.4) and (5.5), we see that

$$\|\nabla \boldsymbol{d}^{n+1}(h) - \nabla \boldsymbol{d}_h^{n+1}\| \leq C\, h\, \|\boldsymbol{w}_h^{n+1}\| + C\, \frac{h}{\varepsilon} + C\, h\cdot \tag{5.6}$$

On the other hand, each term on the right hand-side of (5.1) may be rewritten as:

$$\begin{aligned} -\Big((\nabla \boldsymbol{d}_h^n)^t\, \boldsymbol{w}_h^{n+1}, \bar{\boldsymbol{u}}_h\Big) &= \Big((\nabla \boldsymbol{d}_h^n)^t\, \Delta \boldsymbol{d}^{n+1}(h), \bar{\boldsymbol{u}}_h\Big) - \Big((\nabla \boldsymbol{d}_h^n)^t\, \widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d}_h^n), \bar{\boldsymbol{u}}_h\Big) \\ &= \Big(\big(\nabla \boldsymbol{d}^{n+1}(h)\big)^t\, \Delta \boldsymbol{d}^{n+1}(h), \bar{\boldsymbol{u}}_h\Big) - \Big(\big(\nabla \boldsymbol{d}^{n+1}(h) - \nabla \boldsymbol{d}_h^{n+1}\big)^t\, \boldsymbol{z}_h^{n+1}, \bar{\boldsymbol{u}}_h\Big) \\ &\quad - \Big(\big(\nabla \boldsymbol{d}_h^{n+1} - \nabla \boldsymbol{d}_h^n\big)^t\, \boldsymbol{z}_h^{n+1}, \bar{\boldsymbol{u}}_h\Big) - \Big((\nabla \boldsymbol{d}_h^n)^t\, \widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d}_h^n), \bar{\boldsymbol{u}}_h\Big) := \sum_{i=1}^4 I_i^n. \end{aligned} \tag{5.7}$$

Using the fact that

$$(\nabla \boldsymbol{d}^{n+1}(h))^t \Delta \boldsymbol{d}^{n+1}(h) = \nabla \cdot ((\nabla \boldsymbol{d}^{n+1}(h))^t \nabla \boldsymbol{d}^{n+1}(h)) - \frac{1}{2}\nabla(|\nabla \boldsymbol{d}^{n+1}(h)|^2)$$

and integrating by parts, the term I_1^n of (5.7) may be rewritten as:

$$I_1^n = -\Big((\nabla \boldsymbol{d}^{n+1}(h))^t \nabla \boldsymbol{d}^{n+1}(h), \nabla \bar{\boldsymbol{u}}_h\Big) + \frac{1}{2}\Big(|\nabla \boldsymbol{d}^{n+1}(h)|^2, \nabla \cdot \bar{\boldsymbol{u}}_h\Big) := J_1^n + J_2^n.$$

Next, we handle J_1^n until finding the discrete term $-\Big((\nabla \boldsymbol{d}_h^{n+1})^t \nabla \boldsymbol{d}_h^{n+1}, \nabla \bar{\boldsymbol{u}}_h\Big)$ as follows:

$$\begin{aligned} J_1^n &= -\Big((\nabla \boldsymbol{d}_h^{n+1})^t \nabla \boldsymbol{d}_h^{n+1}, \nabla \bar{\boldsymbol{u}}_h\Big) + \Big((\nabla \boldsymbol{d}_h^{n+1})^t (\nabla \boldsymbol{d}_h^{n+1} - \nabla \boldsymbol{d}^{n+1}(h)), \nabla \bar{\boldsymbol{u}}_h\Big) \\ &\quad + \Big((\nabla \boldsymbol{d}^{n+1}(h) - \nabla \boldsymbol{d}_h^{n+1})^t (\nabla \boldsymbol{d}_h^{n+1} - \nabla \boldsymbol{d}^{n+1}(h)), \nabla \bar{\boldsymbol{u}}_h\Big) \\ &\quad + \Big((\nabla \boldsymbol{d}_h^{n+1} - \nabla \boldsymbol{d}^{n+1}(h))^t \nabla \boldsymbol{d}_h^{n+1}, \nabla \bar{\boldsymbol{u}}_h\Big) \\ &:= -\Big((\nabla \boldsymbol{d}_h^{n+1})^t \nabla \boldsymbol{d}_h^{n+1}, \nabla \bar{\boldsymbol{u}}_h\Big) + \sum_{i=1}^3 K_i^n. \end{aligned}$$

Finally, the term I_4^n of (5.7) takes the form (see (1.9))

$$-\Big((\nabla \boldsymbol{d}_h^n)^t \widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d}_h^n), \bar{\boldsymbol{u}}_h\Big) = -\Big(\nabla \widetilde{F}_\varepsilon(\boldsymbol{d}_h^n), \bar{\boldsymbol{u}}_h\Big) = \Big(\widetilde{F}_\varepsilon(\boldsymbol{d}_h^n), \nabla \cdot \bar{\boldsymbol{u}}_h\Big).$$

The above information allows us to obtain the following discrete integration by parts in (5.7):

$$-\Big((\nabla \boldsymbol{d}_h^n)^t \boldsymbol{w}_h^{n+1}, \bar{\boldsymbol{u}}_h\Big) = -\Big((\nabla \boldsymbol{d}_h^{n+1})^t \nabla \boldsymbol{d}_h^{n+1}, \nabla \bar{\boldsymbol{u}}_h\Big) + \sum_{i=2}^3 I_i^n + \sum_{i=1}^3 K_i^n + J_2^n + \Big(\widetilde{F}_\varepsilon(\boldsymbol{d}_h^n), \nabla \cdot \bar{\boldsymbol{u}}_h\Big).$$

Then, (5.1) is expressed as

$$\begin{aligned} &-\int_0^T \Big((\nabla \boldsymbol{d}_{h,k,\varepsilon}(t))^t \nabla \boldsymbol{d}_{h,k,\varepsilon}(t), \boldsymbol{v}_{h,k}(t)\Big)\, \mathrm{d}t + k \sum_{n=0}^{N-1} \left(\sum_{i=1}^3 K_i^n + \sum_{i=2}^3 I_i^n + J_2^n \right) \\ &+k \sum_{n=0}^{N-1} \Big(\frac{1}{2}|\nabla \boldsymbol{d}^{n+1}(h)|^2 + \widetilde{F}_\varepsilon(\boldsymbol{d}_h^n), \nabla \cdot \boldsymbol{v}_h^{n+1}\Big). \end{aligned} \tag{5.8}$$

Notice that the more singular term is $(\nabla \boldsymbol{d}_{h,k,\varepsilon}(t))^t \nabla \boldsymbol{d}_{h,k,\varepsilon}(t)$ which is only bounded in $L^\infty(0,T;\boldsymbol{L}^1(\Omega))$. The following result help us to determine its limit (see [20], Chap. 12).

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Lemma 5.2. *Let $\boldsymbol{A}^m : Q \to \mathbb{R}^{d\times d}$ be a uniformly bounded sequence in $\boldsymbol{L}^2(Q)$. Then there exist a measure $\mu \in \mathcal{M}(Q)$ and a subsequence of $\boldsymbol{A}^m$ (relabed of the same manner) such that*

$$|\boldsymbol{A}^m|^2 \to \mu \quad \text{weak-}\star \text{ in } \mathcal{M}(Q).$$

Moreover, there exists a weak-$\star$ μ-measurable mapping $(\boldsymbol{x},t) \in Q \to \boldsymbol{M}_{\boldsymbol{x},t} \in \mathrm{Prob}(\mathbb{R}^{d\times d}))$ such that, for a equally relabed subsequence of $\boldsymbol{A}^m$,

$$\int_Q ((\boldsymbol{A}^m)^t \boldsymbol{A}^m)(\boldsymbol{x},t) : \varphi(\boldsymbol{x},t)\,\mathrm{d}\boldsymbol{x}\mathrm{d}t \to \int_Q \varphi(\boldsymbol{x},t) : \left(\int_{\mathbb{R}^{d\times d}} \frac{\boldsymbol{y}^t\boldsymbol{y}}{|\boldsymbol{y}|^2}\mathrm{d}\boldsymbol{M}_{\boldsymbol{x},t}(\boldsymbol{y})\right)\mathrm{d}\mu(\boldsymbol{x},t)$$

for all $\varphi \in C_c^\infty([0,T);\mathcal{C}_c^\infty(\Omega))^{d\times d}$.

In our case, we can apply Lemma 5.2 for $m=(h,k,\varepsilon)$ and $\boldsymbol{A}^m = \{\nabla \boldsymbol{d}_{h,k,\varepsilon}\}$ bounded in $\boldsymbol{L}^2(Q)$.
Thus, we can find $\mu \in \mathcal{M}(Q)$ and $\boldsymbol{M}_{\boldsymbol{x},t} \in \mathrm{Prob}(\mathbb{R}^{d\times d})$ such that

$$\int_Q ((\nabla \boldsymbol{d}_{h,k,\varepsilon})^t \nabla \boldsymbol{d}_{h,k,\varepsilon}) : \nabla \boldsymbol{v}_{h,k}\,\mathrm{d}\boldsymbol{x}\mathrm{d}t \to \int_Q \nabla \boldsymbol{v} : \left(\int_{\mathbb{R}^{d\times d}} \frac{\boldsymbol{y}^t\boldsymbol{y}}{|\boldsymbol{y}|^2}\mathrm{d}\boldsymbol{M}_{\boldsymbol{x},t}(\boldsymbol{y})\right)\mathrm{d}\mu(\boldsymbol{x},t)$$

as $(h,k,\varepsilon)\to 0$. Indeed,

$$\begin{aligned}\int_Q ((\nabla \boldsymbol{d}_{h,k,\varepsilon})^t \nabla \boldsymbol{d}_{h,k,\varepsilon}) : \nabla \boldsymbol{v}_{h,k}\,\mathrm{d}\boldsymbol{x}\mathrm{d}t &= \int_Q ((\nabla \boldsymbol{d}_{h,k,\varepsilon})^t \nabla \boldsymbol{d}_{h,k,\varepsilon}) : \nabla(\boldsymbol{v}_{h,k}-\boldsymbol{v})\,\mathrm{d}\boldsymbol{x}\mathrm{d}t \\ &\quad + \int_Q ((\nabla \boldsymbol{d}_{h,k,\varepsilon})^t \nabla \boldsymbol{d}_{h,k,\varepsilon}) : \nabla \boldsymbol{v}\,\mathrm{d}\boldsymbol{x}\mathrm{d}t.\end{aligned}$$

The first term on the right-hand side tends to zero (because $\nabla \boldsymbol{v}_{h,k} \to \nabla \boldsymbol{v}$ in $L^\infty(Q)$) and the second term converges, by Lemma 5.2, to $\displaystyle\int_Q \nabla \boldsymbol{v} : \Big(\int_{\mathbb{R}^{d\times d}} \frac{\boldsymbol{y}^t\boldsymbol{y}}{|\boldsymbol{y}|^2}\mathrm{d}\boldsymbol{M}_{\boldsymbol{x},t}(\boldsymbol{y})\Big)\,\mathrm{d}\mu(\boldsymbol{x},t)$.

Then, all that remains to prove is that the rest of the residual terms of (5.8) go to zero. First, the last term

$$k\sum_{n=0}^{N-1}\left(\frac{1}{2}|\nabla \boldsymbol{d}^{n+1}(h)|^2 + \widetilde{F}_\varepsilon(\boldsymbol{d}_h^n), \nabla\cdot \boldsymbol{v}_h^{n+1}\right) \to 0$$

because of $\nabla\cdot\boldsymbol{v}_h^{n+1} \to 0$ in $L^\infty(0,T;L^\infty(\Omega))$, and $|\nabla \boldsymbol{d}^{n+1}(h)|^2$ and $\widetilde{F}_\varepsilon(\boldsymbol{d}_h^n)$ are bounded in $L^1(0,T;L^1(\Omega))$ (from (5.6) and estimate (vii) of Thm. 1.4, respectively).

Now, we consider the term K_1^n:

$$k\sum_{n=0}^{N-1} K_1^n = k\sum_{n=0}^{N-1}\left(\left(\nabla \boldsymbol{d}_h^{n+1}\right)^t\left(\nabla \boldsymbol{d}_h^{n+1} - \nabla \boldsymbol{d}^{n+1}(h)\right), \nabla \boldsymbol{v}_h^{n+1}\right) := G_1.$$

In virtue of estimate (v) of Theorem 1.4 and (5.6), we bound it as:

$$G_1 \le C\,k\sum_{n=0}^{N-1}\left(h\|\boldsymbol{w}_h^{n+1}\| + \frac{h}{\varepsilon} + h\right)\|\nabla \boldsymbol{v}_h^{n+1}\|_{L^\infty(\Omega)} \le C\,h + C\,\frac{h}{\varepsilon}$$

and hence $G_1 \to 0$ as $(h,k,\varepsilon)\to 0$ owing to (C). The convergence for the term K_3^n is to verify since it is similar and simpler than that of the term K_2^n.

Now, we treat the terms I_2^n and I_3^n as follows:

$$k\sum_{n=0}^{N-1} I_2^n = \lambda\,k\sum_{n=0}^{N-1}\left(\left(\nabla \boldsymbol{d}^{n+1}(h) - \nabla \boldsymbol{d}_h^n\right)^t \boldsymbol{z}_h^{n+1}, \boldsymbol{v}_h^{n+1}\right) := G_2$$

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and

$$k\sum_{n=0}^{N-1} I_3^n = \lambda\, k\sum_{n=0}^{N-1}\Big(\big(\nabla \boldsymbol{d}_h^{n+1}-\nabla \boldsymbol{d}_h^n\big)^t \boldsymbol{z}_h^{n+1}, \boldsymbol{v}_h^{n+1}\Big) := G_3.$$

Thus G_2 and G_3 can be bounded by applying (5.5) and estimates (v) and (vi) of Theorem 1.4, as

$$\begin{aligned} G_2 &\le C\,k\sum_{n=0}^{N-1}\|\nabla \boldsymbol{d}^{n+1}(h)-\nabla \boldsymbol{d}_h^n\|\,\|\boldsymbol{z}_h^{n+1}\|\,\|\boldsymbol{v}_h^{n+1}\|_{L^\infty(\Omega)}\\ &\le C\,h\,k\sum_{n=0}^{N-1}\|\boldsymbol{z}_h^{n+1}\|^2 \le C\,h\,k\sum_{n=0}^{N-1}\|\boldsymbol{w}_h^{n+1}\|^2 + C\,\frac{h}{\varepsilon^2}\le C\,h + C\,\frac{h}{\varepsilon^2}\end{aligned}$$

and

$$\begin{aligned} G_3 &\le C\,k\sum_{n=0}^{N-1}\|\nabla \boldsymbol{d}_h^{n+1}-\nabla \boldsymbol{d}_h^n\|\,\|\boldsymbol{z}_h^{n+1}\|\,\|\boldsymbol{v}_h^{n+1}\|_{L^\infty(\Omega)}\\ &\le C\,k^{1/2}\left(\sum_{n=0}^{N-1}\|\nabla \boldsymbol{d}_h^{n+1}-\nabla \boldsymbol{d}_h^n\|^2\right)^{1/2}\left(k\sum_{n=0}^{N-1}\Big(\|\boldsymbol{w}_h^{n+1}\|^2+\frac{1}{\varepsilon^2}\Big)\right)^{1/2} \le C\,k^{1/2}+C\,\frac{k^{1/2}}{\varepsilon},\end{aligned}$$

and hence $G_2\to 0$ and $G_3\to 0$ as $(h,k,\varepsilon)\to 0$, owing to (C) and (S'), respectively.

Then, the proof of the convergence result, Theorem 1.7, is finished.

Remark 5.3. In order to control the term G_2, we have had to consider the penalty potential $\widetilde{F}_\varepsilon$ for which the inequality $\|\widetilde{\boldsymbol{f}}_\varepsilon(\boldsymbol{d})\| \le C\,\varepsilon^{-1}\|\widetilde{F}_\varepsilon(\boldsymbol{d})\|_{L^1(\Omega)}^{1/2}$ holds. This estimate is the key to controlling $\boldsymbol{z}_h^{n+1}$ in term of $\boldsymbol{w}_h^{n+1}$ and $\boldsymbol{d}_h^n$ depending on a reasonable power of ε, and therefore to making the term G_2 to go to zero. In the non-truncated case this convergence of G_2 to zero is not clear.

Remark 5.4. In two-dimensional domains, the likely existence of defect points implies that the director has infinite energy in the limiting Ericksen–Leslie equations, hence the definition of weak solutions does not make a sense. On the other hand, in three-dimensional domains, defect points have finite energy, and weak solutions may be well defined.

6. Numerical simulations

The numerical experiences that we will study in this section were extracted from [18] which are also performed in many other works as in [3,16]. These tests show the behavior of the two defects (or singularities) of the director vector field.

We have used the penalty function $F_\varepsilon(\boldsymbol{d})$ (without truncating) and computed all the numerical simulations on the two-dimensional square $\Omega=(-1,1)\times(-1,1)$. As used in [18], physical parameters are set as $\lambda=\nu=\gamma=1$, the penalty parameter is set to $\varepsilon=0.05$, and the initial velocity is zero and the director vector is taken to be

$$\boldsymbol{d}_0 = \widehat{\boldsymbol{d}}/\sqrt{|\widehat{\boldsymbol{d}}|^2+0.05^2},\quad \text{where}\quad \widehat{\boldsymbol{d}}=(x^2+y^2-0.25,y).$$

As shown Figure 1, this director vector has initially two defects at $(\pm 1/2,0)$ (points in which $\widehat{\boldsymbol{d}}=(0,0)$). The boundary condition for the director vector are take to be time-independent and equal to $\boldsymbol{d}_0/|\boldsymbol{d}_0|$ on $\partial\Omega$.

In order to avoid to compute the pressure in a zero-average finite space, we introduce a penalty term into the discrete free-divergence term, *i.e.*, (1.16) is replaced by

$$\Big(\nabla\cdot \boldsymbol{u}_h^{n+1},\bar{p}_h\Big)+\delta\Big(p_h^{n+1},\bar{p}_h\Big)=0\quad \forall\,\bar{p}_h\in Q_h,$$

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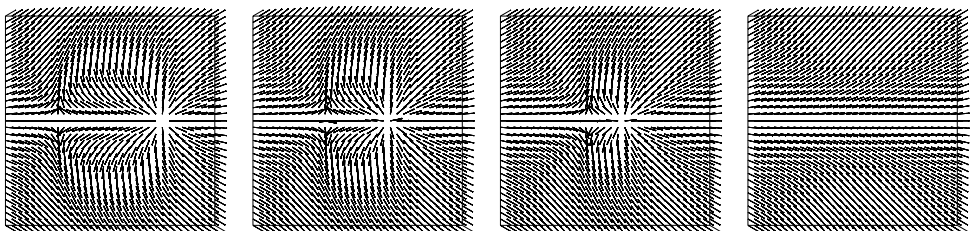


FIGURE 1. Snapshots of $\boldsymbol{d}_{h,k,\varepsilon}(t)$ at times $t = 0$, 0.2, 0.3, 0.4.

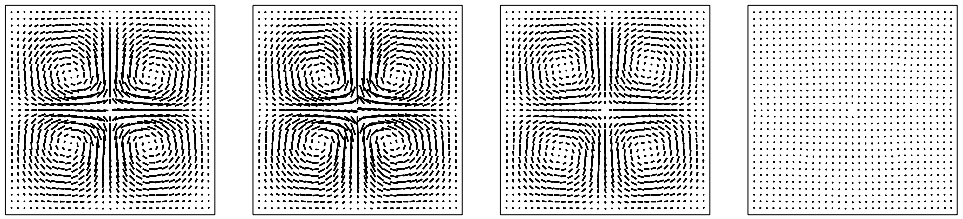


FIGURE 2. Snapshots of $\boldsymbol{u}_{h,k,\varepsilon}(t)$ at times $t = 0.2$, 0.3, 0.4, 0.5.

where δ is chosen to be 10^{-6}. To solve the resulting algebraic linear system from our mixed formulation (1.15)–(1.18), we use the LU direct solver.

For the first simulations, the velocity and pressure $(\boldsymbol{u}, p)$ are approximated by using a pair of finite element spaces known as the mini-element $(\mathbb{P}_1 + bubble, \mathbb{P}_1)$ (which satisfies the Babuska–Brezzi condition (H3)). The director vector and the auxiliary variable $(\boldsymbol{d}, \boldsymbol{w})$ are computed by using the pair of finite element spaces $(\mathbb{P}_1, \mathbb{P}_1)$ agrees with condition (H4). We use a uniform triangular mesh on a 32×32 grid ($h = 1/16$), and the time interval $[0, 1]$ is divided into 400-time steps ($k = 1/400$). Note that $k = \varepsilon^2$ which is agreed with hypothesis (S) (see Rem. 2.3 for $2D$ domains) but $h = 0.0625$ is bigger than ε^2, hence convergence constraint (C) does not hold.

We show the evolution of the two defects at times $t = 0.2$, 0.3, and 0.4, in Figure 1, and the evolution of the velocity field at times $t = 0.2$, 0.3, 0.4 and 0.5, in Figure 2 (note that the elastic tensor $\lambda\nabla \cdot ((\nabla \boldsymbol{d})^t \nabla \boldsymbol{d})$ causes a velocity moving the defects along the axis $x = 0$).

We observe that the annihilation time is around $t = 0.33$. This time is bigger than those obtained in [18] ($t \approx 0.25$) and [16] ($t \approx 0.26$), see Figure 1, where the penalty term is treated in an implicit or semi-implicit manner, respectively. The dependence of this annihilation time with respect to the elasticity constant $\lambda > 0$ can be seen in [17], varying this annihilation time approximately between 0.19 for $\lambda = 10$ and 0.28 for $\lambda = 0.1$.

The annihilation time obtained with our scheme can be improved by considering a smaller time step; for instance, the annihilation time is between $t = 0.27$ and $t = 0.28$ by taking $k = 5 \times 10^{-5}$ (and the same occurs for the scheme given in [16]). It seems to be that this fact is related to the bigger approximation error of the explicit time integration of the penalty term as against the other implicit or semi-implicit treatments.

On the other hand, all the previous annihilation times are smaller than the ones obtained in [3] ($t \approx 0.5$), where a different (Neumann instead of Dirichlet) boundary conditions for the director vector field is considered.

We can observe that our linear coupled scheme is stable (with decreasing discrete energy). Snapshot 1 in Figure 3 shows the behavior of the kinetic energy, $E_{kin} = \frac{1}{2}\int_\Omega |\boldsymbol{u}_h^{n+1}(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x}$, and Snapshopt 2 in Figure 3 shows the elastic energy, $E_{elas} = \frac{\lambda}{2}\int_\Omega |\nabla \boldsymbol{d}_h^{n+1}(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x}$, the penalty energy, $E_{pen} = \frac{\lambda}{2}\int_\Omega F_\varepsilon(\boldsymbol{d}_h^{n+1}(\boldsymbol{x})) \, \mathrm{d}\boldsymbol{x}$, and the total energy $E = E_{\mathrm{kin}} + E_{\mathrm{elas}} + E_{\mathrm{pen}}$.

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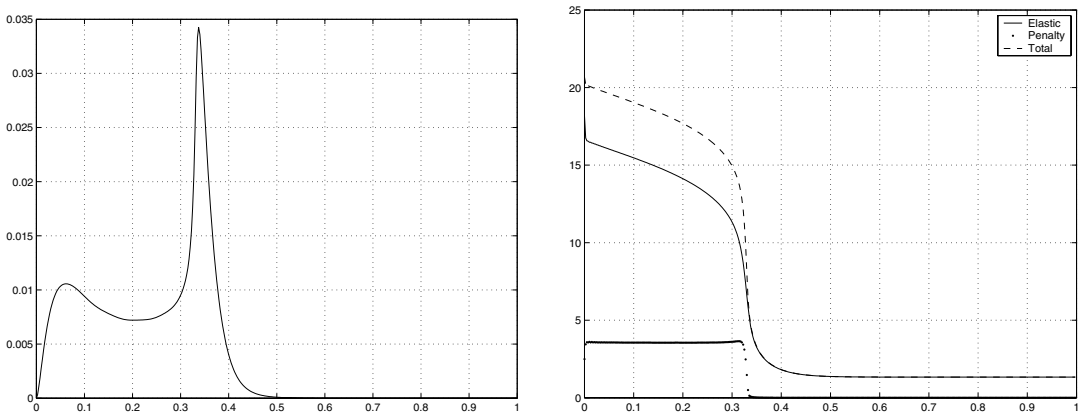


FIGURE 3. Kinetic, elastic, penalty, and total energies.

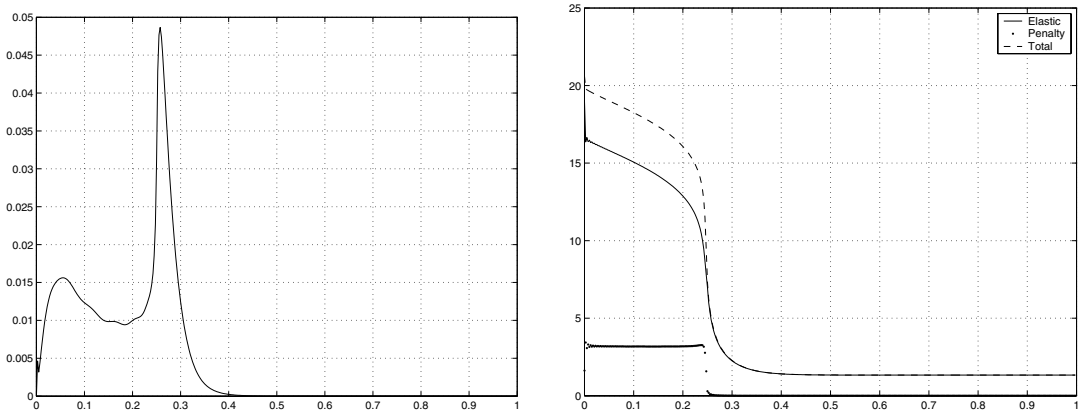


FIGURE 4. Kinetic, elastic, penalty, and total energies in [16].

We now compare the energy decay between scheme (1.15)–(1.18) and the scheme given in [16], which uses the standard piecewise quadratic element, $\mathbb{P}_2$, for both the velocity and the director vector, and piecewise linear elements, $\mathbb{P}_1$, for the pressure. At the beginning of the simulation, we observe (see Snapshots 1 and 2 in Fig. 4) an oscillatory behavior of kinetic, elastic, and penalty energies which could point out that the scheme presented in [16] is less robust with respect to the stability than our approximations.

Concerning the numerical results in [3], we observe that the behavior of the different energies is quite similar despite the authors in [3] took Neumann boundary conditions for the director vector field. The only different is with respect to the size of the kinetic energy.

Figure 5 shows the behavior of the L^2-norm of $\boldsymbol{w}_h^{n+1}$, which represents how far our numerical director is from an equilibrium solution, because $\boldsymbol{w}_h^{n+1}$ is a numerical approximation of the critical point equation for the elastic energy. We can also observe that the dynamic of the annihilation produces an instantaneous increasing of this measure.

In order to be more precise regarding stability constraints, we have changed the finite element approximation, considering now on a uniform 16×16 mesh, $(\mathbb{P}_2, \mathbb{P}_1)$ for the velocity and pressure (which again satisfies the Babuska–Brezzi condition (H3)), and either $(\mathbb{P}_2, \mathbb{P}_2)$ or $(\mathbb{P}_2, \mathbb{P}_0)$ for the director vector and the auxiliary variable $(\boldsymbol{d}, \boldsymbol{w})$ (the first case satisfies $(H4)$ and the second one does not). Both choices are numerically stable

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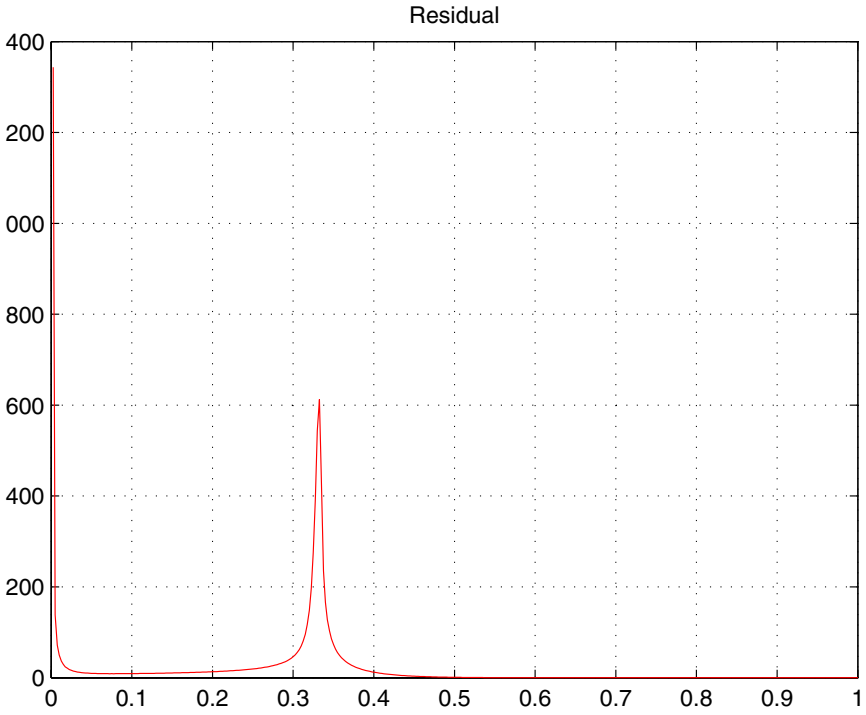


FIGURE 5. L^2-norm of $\boldsymbol{w}_h^{n+1}$ *vs.* time.

(with a decreasing energy) for $k = 0.003$, which is agreed with Remark 2.4, although small oscillations in the kinetic energy are observed. But, for this same $k = 0.003$ and for $(\boldsymbol{d}, \boldsymbol{w})$ being approximated by $(\mathbb{P}_2, \mathbb{P}_1)$, the scheme becomes unstable.

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