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ON THE CONVERGENCE OF AN IEQ-BASED FIRST-ORDER SEMI-DISCRETE SCHEME FOR THE BERIS-EDWARDS SYSTEM

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Abstract. We present a convergence analysis of an unconditionally energy-stable first-order semi-discrete numerical scheme designed for a hydrodynamic Q-tensor model, the so-called Beris-Edwards system, based on the Invariant Energy Quadratization Method (IEQ). The model consists of the Navier–Stokes equations for the fluid flow, coupled to the Q-tensor gradient flow describing the liquid crystal molecule alignment. By using the Invariant Energy Quadratization Method, we obtain a linearly implicit scheme, accelerating the computational speed. However, this introduces an auxiliary variable to replace the bulk potential energy and it is *a priori* unclear whether the reformulated system is equivalent to the Beris-Edward system. In this work, we prove stability properties of the scheme and show its convergence to a weak solution of the coupled liquid crystal system. We also demonstrate the equivalence of the reformulated and original systems in the weak sense.

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1. Introduction

Liquid crystal is an intermediate state of matter between the solid and liquid phase and usually exists in a specific temperature range. On one hand, it possesses the ability to flow of liquids, and on the other hand, the molecules are ordered, (neighboring molecules roughly point in the same direction) similar as in a classical solid. Due to this, liquid crystals have unique physical properties that are used in various real-life applications, such as monitors, screens, clocks, navigation systems, and others. Typically, liquid crystals consist of elongated molecules of identical size which can be pictured as rods. The inter-molecular forces make them align along a common axis [3, 36].

Mathematical models for the dynamics of liquid crystals have been intensively studied in the last decades. For an overview, see [16, 25–27, 37] and the references therein. Here we will consider the Q-tensor model by Landau and de Gennes [15] and its numerical approximation. In this model, the orientation of the liquid crystal molecules is described by the Q-tensor, a symmetric and trace-free $d \times d$-matrix field where $d = 2, 3$ is the spatial dimension. It can be interpreted as the deviation of the second moment of the probability density of the directions of liquid crystal molecules from the isotropic state [29]. When the liquid crystal is in an equilibrium,

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the Q-tensor minimizes a free energy, the so-called Landau–de Gennes free energy [5, 30],

$$E_{\mathrm{LG}}(\boldsymbol{Q}) = \int_\Omega \mathcal{F}_B(\boldsymbol{Q}) + \mathcal{F}_E(\boldsymbol{Q}),$$

where $\Omega \subset \mathbb{R}^d$, is the spatial domain, and we assume that it has a sufficiently smooth boundary. $\mathcal{F}_B$ is the bulk potential and $\mathcal{F}_E$ is the elastic energy density given by

$$\mathcal{F}_B(\boldsymbol{Q}) = \frac{a}{2}\operatorname{tr}(\boldsymbol{Q}^2) - \frac{b}{3}\operatorname{tr}(\boldsymbol{Q}^3) + \frac{c}{4}\big(\operatorname{tr}(\boldsymbol{Q}^2)\big)^2, \quad \mathcal{F}_E(\boldsymbol{Q}) = \frac{L}{2}|\nabla \boldsymbol{Q}|^2,$$

where a, b, c, L are constants with $c, L > 0$. In particular, $c > 0$ will guarantee the existence of a lower bound of the bulk potential, which is vital for the following analysis. In a non-equilibrium situation, the dynamics of the Q-tensor are governed by a nonlinear system of PDEs, consisting of the gradient flow for the Q-tensor field coupled to the Navier–Stokes equations for the underlying fluid flow [7, 43, 44],

$$\begin{cases} \boldsymbol{u}_t + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = -\nabla p + \mu\Delta\boldsymbol{u} + \nabla\cdot\boldsymbol{\Sigma} - \boldsymbol{H}\nabla\boldsymbol{Q}, & (1.1a)\\ \nabla\cdot\boldsymbol{u} = 0, & (1.1b)\\ \boldsymbol{Q}_t + \boldsymbol{u}\cdot\nabla\boldsymbol{Q} - \boldsymbol{S} = M\boldsymbol{H}, & (1.1c)\end{cases}$$

subject to initial and boundary conditions,

$$\begin{cases} \boldsymbol{Q}|_{t=0} = \boldsymbol{Q}_0, \qquad \boldsymbol{Q}|_{\partial\Omega\times[0,T]} = 0, & (1.2a)\\ \boldsymbol{u}|_{t=0} = \boldsymbol{u}_0, \qquad \boldsymbol{u}|_{\partial\Omega\times[0,T]} = 0, & (1.2b)\end{cases}$$

where $(\boldsymbol{H}\nabla\boldsymbol{Q})_k = \sum_{i,j=1}^d H_{ij}\partial_k Q_{ij}$ and $(\boldsymbol{u}\cdot\nabla\boldsymbol{Q})_{ij} = \sum_{k=1}^d u_k\partial_k Q_{ij}$ for all $1 \le k, i, j \le d$. $\boldsymbol{u}$ denotes the velocity field, and p represents the pressure. The tensors $\boldsymbol{S}$ and $\boldsymbol{\Sigma}$ appearing in the system (1.1a)–(1.1c) above are given by

$$\boldsymbol{S} = S(\boldsymbol{u}, \boldsymbol{Q}) = \boldsymbol{W}\boldsymbol{Q} - \boldsymbol{Q}\boldsymbol{W} + \xi(\boldsymbol{Q}\boldsymbol{D} + \boldsymbol{D}\boldsymbol{Q}) + \frac{2\xi}{d}\boldsymbol{D} - 2\xi(\boldsymbol{D}:\boldsymbol{Q})\left(\boldsymbol{Q} + \frac{1}{d}\boldsymbol{I}\right), \tag{1.3}$$

and

$$\boldsymbol{\Sigma} = \Sigma(\boldsymbol{Q}, \boldsymbol{H}) = \boldsymbol{Q}\boldsymbol{H} - \boldsymbol{H}\boldsymbol{Q} - \xi(\boldsymbol{H}\boldsymbol{Q} + \boldsymbol{Q}\boldsymbol{H}) - \frac{2\xi}{d}\boldsymbol{H} + 2\xi(\boldsymbol{Q}:\boldsymbol{H})\left(\boldsymbol{Q} + \frac{1}{d}\boldsymbol{I}\right) \tag{1.4}$$

with

$$\boldsymbol{D} = \frac{1}{2}\big(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^\top\big), \quad \boldsymbol{W} = \frac{1}{2}\big(\nabla\boldsymbol{u} - (\nabla\boldsymbol{u})^\top\big) \tag{1.5}$$

representing the symmetric and skew-symmetric parts of the matrix $\nabla\boldsymbol{u}$. Here $\boldsymbol{S}$ denotes the rotational and stretching effects on the liquid crystal molecules generated by the flow. The constant $\xi \in \mathbb{R}$, whose value is contingent upon the specific molecular characteristics of a given liquid crystal, quantifies the proportion between the tumbling effect and the aligning effect that a shear flow would exert on the liquid crystal director [32]. $\boldsymbol{\Sigma}$ is an elastic stress tensor term [10]. The notation $(\cdot : \cdot)$ represents the standard Frobenius inner prodcut of two matrices, see the notation Section 2.1 for further details. The tensor $\boldsymbol{H}$ is the molecular field corresponding to the variational derivative of the free energy $E_{\mathrm{LG}}(\boldsymbol{Q})$ and given by

$$\boldsymbol{H} = -\frac{\partial E_{\mathrm{LG}}}{\partial\boldsymbol{Q}} = L\Delta\boldsymbol{Q} - \left[a\boldsymbol{Q} - b\left(\boldsymbol{Q}^2 - \frac{1}{d}\operatorname{tr}(\boldsymbol{Q}^2)\boldsymbol{I}\right) - c\operatorname{tr}(\boldsymbol{Q}^2)\,\boldsymbol{Q}\right]. \tag{1.6}$$

Notice that the last term in the definition of $\boldsymbol{\Sigma}$, (1.4) results in a gradient term after taking the divergence as it is the case in (1.1a). Hence we can modify the pressure to include this term and instead use the modified definition of $\boldsymbol{\Sigma}$:

$$\boldsymbol{\Sigma} = \Sigma(\boldsymbol{Q}, \boldsymbol{H}) = \boldsymbol{Q}\boldsymbol{H} - \boldsymbol{H}\boldsymbol{Q} - \xi(\boldsymbol{H}\boldsymbol{Q} + \boldsymbol{Q}\boldsymbol{H}) - \frac{2\xi}{d}\boldsymbol{H} + 2\xi(\boldsymbol{Q}:\boldsymbol{H})\boldsymbol{Q}. \tag{1.7}$$

Indeed, as we will be concerned with Leray-Hopf solutions in the following, these definitions can be used interchangeably. In the following, we will always use definition (1.7) for $\boldsymbol{\Sigma}$ and the accordingly modified definition of the pressure. System (1.1a)–(1.7) is equivalent to the Beris-Edwards model as it is shown in Section 2.1 of [1].

Our goal in this work is to provide a convergence proof for a semi-discrete numerical scheme for (1.1a)–(1.7). The existence, uniqueness and regularity theory for this system have been studied in, *e.g.*, [1, 2, 10, 21, 22, 32, 33]. Numerical simulation and analysis of this and related models have been undertaken in, *e.g.*, [4, 6, 8, 13, 14, 28]. Due to the system being highly nonlinear, for stability of the numerical method, it is crucial to retain a discrete version of the energy dissipation law satisfied by the system at the level of the numerical scheme. However, this often results in nonlinearly implicit schemes which require the iterative solution of a nonlinear algebraic system at every timestep. In order to circumvent this issue, the invariant energy quadratization (IEQ) method has been introduced for nonlinear gradient flows [23, 24, 39–42, 44]. The key idea is to introduce an auxiliary variable for the bulk potential term which is then discretized as an independent variable. This results in a linearly implicit scheme which is unconditionally energy-stable. A discrete version of the energy dissipation property is retained while enhancing computational efficiency.

Specifically, in the case of system (1.1a)–(1.7), the auxiliary variable r is introduced [44]:

$$r(\boldsymbol{Q}) = \sqrt{2\left(\frac{a}{2}\operatorname{tr}(\boldsymbol{Q}^2) - \frac{b}{3}\operatorname{tr}(\boldsymbol{Q}^3) + \frac{c}{4}\operatorname{tr}^2(\boldsymbol{Q}^2) + A_0\right)}, \tag{1.8}$$

where $A_0 > 0$ is a constant ensuring that r is always positive for any $\boldsymbol{Q} \in \mathbb{R}^{d\times d}$. This is possible since one can show that the bulk potential $\mathcal{F}_B(\boldsymbol{Q})$ has a lower bound, see Theorem 2.1 of [44]. If we then define

$$V(\boldsymbol{Q}) = a\boldsymbol{Q} - b\left[\boldsymbol{Q}^2 - \frac{1}{d}\operatorname{tr}(\boldsymbol{Q}^2)\boldsymbol{I}\right] + c\operatorname{tr}(\boldsymbol{Q}^2)\boldsymbol{Q},$$

it follows that

$$\frac{\delta r(\boldsymbol{Q})}{\delta \boldsymbol{Q}} = \frac{V(\boldsymbol{Q})}{r(\boldsymbol{Q})} := P(\boldsymbol{Q}), \tag{1.9}$$

for a trace-free, symmetric tensor $\boldsymbol{Q}$. Then system (1.1a)–(1.1c) can be reformulated as

$$\begin{cases} \boldsymbol{u}_t + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = -\nabla p + \mu\Delta\boldsymbol{u} + \nabla\cdot\boldsymbol{\Sigma} - \boldsymbol{H}\nabla\boldsymbol{Q}, & (1.10\text{a})\\ \nabla\cdot\boldsymbol{u} = 0, & (1.10\text{b})\\ \boldsymbol{Q}_t + \boldsymbol{u}\cdot\boldsymbol{Q} - \boldsymbol{S} = M\boldsymbol{H}, & (1.10\text{c})\\ r_t = P(\boldsymbol{Q}) : \boldsymbol{Q}_t, & (1.10\text{d})\\ \boldsymbol{H} = L\Delta\boldsymbol{Q} - rP(\boldsymbol{Q}). & (1.10\text{e}) \end{cases}$$

In [44], the authors proposed an energy stable scheme for the reformulated system (1.10a)–(1.10e), and proved that it satisfies a discrete version of the energy dissipation law. Yet, to the extent of our knowledge, there is no convergence proof for a numerical scheme developed for the Beris-Edwards model utilizing the IEQ method, nor is there any existing proof of convergence to weak solutions to the Beris-Edwards for any numerical scheme. The main issue is that the reformulation of (1.1a)–(1.7) to (1.10a)–(1.10e) is only valid at the formal level assuming solutions are smooth. However, this may not be the case for this system, given that it involves coupling to the incompressible Navier–Stokes equations. Therefore, at least in three space dimensions, at most global weak solutions can be expected. Specifically, the existence of weak solutions in $\mathbb{R}^3$ was proven in the work of Paicu and Zarnescu [32], and the existence of weak solutions in bounded domains with Dirichlet boundary conditions was shown by Guillén-González *et al.* [22]. To the best of our knowledge, this is the state-to-the-art regarding this system. Furthermore, *a priori*, the auxiliary variable r has less integrability than the square root of the bulk potential. While the square root of the bulk potential is expected to be in the Lebesgue space L^3 in space, the auxiliary variable is only expected to be in L^2 according to the reformulated energy dissipation law. In this work, we will show how to circumvent this issue and obtain *a priori* estimates for the numerical approximations which are sufficient for passing to the limit and obtaining a weak solution of (1.1a)–(1.7). Hence, this can also be seen as an alternative proof of existence of global weak solutions for the Beris-Edwards system.

The focus of this work is on a semi-discrete scheme for the reformulated system (1.10) that uses the projection method by Chorin and Temam [11,38] for the discretization of the Navier–Stokes subsystem. A version of this scheme was initially proposed in [44]. We believe that many of the new ideas we are introducing could facilitate the convergence proof for a fully-discrete scheme also. In particular, we show here how to overcome the lack of regularity for the auxiliary variable r, one of the main obstacles encountered for proving convergence. This issue needs to be solved in the fully-discrete case as well. Nevertheless, further challenges can be expected in the fully-discrete case: A suitable spatial discretization will need to respect a discrete version of the energy law of system (1.10). For a finite difference scheme, due to the coupling between variables and the nonlinear terms, this will require the careful design of discrete chain rules and integration by parts identities, possibly using staggered grids. For a finite element scheme, since the incompressible Navier–Stokes equation appear as a subsystem in the Beris-Edwards equations, any convergence proof requires a convergence proof of a fully-discrete scheme for the Navier–Stokes equations. As far as we know, such a proof is currently not available for a discretization using finite elements and the projection method in 3D under no additional regularity assumptions. For these reasons, we here focus on the semi-discrete scheme, while the fully-discrete is the subject of future research.

The rest of this article is structured as follows: In Section 2, we introduce the notations and some standard results that will be used in the following. Then we will construct and analyze a numerical scheme designed for system (1.10a)–(1.10e) in Section 3. We will also provide a discrete energy dissipation law in this section. In Section 4, we provide the convergence argument. Finally, we will show the equivalence between weak solutions for the reformulated system and weak solutions of the original system (1.1a)–(1.6).

2. Preliminaries

2.1. Notation

Let $\Omega \subset \mathbb{R}^d$ be a bounded domain with C^2 boundary. We denote the norm of a Banach space X as $\|\cdot\|_X$ and its dual space by X^*. If we omit the subscript X, it represents the norm of the space $L^2(\Omega)$. For simplicity, when used as a subscript, we will not write the symbol Ω if we refer to a function space over domain Ω, *i.e.*, $L^2 = L^2(\Omega)$. The inner product on L^2 will be denoted by $\langle\cdot,\cdot\rangle$. Vector-valued and matrix-valued functions will be denoted in bold form.

For two vectors $\boldsymbol{u},\boldsymbol{v} \in \mathbb{R}^d$, we set their inner product to be $\boldsymbol{u}\cdot\boldsymbol{v} = \sum_{i=1}^d u_i v_i$ and for two matrices $\boldsymbol{A},\boldsymbol{B} \in \mathbb{R}^{d\times d}$, we use the Frobenius inner product $\boldsymbol{A} : \boldsymbol{B} = \operatorname{tr}(\boldsymbol{A}^\top \boldsymbol{B}) = \sum_{i,j=1}^d A_{ij}B_{ij}$. The norm of matrix $\mathbf{A}$ is then given by $|\boldsymbol{A}| = |\boldsymbol{A}|_F = \sqrt{\boldsymbol{A}:\boldsymbol{A}}$. Finally, the derivatives of matrix $\boldsymbol{A}$ are defined as a matrix, that is, $\partial_i \boldsymbol{A} = (\partial_i A_{jk})_{jk}$ and $\nabla \boldsymbol{A} = (\partial_1 \boldsymbol{A}, \cdots, \partial_d \boldsymbol{A})$. When we write $\|\boldsymbol{A}\|$, $\|\nabla \boldsymbol{A}\|$, we mean $\|\boldsymbol{A}\| = \left(\int_\Omega |A|^2 \,\mathrm{d}x\right)^{\frac{1}{2}}$ and $\|\nabla \boldsymbol{A}\| = \left(\int_\Omega \sum_{i=1}^d |\partial_i \boldsymbol{A}|^2 \,\mathrm{d}x\right)^{\frac{1}{2}}$.

Throughout this paper, we will denote L^p spaces (*e.g.*, $L^2(\Omega)$ for square integrable functions defined over Ω), Sobolev spaces and Bochner spaces in standard ways, and will not distinguish between scalar, vector-valued and tensor-valued function spaces when it is clear from the context. In particular, we use $L^p(0,T;X)$ to denote the space of functions $f : [0,T) \to X$ which are L^p-integrable in the time variable $t \in [0,T)$. We will denote the space $L^p(0,T;L^p)$ as $L^p([0,T)\times\Omega)$ in the following. We define $\mathcal{S}_0^d$ to be the space of trace-free symmetric $\mathbb{R}^{d\times d}$ matrices,

$$\mathcal{S}_0^d := \left\{ \boldsymbol{A} \in \mathbb{R}^{d\times d} : A_{ij} = A_{ji}, \sum_{i=1}^d A_{ii} = 0, 1 \le i,j \le d \right\}.$$

If there is no additional explanation, when we refer to a matrix-valued function $\boldsymbol{Q}$ (including $\boldsymbol{Q}^{n+1}, \boldsymbol{Q}^n, \boldsymbol{Q}_{\Delta t}, \boldsymbol{Q}_{\Delta t_m}$, etc.), we mean $\boldsymbol{Q} : \Omega \to \mathcal{S}_0^d$. We will use the subscript σ to indicate the divergence-free vector spaces, for example,

$$C_{c,\sigma}^\infty(\Omega) = \{\boldsymbol{\phi} \in C_c^\infty(\Omega); \nabla \cdot \boldsymbol{\phi} = 0\}, \quad L_\sigma^2(\Omega) = \left\{\boldsymbol{\phi} \in L^2(\Omega) : \nabla \cdot \boldsymbol{\phi} = 0, \boldsymbol{\phi} \cdot \boldsymbol{n}|_{\partial\Omega} = 0\right\} = \overline{C_{c,\sigma}^\infty(\Omega)}^{L^2(\Omega)},$$
$$H_{0,\sigma}^1(\Omega) = H_0^1(\Omega) \cap L_\sigma^2(\Omega).$$

We denote the Leray projector by $\mathcal{P} : L^2(\Omega) \to L_\sigma^2(\Omega)$, which is an orthogonal projection induced by the Helmholtz-Hodge decomposition [38] $\boldsymbol{f} = \nabla g + \boldsymbol{h}$ for any $\boldsymbol{f} \in L^2(\Omega)$. Here, $g \in H^1(\Omega)$ is a scalar field, and $\boldsymbol{h} \in L_\sigma^2(\Omega)$ is a divergence-free vector field. Then for all $\boldsymbol{f} \in L^2(\Omega)$, it holds that $\mathcal{P}\boldsymbol{f} = \boldsymbol{h}$.

We will use C to denote a generic constant, which might depend on parameters $\mu, a, b, c, M, L, \xi, d$, domain Ω, and initial values $(\boldsymbol{u}_{in}, \boldsymbol{Q}_{in})$. If a constant depends on any other factors, it will be specified. The product space of two Banach spaces X and Y will be denoted as $X \times Y$ for all $(x, y) \in X \times Y$ where $x \in X, y \in Y$.

2.2. Technical lemmas and definition of weak solutions

Here we will list the technical tools that will be frequently used in the following analysis. To obtain higher order regularity of $\boldsymbol{Q}$ in space, we recall Agmon's inequality ([12], Lem. 4.10).

Lemma 2.1. *For any $f \in H^2(\Omega) \cap H_0^1(\Omega)$,*

$$\|f\|_{L^\infty} \le C\|f\|_{H^1}^{\frac{1}{2}} \|f\|_{H^2}^{\frac{1}{2}}. \tag{2.1}$$

The following lemma states an *a priori* estimate for Laplace operator ([19], Thm. 3.1.2.1).

Lemma 2.2. *There exists a constant C which only depends on the diameter of Ω, such that*

$$\|f\|_{H^2} \le C\|\Delta f\|, \tag{2.2}$$

for all $f \in H^2(\Omega) \cap H_0^1(\Omega)$.

We will also use the Aubin–Lions lemma [9, 35]:

Lemma 2.3. *Let $X_0 \subset X_1 \subset X_2$ be three Banach spaces. Assume that the embedding of X_1 into X_2 is continuous and that the embedding of X_0 into X_1 is compact. Let $p, r \in [1, \infty]$. Now if a family of functions $\mathcal{F}$ satisfies that for any $f \in \mathcal{F}$,*

$$f \in L^p([0,T); X_0), \qquad \frac{\mathrm{d}f}{\mathrm{d}t} \in L^r([0,T); X_2).$$

Then if $p < \infty$, $\mathcal{F}$ is a compact family in $L^p([0,T); X_1)$. If $p = \infty$, then $\mathcal{F}$ is a compact family in $C([0,T); X_1)$.

Definition 2.4. By a weak solution of system (1.1a)–(1.1c), we mean a triple $(\boldsymbol{u}, \boldsymbol{Q}, \boldsymbol{H})$, with $\boldsymbol{u} : [0,T) \times \Omega \to \mathbb{R}^d$, $\boldsymbol{Q} : [0,T) \times \Omega \to \mathbb{R}^{d\times d}$ and $\boldsymbol{H} : [0,T) \times \Omega \to \mathbb{R}^{d\times d}$ which satisfy

(i) $\boldsymbol{Q}(t,x)$ and $\boldsymbol{H}(t,x)$ are trace-free and symmetric and $\boldsymbol{u}(t,x)$ is divergence free for almost every (t,x).
(ii) They attain the initial values

$$\boldsymbol{Q}(0,x) = \boldsymbol{Q}_0(x) \in H^1(\Omega), \quad \boldsymbol{u}(0,x) = \boldsymbol{u}_0(x) \in L^2(\Omega), \quad \langle \boldsymbol{u}_0, \nabla\psi \rangle = 0,$$

for any smooth function $\psi \in C_c^\infty(\Omega)$.

(iii) The triple $(\boldsymbol{u},\boldsymbol{Q},\boldsymbol{H})$ satisfies the regularity condition

$$\boldsymbol{Q}\in L^\infty\big(0,T;H_0^1(\Omega)\big)\cap L^2\big(0,T;H^2(\Omega)\big),\quad \boldsymbol{u}\in L^\infty\big(0,T;L^2_\sigma(\Omega)\big)\cap L^2\big(0,T;H^1(\Omega)\big),\quad \boldsymbol{H}\in L^2([0,T)\times\Omega).$$

(iv) $(\boldsymbol{u},\boldsymbol{Q},\boldsymbol{H})$ satisfy the weak formulations

$$\begin{aligned}
&\int_0^T\int_\Omega \boldsymbol{u}\cdot\partial_t\boldsymbol{\psi}\,\mathrm{d}x\,\mathrm{d}t+\int_\Omega \boldsymbol{u}_0(x)\cdot\boldsymbol{\psi}(0,x)\,\mathrm{d}x+\int_0^T\int_\Omega\sum_{i,j=1}^d u_iu_j\partial_i\psi_j\,\mathrm{d}x\,\mathrm{d}t\\
&\qquad=\int_0^T\int_\Omega\Big[(\boldsymbol{Q}\boldsymbol{H}-\boldsymbol{H}\boldsymbol{Q})-\xi(\boldsymbol{H}\boldsymbol{Q}+\boldsymbol{Q}\boldsymbol{H})-\frac{2\xi}{d}\boldsymbol{H}+2\xi(\boldsymbol{Q}:\boldsymbol{H})\boldsymbol{Q}\Big]:\nabla\boldsymbol{\psi}\,\mathrm{d}x\,\mathrm{d}t\\
&\qquad\quad+\mu\int_0^T\int_\Omega\nabla\boldsymbol{u}:\nabla\boldsymbol{\psi}\,\mathrm{d}x\,\mathrm{d}t+\int_0^T\int_\Omega(\boldsymbol{H}\nabla\boldsymbol{Q})\cdot\boldsymbol{\psi}\,\mathrm{d}x\,\mathrm{d}t, \qquad (2.3a)\\
&\int_0^T\int_\Omega \boldsymbol{Q}:\partial_t\boldsymbol{\varphi}\,\mathrm{d}x\mathrm{d}t+\int_\Omega\boldsymbol{Q}_0(x):\boldsymbol{\varphi}(0,x)\,\mathrm{d}x+\int_0^T\int_\Omega\boldsymbol{Q}:(\boldsymbol{u}\cdot\nabla\boldsymbol{\varphi})\,\mathrm{d}x\,\mathrm{d}t\\
&\qquad\quad+\int_0^T\int_\Omega\Big[\boldsymbol{W}\boldsymbol{Q}-\boldsymbol{Q}\boldsymbol{W}+\xi(\boldsymbol{Q}\boldsymbol{D}+\boldsymbol{D}\boldsymbol{Q})+\frac{2\xi}{d}\boldsymbol{D}-2\xi(\boldsymbol{D}:\boldsymbol{Q})\boldsymbol{Q}\Big]:\boldsymbol{\varphi}\,\mathrm{d}x\,\mathrm{d}t\\
&\qquad=-\int_0^T\int_\Omega M\boldsymbol{H}:\boldsymbol{\varphi}\,\mathrm{d}x\,\mathrm{d}t, \qquad (2.3b)\\
&\int_0^T\int_\Omega\boldsymbol{H}:\boldsymbol{\phi}\,\mathrm{d}x\,\mathrm{d}t=-\int_0^T\int_\Omega\left(L\sum_{i,j=1}^d\nabla Q_{ij}\cdot\nabla\phi_{ij}\right)\mathrm{d}x\,\mathrm{d}t\\
&\qquad\quad-\int_0^T\int_\Omega\left(a\boldsymbol{Q}-b\Big((\boldsymbol{Q}^2)-\frac{1}{d}\operatorname{tr}(\boldsymbol{Q}^2)\Big)+c\operatorname{tr}(\boldsymbol{Q}^2)\boldsymbol{Q}\right):\boldsymbol{\phi}\,\mathrm{d}x\,\mathrm{d}t, \qquad (2.3c)
\end{aligned}$$

for all smooth divergence-free function $\boldsymbol{\psi}:[0,T)\times\Omega\to\mathbb{R}^d$ and all smooth matrix function $\boldsymbol{\varphi}=(\varphi_{ij})_{i,j=1}^d,\boldsymbol{\phi}=(\phi_{ij})_{i,j=1}^d:[0,T)\times\Omega\to\mathbb{R}^{d\times d}$ which are compactly supported within $[0,T)\times\Omega$.

Definition 2.5. By a weak solution of system (1.10a)–(1.10e), we mean a quadruple $(\boldsymbol{u},\boldsymbol{Q},\boldsymbol{H},r)$, with $\boldsymbol{u}:[0,T)\times\Omega\to\mathbb{R}^d$, $\boldsymbol{Q}:[0,T)\times\Omega\to\mathbb{R}^{d\times d}$, $\boldsymbol{H}:[0,T)\times\Omega\to\mathbb{R}^{d\times d}$ and $r:[0,T)\times\Omega\to\mathbb{R}$,

(i) $\boldsymbol{Q}(t,x)$ and $\boldsymbol{H}(t,x)$ are trace-free and symmetric and $\boldsymbol{u}(t,x)$ is divergence free for almost every (t,x).
(ii) They attain the initial values

$$\boldsymbol{Q}(0,x)=\boldsymbol{Q}_0(x)\in H^1(\Omega),\quad \boldsymbol{u}(0,x)=\boldsymbol{u}_0(x)\in L^2(\Omega),\quad r(0,x)=r(Q_0(x)),\quad \langle\boldsymbol{u}_0,\nabla\psi\rangle=0,$$

for any smooth function $\psi\in C_c^\infty(\Omega)$.
(iii) $(\boldsymbol{u},\boldsymbol{Q},r)$ satisfy the regularity condition

$$\begin{aligned}
&\boldsymbol{Q}\in L^\infty\big(0,T;H_0^1(\Omega)\big)\cap L^2\big(0,T;H^2(\Omega)\big), &&\boldsymbol{u}\in L^\infty\big(0,T;L^2_\sigma(\Omega)\big)\cap L^2\big(0,T;H^1(\Omega)\big),\\
&\boldsymbol{H}\in L^2\big(0,T;L^2(\Omega)\big), &&r\in L^\infty\big(0,T;L^2(\Omega)\big).
\end{aligned}$$

(iv) $(\boldsymbol{u}, \boldsymbol{Q}, \boldsymbol{H}, r)$ satisfy the weak formulations

$$\begin{aligned}
&\int_0^T \int_\Omega \boldsymbol{u} \cdot \partial_t \boldsymbol{\psi} \, \mathrm{d}x \, \mathrm{d}t + \int_\Omega \boldsymbol{u}_0(x) \cdot \boldsymbol{\psi}(0,x) \, \mathrm{d}x + \int_0^T \int_\Omega \sum_{i,j=1}^d u_i u_j \partial_i \psi_j \, \mathrm{d}x \, \mathrm{d}t \\
&\quad = \int_0^T \int_\Omega \left[(\boldsymbol{Q}\boldsymbol{H} - \boldsymbol{H}\boldsymbol{Q}) - \xi(\boldsymbol{H}\boldsymbol{Q} + \boldsymbol{Q}\boldsymbol{H}) - \frac{2\xi}{d} \boldsymbol{H} + 2\xi(\boldsymbol{Q} : \boldsymbol{H})\boldsymbol{Q} \right] : \nabla \boldsymbol{\psi} \, \mathrm{d}x \, \mathrm{d}t \\
&\qquad + \mu \int_0^T \int_\Omega \nabla \boldsymbol{u} : \nabla \boldsymbol{\psi} \, \mathrm{d}x \, \mathrm{d}t + \int_0^T \int_\Omega (\boldsymbol{H} \nabla \boldsymbol{Q}) \cdot \boldsymbol{\psi} \, \mathrm{d}x \, \mathrm{d}t, \qquad (2.4a)
\end{aligned}$$

$$\begin{aligned}
&\int_0^T \int_\Omega \boldsymbol{Q} : \partial_t \boldsymbol{\varphi} \, \mathrm{d}x \, \mathrm{d}t + \int_\Omega \boldsymbol{Q}_0(x) : \boldsymbol{\varphi}(0,x) \, \mathrm{d}x - \int_0^T \int_\Omega ((\boldsymbol{u} \cdot \nabla)\boldsymbol{Q}) : \boldsymbol{\varphi} \, \mathrm{d}x \, \mathrm{d}t \\
&\qquad + \int_0^T \int_\Omega \left[\boldsymbol{W}\boldsymbol{Q} - \boldsymbol{Q}\boldsymbol{W} + \xi(\boldsymbol{Q}\boldsymbol{D} + \boldsymbol{D}\boldsymbol{Q}) + \frac{2\xi}{d} \boldsymbol{D} - 2\xi(\boldsymbol{D} : \boldsymbol{Q})\boldsymbol{Q} \right] : \boldsymbol{\varphi} \, \mathrm{d}x \, \mathrm{d}t \\
&\quad = - \int_0^T \int_\Omega M \boldsymbol{H} : \boldsymbol{\varphi} \, \mathrm{d}x \, \mathrm{d}t \qquad (2.4b)
\end{aligned}$$

$$\int_0^T \int_\Omega r \, \phi_t \, \mathrm{d}x \, \mathrm{d}t + \int_\Omega r_0(x) \phi(0,x) \, \mathrm{d}x = - \int_0^T \int_\Omega P(\boldsymbol{Q}) : \boldsymbol{Q}_t \, \phi \, \mathrm{d}x \, \mathrm{d}t, \qquad (2.4c)$$

and

$$\int_0^T \int_\Omega \boldsymbol{H} : \boldsymbol{\phi} \, \mathrm{d}x \, \mathrm{d}t = - \int_0^T \int_\Omega L \sum_{i,j=1}^d \nabla Q_{ij} \cdot \nabla \phi_{ij} \mathrm{d}x \, \mathrm{d}t - \int_0^T \int_\Omega r P(\boldsymbol{Q}) : \boldsymbol{\phi} \, \mathrm{d}x \, \mathrm{d}t, \qquad (2.4d)$$

for all smooth divergence-free function $\boldsymbol{\psi} : [0,T) \times \Omega \to \mathbb{R}^d$, all smooth matrix function $\boldsymbol{\varphi} = (\varphi_{ij})_{i,j=1}^d, \boldsymbol{\phi} = (\phi_{ij})_{i,j=1}^d : [0,T) \times \Omega \to \mathbb{R}^{d \times d}$ and smooth function $\phi : [0,T) \times \Omega \to \mathbb{R}$ which are compactly supported within $[0,T) \times \Omega$.

Remark 2.6. Due to the density of smooth functions with compact support in $L^q(0,T; L^p(\Omega))$ and $L^q(0,T; W_0^{1,p}(\Omega))$ for $1 \le p, q < \infty$ and the regularity requirements on $(\boldsymbol{u}, \boldsymbol{Q}, \boldsymbol{H}, r)$ (together with the upcoming Lems. 3.9, 3.10 and Cor. 3.11 for the regularity of the time derivatives), we can reexamine the weak formulations (2.4) and integrate the time derivatives by part to weaken the requirements on the test functions to $\boldsymbol{\psi} \in L^2(0,T; H^1_{0,\sigma}(\Omega) \cap W^{1,6}(\Omega))$, $\boldsymbol{\varphi} \in L^2(0,T; L^6(\Omega))$, $\phi \in L^6([0,T] \times \Omega)$, and $\boldsymbol{\phi} \in L^2(0,T; H_0^1(\Omega))$ (by interpreting $\int_\Omega \partial_t \boldsymbol{u} \cdot \boldsymbol{\psi} \, \mathrm{d}x$ as a duality product in the space $V := H^1_{0,\sigma} \cap W^{1,6}(\Omega)$). By the same argument, the requirments on the test functions in Definition 2.4 can be weakened.

Then for the treatment of the convection term, we consider a bilinear form

$$B(\boldsymbol{u}, \boldsymbol{v}) = (\boldsymbol{u} \cdot \nabla)\boldsymbol{v} + \frac{1}{2}(\nabla \cdot \boldsymbol{u})\boldsymbol{v}. \qquad (2.5)$$

It is not hard to verify the following properties of B (see [31, 34, 38] and the references therein).

Lemma 2.7. *We define the trilinear form*

$$\tilde{B}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{\omega}) = \langle B(\boldsymbol{u}, \boldsymbol{v}), \boldsymbol{\omega} \rangle. \qquad (2.6)$$

Then

$$\tilde{B}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{\omega}) = -\tilde{B}(\boldsymbol{u}, \boldsymbol{\omega}, \boldsymbol{v}), \qquad (2.7)$$

for all $\boldsymbol{u} \in L^2(\Omega)$ *with* $L^2(\Omega)$*-integrable divergence, and* $\boldsymbol{v}, \boldsymbol{\omega} \in H_0^1(\Omega)$. *Moreover,* $\tilde{B}(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{v}) = 0$.

The following cancelation property will play a key role in deducing the discrete energy dissipation law in the next section.

Lemma 2.8. *For any* $\boldsymbol{u} \in H_0^1(\Omega)$*, we have*

$$\langle \nabla \boldsymbol{u}, \Sigma(\boldsymbol{Q}, \boldsymbol{H})\rangle + \langle \boldsymbol{H}, S(\boldsymbol{u}, \boldsymbol{Q})\rangle = 0, \tag{2.8}$$

for all symmetric trace-free matrices $\boldsymbol{Q} \in L^\infty(\Omega), \boldsymbol{H} \in L^2(\Omega)$.

Proof. From definitions (1.3) and (1.7), we have

$$\langle \boldsymbol{H}, S(\boldsymbol{u}, \boldsymbol{Q})\rangle = \left\langle \boldsymbol{H}, \boldsymbol{W}\boldsymbol{Q} - \boldsymbol{Q}\boldsymbol{W} + \xi(\boldsymbol{Q}\boldsymbol{D} + \boldsymbol{D}\boldsymbol{Q}) + \frac{2\xi}{d}\boldsymbol{D} - 2\xi(\boldsymbol{D} : \boldsymbol{Q})\left(\boldsymbol{Q} + \frac{1}{d}\boldsymbol{I}\right)\right\rangle,$$
$$\langle \nabla \boldsymbol{u}, \Sigma(\boldsymbol{Q}, \boldsymbol{H})\rangle = \left\langle \nabla \boldsymbol{u}, \boldsymbol{Q}\boldsymbol{H} - \boldsymbol{H}\boldsymbol{Q} - \xi(\boldsymbol{H}\boldsymbol{Q} + \boldsymbol{Q}\boldsymbol{H}) - \frac{2\xi}{d}\boldsymbol{H} + 2\xi(\boldsymbol{Q} : \boldsymbol{H})\boldsymbol{Q}\right\rangle.$$

Comparing these terms and utilizing the symmetry and trace-free property of $\boldsymbol{H}$ and $\boldsymbol{Q}$, we observe that

$$\begin{aligned}
\langle \boldsymbol{H}, \boldsymbol{W}\boldsymbol{Q} - \boldsymbol{Q}\boldsymbol{W}\rangle &= \int_\Omega \sum_{i,j,k=1}^d H_{ij}(W_{ik}Q_{kj} - Q_{ik}W_{kj}) \\
&= \int_\Omega \sum_{i,j,k=1}^d (W_{ik}H_{ij}Q_{jk} - W_{kj}Q_{ki}H_{ij}) = \langle \boldsymbol{W}, \boldsymbol{H}\boldsymbol{Q} - \boldsymbol{Q}\boldsymbol{H}\rangle = -\langle \nabla \boldsymbol{u}, \boldsymbol{Q}\boldsymbol{H} - \boldsymbol{H}\boldsymbol{Q}\rangle, \\
\langle \boldsymbol{H}, \xi(\boldsymbol{Q}\boldsymbol{D} + \boldsymbol{D}\boldsymbol{Q})\rangle &= \int_\Omega \sum_{i,j,k=1}^d \xi H_{ij}(Q_{ik}D_{kj} + D_{ik}Q_{kj}) = \int_\Omega \sum_{i,j,k=1}^d \xi(D_{ik}H_{ij}Q_{jk} + D_{kj}Q_{ki}H_{ij}) \\
&= \langle \boldsymbol{D}, \xi(\boldsymbol{H}\boldsymbol{Q} + \boldsymbol{Q}\boldsymbol{H})\rangle = \xi\langle \nabla \boldsymbol{u}, \boldsymbol{H}\boldsymbol{Q} + \boldsymbol{Q}\boldsymbol{H}\rangle, \\
\left\langle \boldsymbol{H}, \frac{2\xi}{d}\boldsymbol{D}\right\rangle &= \left\langle \nabla \boldsymbol{u}, \frac{2\xi}{d}\boldsymbol{H}\right\rangle, \quad \langle \boldsymbol{H}, -2\xi(\boldsymbol{D} : \boldsymbol{Q})\boldsymbol{Q}\rangle = -2\xi \int_\Omega (\nabla \boldsymbol{u} : \boldsymbol{Q})(\boldsymbol{H} : \boldsymbol{Q})\,\mathrm{d}x = -\langle \nabla \boldsymbol{u}, 2\xi(\boldsymbol{Q} : \boldsymbol{H})\boldsymbol{Q}\rangle, \\
\left\langle \boldsymbol{H}, \frac{2\xi}{d}(\boldsymbol{D} : \boldsymbol{Q})\boldsymbol{I}\right\rangle &= \frac{2\xi}{d}\int_\Omega (\boldsymbol{D} : \boldsymbol{Q})\operatorname{tr}(\boldsymbol{H})\,\mathrm{d}x = 0.
\end{aligned}$$

From these calculations, we can conclude that (2.8) holds true. □

We also recall the following lemma from Theorem 4.11 of [20], establishing Lipschitz continuity of P. We will use this lemma to pass to the limit in the numerical approximations introduced below and obtain convergence to a weak solution as in Definition 2.5.

Lemma 2.9. *The function* P *is Lipschitz continuous, that is, there exists constant* $\tilde{L} > 0$ *such that for any matrix* $\boldsymbol{Q}, \delta\boldsymbol{Q} \in \mathbb{R}^{3\times 3}$,

$$|P(\boldsymbol{Q} + \delta\boldsymbol{Q}) - P(\boldsymbol{Q})| \le \tilde{L}\,|\delta\boldsymbol{Q}|. \tag{2.9}$$

3. Construction and analysis of the numerical scheme

We start by describing the first-order semi-discrete numerical scheme for system (1.10a)–(1.10e). It is based on the projection method, a fractional step method widely used for the numerical approximation of the Navier–Stokes equations [11, 34, 38]. It consists of two steps. Let $\Delta t > 0$ be the time step size.

Given initial data $(\boldsymbol{u}^0, \boldsymbol{Q}^0, p^0) \in H_0^1(\Omega) \times \left(H_0^1(\Omega) \cap H^2(\Omega)\right) \times H^2(\Omega)$, we set $\boldsymbol{P}^0 = P(\boldsymbol{Q}^0), r^0 = r(\boldsymbol{Q}^0)$ and $(\boldsymbol{u}^{-1}, \boldsymbol{Q}^{-1}, p^{-1}, r^{-1}) = (\boldsymbol{u}^0, \boldsymbol{Q}^0, p^0, r^0)$. Then for $n = 0, 1, \ldots$, we update $(\boldsymbol{u}^{n+1}, \boldsymbol{Q}^{n+1}, p^{n+1}, \boldsymbol{H}^{n+1}, r^{n+1})$ through the following two steps.

Step 1. Given $(\boldsymbol{u}^n, \boldsymbol{Q}^n, p^n, r^n) \in H_0^1(\Omega) \times \big(H_0^1(\Omega)\cap H^2(\Omega)\big) \times H^2(\Omega) \times L^2(\Omega)$, we seek $(\tilde{\boldsymbol{u}}^{n+1}, \boldsymbol{Q}^{n+1}, \boldsymbol{H}^{n+1}, r^{n+1}) \in H_0^1(\Omega) \times \big(H_0^1(\Omega)\cap H^2(\Omega)\big) \times L^2(\Omega) \times L^2(\Omega)$ as a weak solution of the following system with boundary conditions $\tilde{\boldsymbol{u}}^{n+1}|_{\partial\Omega} = 0$, $\boldsymbol{Q}^{n+1}|_{\partial\Omega} = 0$,

$$\left\langle \frac{\tilde{\boldsymbol{u}}^{n+1} - \boldsymbol{u}^n}{\Delta t}, \boldsymbol{\psi} \right\rangle + \tilde{B}\big(\boldsymbol{u}^n, \tilde{\boldsymbol{u}}^{n+1}, \boldsymbol{\psi}\big) = -\langle \nabla p^n, \boldsymbol{\psi}\rangle - \mu\big\langle \nabla \tilde{\boldsymbol{u}}^{n+1}, \nabla\boldsymbol{\psi}\big\rangle - \big\langle \boldsymbol{\Sigma}^{n+1}, \nabla\boldsymbol{\psi}\big\rangle, \tag{3.1a}$$
$$- \big\langle \boldsymbol{H}^{n+1}\nabla\boldsymbol{Q}^n, \boldsymbol{\psi}\big\rangle$$

$$\left\langle \frac{\boldsymbol{Q}^{n+1} - \boldsymbol{Q}^n}{\Delta t}, \boldsymbol{\varphi} \right\rangle + \big\langle \tilde{\boldsymbol{u}}^{n+1}\cdot\nabla\boldsymbol{Q}^n, \boldsymbol{\varphi}\big\rangle = \big\langle \boldsymbol{s}^{n+1}, \boldsymbol{\varphi}\big\rangle + M\big\langle \boldsymbol{H}^{n+1}, \boldsymbol{\varphi}\big\rangle, \tag{3.1b}$$

$$\big\langle r^{n+1} - r^n, \eta\big\rangle = \big\langle \boldsymbol{P}^n : \big(\boldsymbol{Q}^{n+1} - \boldsymbol{Q}^n\big), \eta\big\rangle, \tag{3.1c}$$

$$\big\langle \boldsymbol{H}^{n+1}, \boldsymbol{\phi}\big\rangle = -L\big\langle \nabla\boldsymbol{Q}^{n+1}, \nabla\boldsymbol{\phi}\big\rangle - \big\langle r^{n+1}\boldsymbol{P}^n, \boldsymbol{\phi}\big\rangle \tag{3.1d}$$

for all smooth vector-valued function $\boldsymbol{\psi}$, smooth scalar function η and smooth matrix-valued function $\boldsymbol{\varphi}, \boldsymbol{\phi}$ with compact support in $[0, T) \times \Omega$. Here

$$\boldsymbol{s}^{n+1} = s(\tilde{\boldsymbol{u}}^{n+1}, \boldsymbol{Q}^n), \qquad \boldsymbol{\Sigma}^{n+1} = \Sigma(\boldsymbol{Q}^n, \boldsymbol{H}^{n+1}), \qquad \boldsymbol{P}^n = P(\boldsymbol{Q}^n) \qquad \text{for all } n \geq 0. \tag{3.2}$$

Step 2. Then we project $\tilde{\boldsymbol{u}}^{n+1}$ onto a divergence free function $\boldsymbol{u}^{n+1}$ using the following procedure: We define $(\boldsymbol{u}^{n+1}, p^{n+1}) \in H^1(\Omega) \times H^2(\Omega)$ through the following equations with boundary condition $\boldsymbol{u}^{n+1}\cdot\boldsymbol{n}|_{\partial\Omega} = 0$ and $\frac{\partial p^{n+1}}{\partial n} = 0$,

$$\left\langle \frac{\boldsymbol{u}^{n+1} - \tilde{\boldsymbol{u}}^{n+1}}{\Delta t}, \boldsymbol{v} \right\rangle = 2\big\langle p^{n+1} - p^n, \nabla\cdot\boldsymbol{v}\big\rangle, \tag{3.3a}$$

$$\big\langle \nabla p^{n+1}, \nabla\zeta\big\rangle = \frac{1}{2\Delta t}\big\langle \tilde{\boldsymbol{u}}^{n+1}, \nabla\zeta\big\rangle + \langle \nabla p^n, \nabla\zeta\rangle, \tag{3.3b}$$

for all vector-valued $\boldsymbol{v} \in L^2(\Omega)$ with square integrable divergence and scalar function $\zeta \in H^1(\Omega)$.

Remark 3.1. The second step can be understood as applying the Helmholtz decomposition to $\tilde{\boldsymbol{u}}^{n+1}$, in particular, $\boldsymbol{u}^{n+1} = \mathcal{P}\tilde{\boldsymbol{u}}^{n+1}$. In particular, using $\nabla\eta$ for any $\eta \in H^1(\Omega)$ as a test function in (3.3a), we obtain

$$\big\langle \boldsymbol{u}^{n+1}, \nabla\eta\big\rangle = 0. \tag{3.4}$$

Here $s = s(\boldsymbol{u}, \boldsymbol{Q})$ is given by

$$s(\boldsymbol{u}, \boldsymbol{Q}) := S(\boldsymbol{u}, \boldsymbol{Q}) - \frac{2\xi}{d^2}(\nabla\cdot\boldsymbol{u})\,\boldsymbol{I}. \tag{3.5}$$

Clearly, if $\boldsymbol{u}$ is divergence free, this definition coincides with the definition of S in (1.3). However, the velocity field $\tilde{\boldsymbol{u}}^{n+1}$ obtained in the first step of the scheme is not necessarily divergence free and hence S may not be trace-free, a fact which is needed to show that the scheme conserves the trace-free properties of $\boldsymbol{Q}$ and $\boldsymbol{H}$, as we will see later. From the proof of Lemma 2.8, we notice that the trace-free property of $\boldsymbol{H}$ is in fact necessary for obtaining the cancellation property (2.8), which in turn is needed for showing the discrete energy balance.

Then the following version of Lemma 2.8 holds:

Lemma 3.2. *For any* $\boldsymbol{u} \in H_0^1(\Omega)$*, we have*

$$\langle \nabla\boldsymbol{u}, \Sigma(\boldsymbol{Q}, \boldsymbol{H})\rangle + \langle \boldsymbol{H}, s(\boldsymbol{u}, \boldsymbol{Q})\rangle = 0, \tag{3.6}$$

for every symmetric trace-free matrix $\boldsymbol{Q} \in H_0^1(\Omega) \cap H^2(\Omega)$*,* $\boldsymbol{H} \in L^2(\Omega)$*.*

Proof. The proof is the same as the proof of Lemma 2.8 after noting that $\frac{2\xi}{d^2}(\nabla\cdot\boldsymbol{u})\operatorname{tr}\boldsymbol{H} = 0$. □

3.1. Well-posedness of the scheme

First, we need to guarantee a solution of (3.1)–(3.3) with the required properties exists at every step n. We start by noting that the scheme preserves the trace-free and symmetry property of $\boldsymbol{Q}$ and $\boldsymbol{H}$, *i.e.*, if $\boldsymbol{Q}^n$ is trace-free and symmetric, then $\boldsymbol{Q}^{n+1}$ and $\boldsymbol{H}^{n+1}$ will be also. Since the second step of the scheme does not modify $\boldsymbol{Q}$ and $\boldsymbol{H}$, we only need to consider the first step:

Lemma 3.3. *If $\boldsymbol{Q}^n$ is trace-free and symmetric, then $\boldsymbol{Q}^{n+1}$ and $\boldsymbol{H}^{n+1}$ computed through (3.1) are also trace-free and symmetric almost everywhere.*

Proof. We use $\operatorname{tr}(\boldsymbol{Q}^{n+1})\mathbf{I}$ (where $\mathbf{I}$ is the $d\times d$ identity matrix) as a test function in (3.1b):

$$\left\langle \frac{\boldsymbol{Q}^{n+1}-\boldsymbol{Q}^n}{\Delta t}, \operatorname{tr}(\boldsymbol{Q}^{n+1})\mathbf{I}\right\rangle + \left\langle \tilde{\boldsymbol{u}}^{n+1}\cdot\nabla\boldsymbol{Q}^n, \operatorname{tr}(\boldsymbol{Q}^{n+1})\mathbf{I}\right\rangle - \left\langle \boldsymbol{s}^{n+1}, \operatorname{tr}(\boldsymbol{Q}^{n+1})\mathbf{I}\right\rangle = M\left\langle \boldsymbol{H}^{n+1}, \operatorname{tr}(\boldsymbol{Q}^{n+1})\mathbf{I}\right\rangle$$

which can be rewritten as

$$\begin{aligned}\left\langle \frac{\operatorname{tr}(\boldsymbol{Q}^{n+1})-\operatorname{tr}(\boldsymbol{Q}^n)}{\Delta t}, \operatorname{tr}(\boldsymbol{Q}^{n+1})\right\rangle + \left\langle \tilde{\boldsymbol{u}}^{n+1}\cdot\nabla\operatorname{tr}(\boldsymbol{Q}^n), \operatorname{tr}(\boldsymbol{Q}^{n+1})\right\rangle - \left\langle \operatorname{tr}(\boldsymbol{s}^{n+1}), \operatorname{tr}(\boldsymbol{Q}^{n+1})\right\rangle \\ = M\left\langle \operatorname{tr}(\boldsymbol{H}^{n+1}), \operatorname{tr}(\boldsymbol{Q}^{n+1})\right\rangle.\end{aligned}$$

By assumption, $\boldsymbol{Q}^n$ is trace-free, hence this becomes

$$\frac{1}{\Delta t}\left\|\operatorname{tr}(\boldsymbol{Q}^{n+1})\right\|^2 - \left\langle \operatorname{tr}(\boldsymbol{s}^{n+1}), \operatorname{tr}(\boldsymbol{Q}^{n+1})\right\rangle = M\left\langle \operatorname{tr}(\boldsymbol{H}^{n+1}), \operatorname{tr}(\boldsymbol{Q}^{n+1})\right\rangle. \tag{3.7}$$

From the definition of $\boldsymbol{s}^{n+1}$ in (3.5) and (3.2), it follows that

$$\begin{aligned}\left\langle \operatorname{tr}(\boldsymbol{s}^{n+1}), \phi\right\rangle &= \left\langle \operatorname{tr}\left(S(\tilde{\boldsymbol{u}}^{n+1}, \boldsymbol{Q}^n)\right), \phi\right\rangle - \left\langle \frac{2\xi}{d^2}(\nabla\cdot\tilde{\boldsymbol{u}}^{n+1})\operatorname{tr}(\boldsymbol{I}), \phi\right\rangle \\ &= \left\langle \operatorname{tr}\left(\tilde{\boldsymbol{W}}^{n+1}\boldsymbol{Q}^n - \boldsymbol{Q}^n\tilde{\boldsymbol{W}}^{n+1}\right) + \xi\operatorname{tr}\left(\boldsymbol{Q}^n\tilde{\boldsymbol{D}}^{n+1} + \tilde{\boldsymbol{D}}^{n+1}\boldsymbol{Q}^n\right) + \frac{2\xi}{d}\operatorname{tr}\left(\tilde{\boldsymbol{D}}^{n+1}\right)\right. \\ &\quad \left. - 2\xi\left(\tilde{\boldsymbol{D}}^{n+1} : \boldsymbol{Q}^n\right)\operatorname{tr}(\boldsymbol{Q}^n) - \frac{2\xi}{d}\left(\tilde{\boldsymbol{D}}^{n+1} : \boldsymbol{Q}^n\right)\operatorname{tr}(\boldsymbol{I}) - \frac{2\xi}{d}(\nabla\cdot\tilde{\boldsymbol{u}}^{n+1}), \phi\right\rangle = 0\end{aligned} \tag{3.8}$$

for any test function $\phi:\Omega\to\mathbb{R}$ with zero trace and contained in $H^2(\Omega)$. In order to deal with the last term, we take $\operatorname{tr}(\boldsymbol{Q}^{n+1})\mathbf{I}$ as a test function in (3.1d):

$$\left\langle \boldsymbol{H}^{n+1}, \operatorname{tr}(\boldsymbol{Q}^{n+1})\mathbf{I}\right\rangle = -L\left\langle \nabla\boldsymbol{Q}^{n+1}, \nabla\left(\operatorname{tr}(\boldsymbol{Q}^{n+1})\mathbf{I}\right)\right\rangle - \left\langle r^{n+1}\boldsymbol{P}^n, \operatorname{tr}(\boldsymbol{Q}^{n+1})\mathbf{I}\right\rangle,$$

which again, we can write as

$$\left\langle \operatorname{tr}\left(\boldsymbol{H}^{n+1}\right), \operatorname{tr}\left(\boldsymbol{Q}^{n+1}\right)\right\rangle = -L\left\|\nabla\operatorname{tr}\left(\boldsymbol{Q}^{n+1}\right)\right\|^2 - \left\langle r^{n+1}\operatorname{tr}(\boldsymbol{P}^n), \operatorname{tr}\left(\boldsymbol{Q}^{n+1}\right)\right\rangle.$$

From equation (1.9), where due to $\boldsymbol{P}^n = P(\boldsymbol{Q}^n)$ and the condition $\operatorname{tr}(\boldsymbol{Q}^n) = 0$, it follows that $\operatorname{tr}(\boldsymbol{P}^n) = 0$. Therefore the last equation simplifies to

$$\left\langle \operatorname{tr}\left(\boldsymbol{H}^{n+1}\right), \operatorname{tr}\left(\boldsymbol{Q}^{n+1}\right)\right\rangle = -L\left\|\nabla\operatorname{tr}\left(\boldsymbol{Q}^{n+1}\right)\right\|^2.$$

Plugging this into (3.7), we obtain

$$\frac{1}{\Delta t}\left\|\operatorname{tr}\left(\boldsymbol{Q}^{n+1}\right)\right\|^2 - \left\langle \operatorname{tr}\left(\boldsymbol{s}^{n+1}\right), \operatorname{tr}\left(\boldsymbol{Q}^{n+1}\right)\right\rangle = -ML\left\|\nabla\operatorname{tr}\left(\boldsymbol{Q}^{n+1}\right)\right\|^2 \le 0$$

and so $\operatorname{tr}(\boldsymbol{Q}^{n+1}) = 0$ almost everywhere.

For the symmetry, we consider $\boldsymbol{Z}^{n+1} = \boldsymbol{Q}^{n+1} - (\boldsymbol{Q}^{n+1})^\top$ as a test function in (3.1b):

$$\left\langle \frac{\boldsymbol{Q}^{n+1} - \boldsymbol{Q}^n}{\Delta t}, \boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top \right\rangle + \left\langle \tilde{\boldsymbol{u}}^{n+1} \cdot \nabla \boldsymbol{Q}^n, \boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top \right\rangle - \left\langle \boldsymbol{s}^{n+1}, \boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top \right\rangle$$
$$= M\left\langle \boldsymbol{H}^{n+1}, \boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top \right\rangle$$

which can be rewritten as

$$\frac{1}{2}\left\langle \frac{\boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top - \left(\boldsymbol{Q}^n - (\boldsymbol{Q}^n)^\top\right)}{\Delta t}, \boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top \right\rangle + \frac{1}{2}\left\langle \tilde{\boldsymbol{u}}^{n+1} \cdot \nabla\big(\boldsymbol{Q}^n - (\boldsymbol{Q}^n)^\top\big), \boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top \right\rangle$$
$$- \frac{1}{2}\left\langle \boldsymbol{s}^{n+1} - \left(\boldsymbol{s}^{n+1}\right)^\top, \boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top \right\rangle = \frac{M}{2}\left\langle \boldsymbol{H}^{n+1} - \left(\boldsymbol{H}^{n+1}\right)^\top, \boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top \right\rangle.$$

Since $\boldsymbol{Q}^n$ is assumed to be symmetric, a simple calculation reveals that $\boldsymbol{s}^{n+1}$ is also symmetric and so the previous identity simplifies to

$$\frac{1}{2\Delta t}\left\| \boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top \right\|^2 = \frac{M}{2}\left\langle \boldsymbol{H}^{n+1} - \left(\boldsymbol{H}^{n+1}\right)^\top, \boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top \right\rangle. \tag{3.9}$$

We use $\boldsymbol{Z}^{n+1}$ as a test function in the equation for $\boldsymbol{H}^{n+1}$, equation (3.1d):

$$\left\langle \boldsymbol{H}^{n+1}, \boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top \right\rangle = -L\left\langle \nabla \boldsymbol{Q}^{n+1}, \nabla\left(\boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top\right) \right\rangle - \left\langle r^{n+1}\boldsymbol{P}^n, \boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top \right\rangle,$$

which we can rewrite as

$$\frac{1}{2}\left\langle \boldsymbol{H}^{n+1} - \left(\boldsymbol{H}^{n+1}\right)^\top, \boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top \right\rangle = -\frac{L}{2}\left\| \nabla\left(\boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top\right) \right\|^2$$
$$- \frac{1}{2}\left\langle r^{n+1}\left(\boldsymbol{P}^n - (\boldsymbol{P}^n)^\top\right), \boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top \right\rangle,$$

which noticing that $\boldsymbol{P}^n$ is symmetric since $\boldsymbol{Q}^n$ is, becomes

$$\frac{1}{2}\left\langle \boldsymbol{H}^{n+1} - \left(\boldsymbol{H}^{n+1}\right)^\top, \boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top \right\rangle = -\frac{L}{2}\left\| \nabla\left(\boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top\right) \right\|^2.$$

Thus (3.9) becomes

$$\frac{1}{2\Delta t}\left\| \boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top \right\|^2 = -\frac{LM}{2}\left\| \nabla\left(\boldsymbol{Q}^{n+1} - \left(\boldsymbol{Q}^{n+1}\right)^\top\right) \right\|^2 \leq 0.$$

This implies that $\boldsymbol{Q}^{n+1}$ is symmetric almost everywhere. □

Next, we turn to the solvability of our numerical scheme, that is, given $(\boldsymbol{u}^n, \boldsymbol{Q}^n, p^n, \boldsymbol{H}^n, r^n) \in H^1(\Omega) \times \left(H^2(\Omega) \cap H_0^1(\Omega)\right) \times H^2(\Omega) \times L^2(\Omega) \times L^2(\Omega)$, whether there exists $(\boldsymbol{u}^{n+1}, \boldsymbol{Q}^{n+1}, p^{n+1}, \boldsymbol{H}^{n+1}, r^{n+1}) \in H^1(\Omega) \times \left(H^2(\Omega) \cap H_0^1(\Omega)\right) \times H^2(\Omega) \times L^2(\Omega) \times L^2(\Omega)$ solving equations (3.1)–(3.3). To see this, we will rewrite the scheme into a more straightforward form to implement and analyze. From (3.1c), we can express r^{n+1} in terms of $\boldsymbol{Q}^n$, $\boldsymbol{Q}^{n+1}$ and r^n as

$$r^{n+1} = r^n + \boldsymbol{P}^n : \left(\boldsymbol{Q}^{n+1} - \boldsymbol{Q}^n\right),$$

interpreted in the distributional sense. Substituting r^{n+1} into the formula for $\boldsymbol{H}^{n+1}$ in (3.1d), we obtain

$$\langle \boldsymbol{H}^{n+1}, \boldsymbol{\phi} \rangle = -L\langle \nabla \boldsymbol{Q}^{n+1}, \nabla \boldsymbol{\phi} \rangle - \langle (\boldsymbol{P}^n : \boldsymbol{Q}^{n+1})\boldsymbol{P}^n, \boldsymbol{\phi} \rangle + \langle \boldsymbol{F}^n, \boldsymbol{\phi} \rangle \tag{3.10}$$

where we denoted $\boldsymbol{F}^n := (\boldsymbol{P}^n : \boldsymbol{Q}^n)\boldsymbol{P}^n - r^n\boldsymbol{P}^n$. This leads to the following problem: Given $(\boldsymbol{u}^n, \boldsymbol{Q}^n, p^n, \boldsymbol{H}^n, r^n) \in H^1(\Omega) \times \big(H^2(\Omega) \cap H_0^1(\Omega)\big) \times H^2(\Omega) \times L^2(\Omega) \times L^2(\Omega)$, find a unique $\big(\boldsymbol{u}, \boldsymbol{Q}, \boldsymbol{H}\big) \in H_0^1(\Omega) \times H_0^1(\Omega) \times L^2(\Omega)$ such that

$$a_{n+1}\big(\big(\boldsymbol{u}, \boldsymbol{Q}, \boldsymbol{H}\big), \big(\boldsymbol{\psi}, \boldsymbol{\varphi}, \boldsymbol{\phi}\big)\big) = f_n\big(\big(\boldsymbol{\psi}, \boldsymbol{\varphi}, \boldsymbol{\phi}\big)\big) \tag{3.11}$$

holds for all $\big(\boldsymbol{\psi}, \boldsymbol{\varphi}, \boldsymbol{\phi}\big) \in H_0^1(\Omega) \times H_0^1(\Omega) \times L^2(\Omega)$. Here the bilinear form $a_{n+1}(\cdot,\cdot) : \big(H_0^1(\Omega) \times H_0^1(\Omega) \times L^2(\Omega)\big) \times \big(H_0^1(\Omega) \times H_0^1(\Omega) \times L^2(\Omega)\big) \to \mathbb{R}$ is defined as:

$$\begin{aligned}
&a_{n+1}\big(\big(\boldsymbol{u}, \boldsymbol{Q}, \boldsymbol{H}\big), \big(\boldsymbol{\psi}, \boldsymbol{\varphi}, \boldsymbol{\phi}\big)\big)\\
&\quad= \frac{1}{\Delta t}\int_\Omega \boldsymbol{u}\cdot\boldsymbol{\psi}\,\mathrm{d}x + \tilde{B}(\boldsymbol{u}^n, \boldsymbol{u}, \boldsymbol{\psi}) + \mu\int_\Omega \nabla\boldsymbol{u}\cdot\nabla\boldsymbol{\psi}\,\mathrm{d}x + \int_\Omega \Sigma(\boldsymbol{Q}^n, \boldsymbol{H}) : \nabla\boldsymbol{\psi}\,\mathrm{d}x + \int_\Omega \boldsymbol{H}\nabla\boldsymbol{Q}^n\cdot\boldsymbol{\psi}\,\mathrm{d}x\\
&\qquad - \frac{1}{\Delta t}\int_\Omega \boldsymbol{Q} : \boldsymbol{\phi}\,\mathrm{d}x - \int_\Omega (\boldsymbol{u}\cdot\nabla\boldsymbol{Q}^n) : \boldsymbol{\phi}\,\mathrm{d}x + \int_\Omega s(\boldsymbol{u}, \boldsymbol{Q}^n) : \boldsymbol{\phi}\,\mathrm{d}x + M\int_\Omega \boldsymbol{H} : \boldsymbol{\phi}\,\mathrm{d}x\\
&\qquad + \frac{1}{\Delta t}\int_\Omega \boldsymbol{H} : \boldsymbol{\varphi}\,\mathrm{d}x + \frac{L}{\Delta t}\int_\Omega \nabla\boldsymbol{Q} : \nabla\boldsymbol{\varphi}\,\mathrm{d}x + \frac{1}{\Delta t}\int_\Omega (\boldsymbol{P}^n : \boldsymbol{Q})(\boldsymbol{P}^n : \boldsymbol{\varphi})\,\mathrm{d}x := \sum_{k=1}^{12} A_k^{n+1},
\end{aligned} \tag{3.12a}$$

and the right-hand side is

$$f_n\big(\big(\boldsymbol{\psi}, \boldsymbol{\varphi}, \boldsymbol{\phi}\big)\big) = \frac{1}{\Delta t}\langle \boldsymbol{u}^n, \boldsymbol{\psi}\rangle - \langle \nabla p^n, \boldsymbol{\psi}\rangle + \frac{1}{\Delta t}\langle \boldsymbol{Q}^n, \boldsymbol{\phi}\rangle + \frac{1}{\Delta t}\langle \boldsymbol{F}^n, \boldsymbol{\varphi}\rangle. \tag{3.12b}$$

By the Lax–Milgram theorem [17], we infer that it is enough to show that a_{n+1} is bounded and coercive. We will start with the boundedness. Given $(\boldsymbol{u}^n, \boldsymbol{Q}^n, \boldsymbol{H}^n) \in H_0^1(\Omega) \times \big(H_0^1(\Omega) \cap H^2(\Omega)\big) \times L^2(\Omega)$ and a fixed Δt, the terms $A_1^{n+1}, A_3^{n+1}, A_6^{n+1}, A_9^{n+1}, A_{10}^{n+1}, A_{11}^{n+1}$ can be bounded by Cauchy–Schwarz inequality as

$$\begin{aligned}
\big|A_1^{n+1}\big| &\le \frac{1}{\Delta t}\|\boldsymbol{u}\|\,\|\boldsymbol{\psi}\| \le \frac{1}{\Delta t}\|\boldsymbol{u}\|_{H_0^1}\,\|\boldsymbol{\psi}\|_{H_0^1},\\
\big|A_3^{n+1}\big| &\le \mu\|\nabla\boldsymbol{u}\|\,\|\nabla\boldsymbol{\psi}\| \le \mu\|\boldsymbol{u}\|_{H_0^1}\,\|\boldsymbol{\psi}\|_{H_0^1},\\
\big|A_6^{n+1}\big| &\le \frac{1}{\Delta t}\|\boldsymbol{Q}\|\,\|\boldsymbol{\phi}\| \le \frac{1}{\Delta t}\|\boldsymbol{Q}\|_{H_0^1}\,\|\boldsymbol{\phi}\|,\\
\big|A_9^{n+1}\big| &\le M\|\boldsymbol{H}\|\,\|\boldsymbol{\phi}\|,\\
\big|A_{10}^{n+1}\big| &\le \frac{1}{\Delta t}\|\boldsymbol{H}\|\,\|\boldsymbol{\varphi}\| \le \frac{1}{\Delta t}\|\boldsymbol{H}\|\,\|\boldsymbol{\varphi}\|_{H_0^1},\\
\big|A_{11}^{n+1}\big| &\le \frac{L}{\Delta t}\|\nabla\boldsymbol{Q}\|\,\|\nabla\boldsymbol{\varphi}\| \le \frac{L}{\Delta t}\|\boldsymbol{Q}\|_{H_0^1}\,\|\boldsymbol{\varphi}\|_{H_0^1}.
\end{aligned}$$

Using the Hölder inequality and the Sobolev inequality, we can estimate A_2^{n+1} as

$$\big|A_2^{n+1}\big| \le \|\boldsymbol{u}^n\|_{L^4}\,\|\nabla\boldsymbol{u}\|\,\|\boldsymbol{\psi}\|_{L^4} \le C\|\boldsymbol{u}^n\|_{H_0^1}\,\|\boldsymbol{u}\|_{H_0^1}\,\|\boldsymbol{\psi}\|_{H_0^1} \le C\|\boldsymbol{u}\|_{H_0^1}\,\|\boldsymbol{\psi}\|_{H_0^1}.$$

Similar tricks can be applied to control A_5^k and A_7^k. Specifically, we have

$$\big|A_5^{n+1}\big| \le \|\boldsymbol{H}\|\,\|\nabla\boldsymbol{Q}^n\|_{L^4}\,\|\boldsymbol{\psi}\|_{L^4} \le C\|\boldsymbol{H}\|\,\|\boldsymbol{Q}^n\|_{H^2}\,\|\boldsymbol{\psi}\|_{H_0^1} \le C\|\boldsymbol{H}\|\,\|\boldsymbol{\psi}\|_{H_0^1},$$

and

$$\big|A_7^{n+1}\big| \le \|\boldsymbol{u}\|_{L^4}\,\|\nabla\boldsymbol{Q}^n\|_{L^4}\,\|\boldsymbol{\phi}\| \le C\|\boldsymbol{u}\|_{H_0^1}\,\|\boldsymbol{Q}^n\|_{H^2}\,\|\boldsymbol{\phi}\| \le C\|\boldsymbol{u}\|_{H_0^1}\,\|\boldsymbol{\phi}\|.$$

Thanks to Lemmas 2.1 and 2.9, we obtain

$$\begin{aligned}
\big|A_{12}^{n+1}\big| \le \frac{1}{\Delta t}\|\boldsymbol{P}^n\|_{L^\infty}^2\,\|\boldsymbol{Q}\|\,\|\boldsymbol{\varphi}\| &\le \frac{\tilde{L}^2}{\Delta t}\|\boldsymbol{Q}^n\|_{L^\infty}^2\,\|\boldsymbol{Q}\|_{H_0^1}\,\|\boldsymbol{\varphi}\|_{H_0^1}\\
&\le C\|\boldsymbol{Q}^n\|_{H_0^1}\,\|\boldsymbol{Q}^n\|_{H^2}\,\|\boldsymbol{Q}\|_{H_0^1}\,\|\boldsymbol{\varphi}\|_{H_0^1} \le C\|\boldsymbol{Q}\|_{H_0^1}\,\|\boldsymbol{\varphi}\|_{H_0^1}.
\end{aligned}$$

Recalling definition (1.3), (3.5) and (1.7) and using Lemma 2.1, we can estimate the remaining two terms A_4^{n+1}, A_8^{n+1} as

$$\begin{aligned}\left|A_4^{n+1}\right| &= \left|\int_\Omega \left[\boldsymbol{Q}^n\boldsymbol{H} - \boldsymbol{H}\boldsymbol{Q}^n - \xi(\boldsymbol{H}\boldsymbol{Q}^n + \boldsymbol{Q}^n\boldsymbol{H}) - \frac{2\xi}{d}\boldsymbol{H} + 2\xi(\boldsymbol{Q}^n : \boldsymbol{H})\boldsymbol{Q}^n\right] : \nabla\boldsymbol{\psi}\,\mathrm{d}x\right| \\ &\le C\left(\|\boldsymbol{Q}^n\|_{L^\infty} + \|\boldsymbol{Q}^n\|_{L^\infty}^2 + 1\right)\|\boldsymbol{H}\|\,\|\nabla\boldsymbol{\psi}\| \le C\|\boldsymbol{H}\|\,\|\boldsymbol{\psi}\|_{H_0^1},\end{aligned}$$

and

$$\begin{aligned}\left|A_8^{n+1}\right| &= \left|\int_\Omega \left[\boldsymbol{W}\boldsymbol{Q}^n - \boldsymbol{Q}^n\boldsymbol{W} + \xi(\boldsymbol{Q}^n\boldsymbol{D} + \boldsymbol{D}\boldsymbol{Q}^n) + \frac{2\xi}{d}\boldsymbol{D} - 2\xi(\boldsymbol{D}:\boldsymbol{Q}^n)\left(\boldsymbol{Q}^n + \frac{1}{d}\boldsymbol{I}\right) - \frac{2\xi}{d^2}(\nabla\cdot\boldsymbol{u})\,\boldsymbol{I}\right] : \boldsymbol{\phi}\,\mathrm{d}x\right| \\ &\le C\left(\|\boldsymbol{Q}^n\|_{L^\infty} + \|\boldsymbol{Q}^n\|_{L^\infty}^2 + 1\right)\|\nabla\boldsymbol{u}\|\,\|\boldsymbol{\phi}\| \le C\|\boldsymbol{u}\|_{H_0^1}\|\boldsymbol{\phi}\|.\end{aligned}$$

Combining these estimates on $A_i, i = 1, 2, \cdots, 12$, we conclude that

$$\begin{aligned}\left|a_{n+1}\big((\boldsymbol{u},\boldsymbol{Q},\boldsymbol{H}),(\boldsymbol{\psi},\boldsymbol{\varphi},\boldsymbol{\phi})\big)\right| &\le C\Big(\|\boldsymbol{u}\|_{H_0^1} + \|\boldsymbol{Q}\|_{H_0^1} + \|\boldsymbol{H}\|\Big)\Big(\|\boldsymbol{\psi}\|_{H_0^1} + \|\boldsymbol{\varphi}\|_{H_0^1} + \|\boldsymbol{\phi}\|\Big) \\ &\le C\left\|\big(\boldsymbol{u},\boldsymbol{Q},\boldsymbol{H}\big)\right\|_{H_0^1(\Omega)\times H_0^1(\Omega)\times L^2(\Omega)}\left\|\big(\boldsymbol{\psi},\boldsymbol{\varphi},\boldsymbol{\phi}\big)\right\|_{H_0^1(\Omega)\times H_0^1(\Omega)\times L^2(\Omega)},\end{aligned} \tag{3.13}$$

which completes the proof of the boundedness of the bilinear form a_{n+1}.

Next we show the coercivity of a_{n+1}. To do so, we choose $\big(\boldsymbol{\psi},\boldsymbol{\varphi},\boldsymbol{\phi}\big) = \big(\boldsymbol{u},\boldsymbol{Q},\boldsymbol{H}\big)$, it follows from Lemmas 2.7, 3.2 that

$$\begin{aligned}&a\big((\boldsymbol{u},\boldsymbol{Q},\boldsymbol{H}),(\boldsymbol{u},\boldsymbol{Q},\boldsymbol{H})\big) \\ &\quad= \frac{1}{\Delta t}\int_\Omega \boldsymbol{u}\cdot\boldsymbol{u}\,\mathrm{d}x + \tilde{B}(\boldsymbol{u}^n,\boldsymbol{u},\boldsymbol{u}) + \mu\int_\Omega \nabla\boldsymbol{u}\cdot\nabla\boldsymbol{u}\,\mathrm{d}x + \int_\Omega \Sigma(\boldsymbol{Q}^n,\boldsymbol{H}) : \nabla\boldsymbol{u}\,\mathrm{d}x + \int_\Omega \boldsymbol{H}\nabla\boldsymbol{Q}^n\cdot\boldsymbol{u}\,\mathrm{d}x \\ &\qquad - \frac{1}{\Delta t}\int_\Omega \boldsymbol{Q}:\boldsymbol{H}\,\mathrm{d}x - \int_\Omega (\boldsymbol{u}\cdot\nabla\boldsymbol{Q}^n):\boldsymbol{H}\,\mathrm{d}x + \int_\Omega s(\boldsymbol{u},\boldsymbol{Q}^n):\boldsymbol{H}\,\mathrm{d}x + M\int_\Omega \boldsymbol{H}:\boldsymbol{H}\,\mathrm{d}x \\ &\qquad + \frac{1}{\Delta t}\int_\Omega \boldsymbol{H}:\boldsymbol{Q}\,\mathrm{d}x + \frac{L}{\Delta t}\int_\Omega \nabla\boldsymbol{Q}:\nabla\boldsymbol{Q}\,\mathrm{d}x + \frac{1}{\Delta t}\int_\Omega (\boldsymbol{P}^n:\boldsymbol{Q})^2\,\mathrm{d}x \\ &\quad= \frac{1}{\Delta t}\|\boldsymbol{u}\|^2 + \mu\|\nabla\boldsymbol{u}\|^2 + M\|\boldsymbol{H}\|^2 + \frac{L}{\Delta t}\|\nabla\boldsymbol{Q}\|^2 + \frac{1}{\Delta t}\|\boldsymbol{P}^n:\boldsymbol{Q}\|^2 \\ &\quad\ge C\Big(\|\boldsymbol{u}\|_{H_0^1}^2 + \|\boldsymbol{Q}\|_{H_0^1}^2 + \|\boldsymbol{H}\|^2\Big),\end{aligned} \tag{3.14}$$

for some constant $C > 0$ which depends on μ, M, and Δt. Thus, given $(\boldsymbol{u}^n,\boldsymbol{Q}^n,\boldsymbol{H}^n,p^n,r^n) \in H_0^1(\Omega)\times\big(H_0^1(\Omega)\cap H^2(\Omega)\big)\times L^2(\Omega)\times L^2(\Omega)\times L^2(\Omega)$, there exists a unique $(\tilde{\boldsymbol{u}}^{n+1},\boldsymbol{Q}^{n+1},\boldsymbol{H}^{n+1}) \in H_0^1(\Omega)\times H_0^1(\Omega)\times L^2(\Omega)$ solving (3.1). Then standard results about elliptic equations [17] lift the regularity of $\boldsymbol{Q}^{n+1}$ to $H^2(\Omega)$ due to (3.10).

As it is stated in Remark 3.1, the uniqueness and existence of $\boldsymbol{u}^{n+1}$ and p^{n+1} are guaranteed by the Helmholtz decomposition. Using (3.3a) and (3.4), for any smooth function $\boldsymbol{\psi}$ with compact support in $[0,T)\times\Omega$, p^{n+1} solves

$$\begin{aligned}\int_\Omega \nabla p^{n+1}\cdot\nabla\boldsymbol{\psi}\,\mathrm{d}x &= \int_\Omega \nabla p^n\cdot\nabla\boldsymbol{\psi}\,\mathrm{d}x - \frac{1}{2\Delta t}\int_\Omega \big(\boldsymbol{u}^{n+1} - \tilde{\boldsymbol{u}}^{n+1}\big)\cdot\nabla\boldsymbol{\psi} \\ &= \int_\Omega \nabla p^n\cdot\nabla\boldsymbol{\psi} - \frac{1}{2\Delta}\int_\Omega \big(\nabla\cdot\tilde{\boldsymbol{u}}^{n+1}\big)\,\boldsymbol{\psi}\,\mathrm{d}x,\end{aligned} \tag{3.15}$$

which implies that $p^{n+1} \in H^2(\Omega)$ given $p^n \in H^2(\Omega)$. In addition, it follows from (3.3a) that $\boldsymbol{u}^{n+1} = \tilde{\boldsymbol{u}}^{n+1} - 2(\nabla p^{n+1} - \nabla p^n)\Delta t \in H^1(\Omega)$. We have shown:

Theorem 3.4. *Given the initial value* $(\boldsymbol{u}^0,\boldsymbol{Q}^0) \in H_0^1(\Omega)\times\big(H_0^1(\Omega)\cap H^2(\Omega)\big)$, *the numerical scheme* (3.1)–(3.3) *can be solved iteratively with* $(\boldsymbol{u}^n,\boldsymbol{Q}^n) \in H^1(\Omega)\times\big(H_0^1(\Omega)\cap H^2(\Omega)\big)$ *for every* $n\in\mathbb{Z}$.

Remark 3.5. Owing to the enhanced regularity obtained, the results established in Lemma 3.3 can be upgraded from holding almost everywhere in Ω to now being valid point-wisely throughout the domain.

3.2. Energy stability

Lemma 3.6. *The numerical scheme* (3.1)–(3.3) *is unconditionally energy stable and satisfies the semi-discrete energy dissipation law*

$$E^{N+1} + \frac{1}{4}\sum_{n=0}^{N-1}\left\|\boldsymbol{u}^{n+1} - \tilde{\boldsymbol{u}}^{n+1}\right\|^2 + \frac{1}{2}\sum_{n=0}^{N}\left\|\tilde{\boldsymbol{u}}^{n+1} - \boldsymbol{u}^n\right\|^2 + \frac{L}{2}\sum_{n=0}^{N}\left\|\nabla\boldsymbol{Q}^{n+1} - \nabla\boldsymbol{Q}^n\right\|^2$$
$$+ \frac{1}{2}\sum_{n=0}^{N}\left\|r^{n+1} - r^n\right\|^2 + \mu\sum_{n=0}^{N}\left\|\nabla\tilde{\boldsymbol{u}}^{n+1}\right\|^2\Delta t + M\sum_{n=0}^{N}\left\|\boldsymbol{H}^{n+1}\right\|^2\Delta t = E^0, \tag{3.16}$$

for all integers $N \in \left[0, \lfloor\frac{T}{\Delta t}\rfloor\right]$ *where*

$$E^{N+1} = \frac{1}{2}\left\|\tilde{\boldsymbol{u}}^{N+1}\right\|^2 + \frac{1}{2}\left\|\boldsymbol{u}^{N+1}\right\|^2 + \frac{L}{2}\left\|\nabla\boldsymbol{Q}^{N+1}\right\|^2 + \frac{1}{2}\left\|r^{N+1}\right\|^2 + \left\|\nabla p^{N+1}\right\|^2\Delta t^2.$$

Proof. According to Theorem 3.4, $\tilde{\boldsymbol{u}}^{n+1} \in H_0^1(\Omega)$ for every $n \geq 0$. It allows us to choose $\boldsymbol{\varphi} = \tilde{\boldsymbol{u}}^{n+1}\Delta t$ as a test function in (3.1a) to get

$$\frac{1}{2}\left(\left\|\tilde{\boldsymbol{u}}^{n+1}\right\|^2 - \|\boldsymbol{u}^n\|^2 + \left\|\tilde{\boldsymbol{u}}^{n+1} - \boldsymbol{u}^n\right\|^2\right) = -\langle\nabla p^n, \tilde{\boldsymbol{u}}^{n+1}\rangle\Delta t - \mu\left\|\nabla\tilde{\boldsymbol{u}}^{n+1}\right\|^2\Delta t - \langle\boldsymbol{\Sigma}^{n+1}, \nabla\tilde{\boldsymbol{u}}^{n+1}\rangle\Delta t$$
$$- \langle\boldsymbol{H}^{n+1}\nabla\boldsymbol{Q}^n, \tilde{\boldsymbol{u}}^{n+1}\rangle\Delta t,$$

where we have used the fact that $\tilde{B}(\boldsymbol{u}^n, \tilde{\boldsymbol{u}}^{n+1}, \tilde{\boldsymbol{u}}^{n+1}) = 0$ by Lemma 2.7. Taking $-\Delta t\boldsymbol{H}^{n+1}$ as a test function in (3.1b) and $\boldsymbol{Q}^{n+1} - \boldsymbol{Q}^n$ in (3.1d), adding the two equations, and using (3.1c), tested by r^{n+1}, we have

$$\frac{L}{2}\left(\left\|\nabla\boldsymbol{Q}^{n+1}\right\|^2 - \|\nabla\boldsymbol{Q}^n\|^2 + \left\|\nabla\boldsymbol{Q}^{n+1} - \nabla\boldsymbol{Q}^n\right\|^2\right) + \frac{1}{2}\left(\left\|\tilde{r}^{n+1}\right\|^2 - \|r^n\|^2 + \left\|\tilde{r}^{n+1} - r^n\right\|^2\right)$$
$$= -M\left\|\boldsymbol{H}^{n+1}\right\|^2\Delta t + \langle\tilde{\boldsymbol{u}}^{n+1}\cdot\nabla\boldsymbol{Q}^n, \boldsymbol{H}^{n+1}\rangle\Delta t - \langle\boldsymbol{s}^{n+1}, \boldsymbol{H}^{n+1}\rangle\Delta t.$$

Lemma 3.2 implies that

$$\langle\nabla\tilde{\boldsymbol{u}}^{n+1}, \boldsymbol{\Sigma}^{n+1}\rangle + \langle\boldsymbol{H}^{n+1}, \boldsymbol{s}^{n+1}\rangle = 0.$$

Next, we take $\frac{1}{2}\boldsymbol{u}^{n+1}\Delta t$ and $\frac{1}{4}\left(\boldsymbol{u}^{n+1} + \tilde{\boldsymbol{u}}^{n+1}\right)\Delta t$ respectively as test functions in (3.3a), and use the divergence free condition (3.4) for $\boldsymbol{u}^{n+1}$. Then we have

$$\frac{1}{4}\|\boldsymbol{u}^{n+1}\|^2 - \frac{1}{4}\|\tilde{\boldsymbol{u}}^{n+1}\|^2 + \frac{1}{4}\left\|\boldsymbol{u}^{n+1} - \tilde{\boldsymbol{u}}^{n+1}\right\|^2 = 0, \tag{3.17a}$$
$$\frac{1}{4}\|\boldsymbol{u}^{n+1}\|^2 - \frac{1}{4}\|\tilde{\boldsymbol{u}}^{n+1}\|^2 = -\frac{1}{2}\left\langle\nabla p^{n+1} - \nabla p^n, \tilde{\boldsymbol{u}}^{n+1}\right\rangle\Delta t. \tag{3.17b}$$

These are admissible test functions, since we have shown that $\tilde{\boldsymbol{u}}^{n+1}, \boldsymbol{u}^{n+1} \in H^1(\Omega)$ with $\tilde{\boldsymbol{u}}^{n+1} = 0$ and $\boldsymbol{u}^{n+1}\cdot\mathbf{n} = 0$ on the boundary. Adding up these estimates together, we obtain

$$\left(\frac{1}{2}\|\boldsymbol{u}^{n+1}\|^2 + \frac{L}{2}\|\nabla\boldsymbol{Q}^{n+1}\|^2 + \frac{1}{2}\|r^{n+1}\|^2\right) - \left(\frac{1}{2}\|u^n\|^2 + \frac{L}{2}\|\nabla Q^n\|^2 + \frac{1}{2}\|r^n\|^2\right)$$
$$+ \frac{1}{4}\|\boldsymbol{u}^{n+1} - \tilde{\boldsymbol{u}}^{n+1}\|^2 + \frac{1}{2}\left\|\tilde{\boldsymbol{u}}^{n+1} - \boldsymbol{u}^n\right\|^2 + \frac{L}{2}\left\|\nabla\boldsymbol{Q}^{n+1} - \nabla\boldsymbol{Q}^n\right\|^2 + \frac{1}{2}\left\|r^{n+1} - r^n\right\|^2$$
$$= -\frac{1}{2}\langle\nabla p^{n+1} + \nabla p^n, \tilde{\boldsymbol{u}}^{n+1}\rangle\Delta t - \mu\left\|\nabla\tilde{\boldsymbol{u}}^{n+1}\right\|^2\Delta t - M\left\|\boldsymbol{H}^{n+1}\right\|^2\Delta t$$
$$= -\frac{1}{2}\langle\nabla p^{n+1} + \nabla p^n, 2\left(\nabla p^{n+1} - \nabla p^n\right)\Delta t\rangle\Delta t - \mu\left\|\nabla\tilde{\boldsymbol{u}}^{n+1}\right\|^2\Delta t - M\left\|\boldsymbol{H}^{n+1}\right\|^2\Delta t$$
$$= -\left(\left\|\nabla p^{n+1}\right\|^2 - \|\nabla p^n\|^2\right)\Delta t^2 - \mu\left\|\nabla\tilde{\boldsymbol{u}}^{n+1}\right\|^2\Delta t - M\left\|\boldsymbol{H}^{n+1}\right\|^2\Delta t.$$

Summing up it from $n=0$ to N, we yield

$$\frac{1}{2}\|\boldsymbol{u}^{N+1}\|^2+\frac{L}{2}\|\nabla\boldsymbol{Q}^{N+1}\|^2+\frac{1}{2}\|r^{n+1}\|^2+\|\nabla p^{N+1}\|^2\Delta t^2 \\ +\frac{1}{4}\sum_{n=0}^{N}\|\boldsymbol{u}^{n+1}-\tilde{\boldsymbol{u}}^{n+1}\|^2+\frac{1}{2}\sum_{n=0}^{N}\|\tilde{\boldsymbol{u}}^{n+1}-\boldsymbol{u}^n\|^2+\frac{L}{2}\sum_{n=0}^{N}\|\nabla\boldsymbol{Q}^{n+1}-\nabla\boldsymbol{Q}^n\|^2+\frac{1}{2}\sum_{n=0}^{N}\|r^{n+1}-r^n\|^2 \\ +\mu\sum_{n=0}^{N}\|\nabla\tilde{\boldsymbol{u}}^{n+1}\|^2\Delta t+M\sum_{n=0}^{N}\|\boldsymbol{H}^{n+1}\|^2\Delta t=\frac{1}{2}\|\boldsymbol{u}^0\|^2+\frac{L}{2}\|\nabla\boldsymbol{Q}^0\|^2+\frac{1}{2}\|r^0\|^2+\|\nabla p^0\|^2\Delta t^2.$$

Using (3.17a) once more, we can also rewrite this equation as

$$\frac{1}{4}\|\tilde{\boldsymbol{u}}^{N+1}\|^2+\frac{1}{4}\|\boldsymbol{u}^{N+1}\|^2+\frac{L}{2}\|\nabla\boldsymbol{Q}^{N+1}\|^2+\frac{1}{2}\|r^{n+1}\|^2+\|\nabla p^{N+1}\|^2\Delta t^2 \\ +\frac{1}{4}\sum_{n=0}^{N-1}\|\boldsymbol{u}^{n+1}-\tilde{\boldsymbol{u}}^{n+1}\|^2+\frac{1}{2}\sum_{n=0}^{N}\|\tilde{\boldsymbol{u}}^{n+1}-\boldsymbol{u}^n\|^2+\frac{L}{2}\sum_{n=0}^{N}\|\nabla\boldsymbol{Q}^{n+1}-\nabla\boldsymbol{Q}^n\|^2 \\ +\frac{1}{2}\sum_{n=0}^{N}\|r^{n+1}-r^n\|^2+\mu\sum_{n=0}^{N}\|\nabla\tilde{\boldsymbol{u}}^{n+1}\|^2\Delta t+M\sum_{n=0}^{N}\|\boldsymbol{H}^{n+1}\|^2\Delta t \\ =\frac{1}{2}\|\boldsymbol{u}^0\|^2+\frac{L}{2}\|\nabla\boldsymbol{Q}^0\|^2+\frac{1}{2}\|r^0\|^2+\|\nabla p^0\|^2\Delta t^2. \tag{3.18}$$

This concludes the proof of the discrete energy law of the system. □

Next, we define piece-wise linear in time interpolations based on the approximants $(\boldsymbol{u}^n,\boldsymbol{Q}^n,p^n,r^n)$, $1\le n\le\lfloor\frac{T}{\Delta t}\rfloor$. Specifically, given $\Delta t>0$, we define $(\boldsymbol{u}_{\Delta t},\boldsymbol{u}^*_{\Delta t},\boldsymbol{Q}_{\Delta t},r_{\Delta t})$ as piece-wise linear interpolation of $\boldsymbol{u}^n,\tilde{\boldsymbol{u}}^{n+1},\boldsymbol{Q}^n,r^n$, that is,

$$\boldsymbol{u}_{\Delta t}(t)=\sum_{n=0}^{N-1}\left[\frac{(n+1)\Delta t-t}{\Delta t}\boldsymbol{u}^n+\frac{t-n\Delta t}{\Delta t}\boldsymbol{u}^{n+1}\right]\chi_{S_n}, \tag{3.19a}$$

$$\boldsymbol{u}^*_{\Delta t}(t)=\sum_{n=0}^{N-1}\left[\frac{(n+1)\Delta t-t}{\Delta t}\tilde{\boldsymbol{u}}^n+\frac{t-n\Delta t}{\Delta t}\tilde{\boldsymbol{u}}^{n+1}\right]\chi_{S_n}, \tag{3.19b}$$

$$\boldsymbol{Q}_{\Delta t}(t)=\sum_{n=0}^{N-1}\left[\frac{(n+1)\Delta t-t}{\Delta t}\boldsymbol{Q}^n+\frac{t-n\Delta t}{\Delta t}\boldsymbol{Q}^{n+1}\right]\chi_{S_n}, \tag{3.19c}$$

$$\boldsymbol{Q}^*_{\Delta t}(t)=\sum_{n=0}^{N-1}\left[\frac{(n+1)\Delta t-t}{\Delta t}\boldsymbol{Q}^{n-1}+\frac{t-n\Delta t}{\Delta t}\boldsymbol{Q}^{n}\right]\chi_{S_n}, \tag{3.19d}$$

$$\boldsymbol{P}_{\Delta t}(t)=\sum_{n=0}^{N-1}\left[\frac{(n+1)\Delta t-t}{\Delta t}\boldsymbol{P}^{n-1}+\frac{t-n\Delta t}{\Delta t}\boldsymbol{P}^{n}\right]\chi_{S_n}, \tag{3.19e}$$

$$\boldsymbol{H}_{\Delta t}(t)=\sum_{n=0}^{N-1}\left[\frac{(n+1)\Delta t-t}{\Delta t}\boldsymbol{H}^n+\frac{t-n\Delta t}{\Delta t}\boldsymbol{H}^{n+1}\right]\chi_{S_n}, \tag{3.19f}$$

$$r_{\Delta t}(t)=\sum_{n=0}^{N-1}\left[\frac{(n+1)\Delta t-t}{\Delta t}r^n+\frac{t-n\Delta t}{\Delta t}r^{n+1}\right]\chi_{S_n}, \tag{3.19g}$$

where $S_n=[n\Delta t,(n+1)\Delta t)$ and χ_{S_n} is the characteristic function on S_n. Our goal is to use the Aubin–Lions lemma, Lemma 2.3 to deduce pre-compactness of these interpolants. To do so, we need a couple of additional *a priori* estimates that are uniform in Δt.

As in [32, 33], we will show that the approximations of $\boldsymbol{Q}$ are uniformly bounded in $L^2(0,T;H^2)$. This is critical for obtaining weak solutions. In [32, 33], this result is obtained *via* Sobolev embeddings and using the integrability of the bulk potential term in the energy. Due to the reformulation with the auxiliary variable, the same integrability is not available for the auxiliary variable r through the *a priori* energy estimate. However, it is possible to obtain the $L^2(0,T;H^2)$-regularity using Lemma 2.1:

Lemma 3.7. *If* $\boldsymbol{Q}^0 \in H^2(\Omega)$*, then*

$$\Delta t \sum_{k=1}^{N} \left\|\Delta \boldsymbol{Q}^k\right\|^2 \leq C. \tag{3.20}$$

Proof. As it is shown in Theorem 3.4, for each $k \in \mathbb{N}$, $\boldsymbol{Q}^k \in H^2(\Omega)$. Therefore, we can integrate by parts in (3.1d) which leads to

$$\left\langle \boldsymbol{H}^{k+1}, \boldsymbol{\phi} \right\rangle = L\left\langle \Delta \boldsymbol{Q}^{k+1}, \boldsymbol{\phi} \right\rangle - \left\langle r^{k+1} \boldsymbol{P}^k, \boldsymbol{\phi} \right\rangle,$$

for any smooth $\boldsymbol{\phi}$ with compact support. By density of $C_c^\infty(\Omega)$ in $L^2(\Omega)$, we can use test functions in $L^2(\Omega)$ and in particular, we can choose $\Delta \boldsymbol{Q}^{k+1}$ as a test function to obtain

$$L\left\langle \Delta \boldsymbol{Q}^{k+1}, \Delta \boldsymbol{Q}^{k+1} \right\rangle = \left\langle \boldsymbol{H}^{k+1}, \Delta \boldsymbol{Q}^{k+1} \right\rangle + \left\langle r^{k+1} \boldsymbol{P}^k, \Delta \boldsymbol{Q}^{k+1} \right\rangle.$$

Using Lemmas 3.6, 2.1, 2.2 and 2.9, we have

$$\begin{aligned}
L\left\|\Delta \boldsymbol{Q}^{k+1}\right\|^2 &\leq C\left(\left\|\boldsymbol{H}^{k+1}\right\|^2 + \left\|r^{k+1} P(\boldsymbol{Q}^k)\right\|^2\right) + \frac{L}{4}\left\|\Delta \boldsymbol{Q}^{k+1}\right\|^2 \\
&\leq C\left(\left\|\boldsymbol{H}^{k+1}\right\|^2 + \left\|P(\boldsymbol{Q}^k)\right\|_{L^\infty}^2 \left\|r^{k+1}\right\|^2\right) + \frac{L}{4}\left\|\Delta \boldsymbol{Q}^{k+1}\right\|^2 \\
&\overset{\text{Lemma 2.9}}{\leq} C\left(\left\|\boldsymbol{H}^{k+1}\right\|^2 + \left\|\boldsymbol{Q}^k\right\|_{L^\infty}^2 \left\|r^{k+1}\right\|^2\right) + \frac{L}{4}\left\|\Delta \boldsymbol{Q}^{k+1}\right\|^2 \\
&\overset{\text{Lemma 2.1}}{\leq} C\left(\left\|\boldsymbol{H}^{k+1}\right\|^2 + \left\|\boldsymbol{Q}^k\right\|_{H^2} + 1\right) + \frac{L}{4}\left\|\Delta \boldsymbol{Q}^{k+1}\right\|^2 \\
&\overset{\text{Lemma 2.2}}{\leq} C\left(\left\|\boldsymbol{H}^{k+1}\right\|^2 + \left\|\Delta \boldsymbol{Q}^k\right\| + 1\right) + \frac{L}{4}\left\|\Delta \boldsymbol{Q}^{k+1}\right\|^2 \\
&\leq C\left(1 + \left\|\boldsymbol{H}^{k+1}\right\|^2\right) + \frac{L}{4}\left\|\Delta \boldsymbol{Q}^k\right\|^2 + \frac{L}{4}\left\|\Delta \boldsymbol{Q}^{k+1}\right\|^2.
\end{aligned}$$

Multiplying Δt on both sides and summing from $k=0$ to $k=N-1$, we have

$$\frac{L}{4}\left\|\Delta \boldsymbol{Q}^N\right\|^2 \Delta t + \frac{L}{2}\sum_{k=1}^{N}\left\|\Delta \boldsymbol{Q}^k\right\|^2 \Delta t \leq \frac{L}{4}\left\|\Delta \boldsymbol{Q}^0\right\|^2 \Delta t + \sum_{k=1}^{N} C\left(1 + \left\|\boldsymbol{H}^{k+1}\right\|^2\right)\Delta t,$$

which is bounded uniformly in Δt thanks to the discrete energy estimate (3.18). ☐

Remark 3.8. When the boundary is smooth enough, this estimate implies that $\boldsymbol{Q}_{\Delta t}, \boldsymbol{Q}^*_{\Delta t} \in L^2(0,T;H^2(\Omega))$ uniformly in Δt, see Lemma 2.2. Using the Gagliardo–Nirenberg interpolation inequality, this implies that

$$\boldsymbol{Q}_{\Delta t} \in L^{\frac{4p}{3p-6}}(0,T;W^{1,p}(\Omega)), \quad 2 \leq p < 6,$$

uniformly in Δt. In particular, we obtain $\boldsymbol{Q}_{\Delta t} \in L^4(0,T;W^{1,3}(\Omega)) \cap L^{8/3}(0,T;W^{1,4}(\Omega)) \cap L^{20/9}(0,T;W^{1,5}(\Omega))$ (and the same estimates for $\boldsymbol{Q}^*_{\Delta t}$).

To apply the Aubin–Lions lemma, we also need to derive uniform (in Δt) estimates on the time derivatives of $\boldsymbol{u}_{\Delta t}$ and $\boldsymbol{Q}_{\Delta t}$. We summarize these estimates for regularity in time in the following two lemmas. The first one states the regularity for time derivative of velocity field $\boldsymbol{u}_{\Delta t}$.

Lemma 3.9. *Let* $V = W^{1,6}(\Omega) \cap H^1_{0,\sigma}(\Omega)$*. For every* $\Delta t > 0$*, we have*

$$\partial_t \boldsymbol{u}_{\Delta t} \in L^2(0,T;V').$$

Proof. From (3.1a), we infer that for any $\boldsymbol{\phi} \in L^2(0,T;V)$,

$$\left\langle \frac{\tilde{\boldsymbol{u}}^{n+1} - \boldsymbol{u}^n}{\Delta t}, \boldsymbol{\phi}(\cdot,t) \right\rangle = -\big\langle B\big(\boldsymbol{u}^n, \tilde{\boldsymbol{u}}^{n+1}\big), \boldsymbol{\phi}(\cdot,t)\big\rangle - \big\langle \mu \nabla \tilde{\boldsymbol{u}}^{n+1}, \nabla \boldsymbol{\phi}(\cdot,t)\big\rangle$$
$$- \big\langle \boldsymbol{\Sigma}^{n+1}, \nabla \boldsymbol{\phi}(\cdot,t)\big\rangle - \big\langle \boldsymbol{H}^{n+1} \nabla \boldsymbol{Q}^n, \boldsymbol{\phi}(\cdot,t)\big\rangle \coloneqq \sum_{k=1}^{4} I_k^n.$$

To derive the regularity estimate, we will control I_1^n to I_4^n separately. Using integration by parts and the energy estimate (3.18), we obtain

$$\begin{aligned}
\left|\sum_{n=0}^{N-1} \int_{n\Delta t}^{(n+1)\Delta t} I_1^n \,\mathrm{d}t\right| &= \left|\sum_{n=0}^{N-1} \int_{n\Delta t}^{(n+1)\Delta t} \int_\Omega (\boldsymbol{u}^n \cdot \nabla)\tilde{\boldsymbol{u}}^{n+1} \cdot \boldsymbol{\phi} \,\mathrm{d}x \,\mathrm{d}t\right| \\
&\le \sum_{n=0}^{N-1} \int_{n\Delta t}^{(n+1)\Delta t} \|\boldsymbol{\phi}(\cdot,t)\|_{L^\infty} \|\boldsymbol{u}^n\| \big\|\nabla \tilde{\boldsymbol{u}}^{n+1}\big\| \,\mathrm{d}t \\
&\overset{(3.18)}{\le} C \sum_{n=0}^{N-1} \int_{n\Delta t}^{(n+1)\Delta t} \|\boldsymbol{\phi}(\cdot,t)\|_{L^\infty} \big\|\nabla \tilde{\boldsymbol{u}}^{n+1}\big\| \,\mathrm{d}t \\
&\le C \sum_{n=0}^{N-1} \int_{n\Delta t}^{(n+1)\Delta t} \|\boldsymbol{\phi}(\cdot,t)\|_{W^{1,6}} \big\|\nabla \tilde{\boldsymbol{u}}^{n+1}\big\| \,\mathrm{d}t \\
&\le C \left(\sum_{n=0}^{N-1} \int_{n\Delta t}^{(n+1)\Delta t} \big\|\nabla \tilde{\boldsymbol{u}}^{n+1}\big\|^2 \,\mathrm{d}t\right)^{\frac{1}{2}} \left(\sum_{n=0}^{N-1} \int_{n\Delta t}^{(n+1)\Delta t} \|\boldsymbol{\phi}(\cdot,t)\|_{W^{1,6}}^2 \,\mathrm{d}t\right)^{\frac{1}{2}} \\
&= C \left(\sum_{n=0}^{N-1} \big\|\nabla \tilde{\boldsymbol{u}}^{n+1}\big\|^2 \Delta t\right)^{\frac{1}{2}} \|\boldsymbol{\phi}\|_{L^2(0,T;W^{1,6})} \overset{(3.18)}{\le} C \|\boldsymbol{\phi}\|_{L^2(0,T;V)}.
\end{aligned}$$

I_2 can be estimated as

$$\begin{aligned}
\left|\sum_{n=0}^{N-1} \int_{n\Delta t}^{(n+1)\Delta t} I_2^n \,\mathrm{d}t\right| &= \left|\sum_{n=0}^{N-1} \int_{n\Delta t}^{(n+1)\Delta t} \int_\Omega \mu \nabla \tilde{\boldsymbol{u}}^{n+1} \cdot \nabla \boldsymbol{\phi} \,\mathrm{d}x \,\mathrm{d}t\right| \\
&\le C \left(\sum_{n=0}^{N-1} \big\|\nabla \tilde{\boldsymbol{u}}^{n+1}\big\|^2 \Delta t\right)^{\frac{1}{2}} \|\nabla \boldsymbol{\phi}\|_{L^2([0,T)\times\Omega)} \overset{(3.18)}{\le} C \|\boldsymbol{\phi}\|_{L^2(0,T;V)}.
\end{aligned}$$

By definitions (1.7) and (3.2), Hölder's inequality, Poincaré's inequality and the Sobolev inequality, we have

$$\begin{aligned}\left|\sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t} I_3^n\,\mathrm{d}t\right| &\le \sum_{n=0}^{N-1}\left|\int_{n\Delta t}^{(n+1)\Delta t}\Big\langle \big(\boldsymbol{Q}^n\boldsymbol{H}^{n+1}-\boldsymbol{H}^{n+1}\boldsymbol{Q}^n\big)-\xi\big(\boldsymbol{H}^{n+1}\boldsymbol{Q}^n+\boldsymbol{Q}^n\boldsymbol{H}^{n+1}\big)\right.\\ &\qquad \left. -\frac{2\xi}{d}\boldsymbol{H}^{n+1}+2\xi\big(\boldsymbol{Q}^n:\boldsymbol{H}^{n+1}\big)\boldsymbol{Q}^n,\nabla\boldsymbol{\phi}(\cdot,t)\Big\rangle\,\mathrm{d}t\right|\\ &\le C\sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t}\Big(\|\boldsymbol{Q}^n\|_{L^3}\left\|\boldsymbol{H}^{n+1}\right\|\|\nabla\boldsymbol{\phi}(\cdot,t)\|_{L^6}\\ &\qquad+\left\|\boldsymbol{H}^{n+1}\right\|\|\nabla\boldsymbol{\phi}(\cdot,t)\|+\left\|\boldsymbol{H}^{n+1}\right\|\|\boldsymbol{Q}^n\|_{L^6}^2\|\nabla\boldsymbol{\phi}(\cdot,t)\|_{L^6}\Big)\,\mathrm{d}t\\ &\le C\sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t}\Big(\|\boldsymbol{Q}^n\|_{H^1}\left\|\boldsymbol{H}^{n+1}\right\|\|\boldsymbol{\phi}(\cdot,t)\|_{W^{1,6}}\\ &\qquad+\left\|\boldsymbol{H}^{n+1}\right\|\|\boldsymbol{\phi}(\cdot,t)\|_{H^1}+\left\|\boldsymbol{H}^{n+1}\right\|\|\boldsymbol{Q}^n\|_{H^1}^2\|\boldsymbol{\phi}(\cdot,t)\|_{W^{1,6}}\Big)\,\mathrm{d}t\\ &\overset{(3.18)}{\le} C\sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t}\big(\left\|\boldsymbol{H}^{n+1}\right\|\|\boldsymbol{\phi}(\cdot,t)\|_{W^{1,6}}+\left\|\boldsymbol{H}^{n+1}\right\|\|\boldsymbol{\phi}(\cdot,t)\|_{H^1}\\ &\qquad+\left\|\boldsymbol{H}^{n+1}\right\|\|\boldsymbol{\phi}(\cdot,t)\|_{W^{1,6}}\big)\,\mathrm{d}t\\ &\le C\left(\sum_{n=0}^{N-1}\left\|\boldsymbol{H}^{n+1}\right\|^2\Delta t\right)^{\frac{1}{2}}\|\boldsymbol{\phi}\|_{L^2(0,T;W^{1,6}\cap H^1_{0,\sigma})}\overset{(3.18)}{\le} C\|\boldsymbol{\phi}\|_{L^2(0,T;V)}.\end{aligned}$$

To control I_4, we apply Lemma 2.1,

$$\begin{aligned}\left|\sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t} I_4^n\,\mathrm{d}t\right| &= \left|\sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t}\int_\Omega \boldsymbol{H}^{n+1}\nabla\boldsymbol{Q}^n\cdot\boldsymbol{\phi}\,\mathrm{d}x\,\mathrm{d}t\right|\\ &\le \sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t}\|\boldsymbol{\phi}(\cdot,t)\|_{L^\infty}\left\|\boldsymbol{H}^{n+1}\right\|\|\nabla\boldsymbol{Q}^n\|\,\mathrm{d}x\,\mathrm{d}t\\ &\overset{(3.18)}{\le} C\sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t}\|\boldsymbol{\phi}(\cdot,t)\|_{W^{1,6}}\left\|\boldsymbol{H}^{n+1}\right\|\,\mathrm{d}x\,\mathrm{d}t\\ &\le C\left(\sum_{n=0}^{N-1}\left\|\boldsymbol{H}^{n+1}\right\|^2\Delta t\right)^{\frac{1}{2}}\left(\int_0^T\|\boldsymbol{\phi}(\cdot,t)\|_{W^{1,6}}^2\,\mathrm{d}t\right)^{\frac{1}{2}}\overset{(3.18)}{\le} C\|\boldsymbol{\phi}\|_{L^2(0,T;V)}.\end{aligned}$$

According to scheme (3.3), for each n, $\boldsymbol{u}^{n+1}$ is the projection of $\tilde{\boldsymbol{u}}^{n+1}$ onto the space of divergence free functions. Therefore, for every $\boldsymbol{\phi}\in L^2(0,T;V)$, we have

$$\int_{n\Delta t}^{(n+1)\Delta t}\langle\partial_t\boldsymbol{u}_{\Delta t},\boldsymbol{\phi}\rangle\,\mathrm{d}t=\int_{n\Delta t}^{(n+1)\Delta t}\left\langle\frac{\boldsymbol{u}^{n+1}-\boldsymbol{u}^n}{\Delta t},\boldsymbol{\phi}\right\rangle\mathrm{d}t=\int_{n\Delta t}^{(n+1)\Delta t}\left\langle\frac{\tilde{\boldsymbol{u}}^{n+1}-\boldsymbol{u}^n}{\Delta t},\boldsymbol{\phi}\right\rangle\mathrm{d}t.$$

Therefore, combining the estimates from I_1 to I_4, we have shown that

$$\|\partial_t\boldsymbol{u}_{\Delta t}\|_{L^2(0,T;V')}=\sup_{\boldsymbol{\phi}\in L^2(0,T;V)}\frac{\left|\sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t}\left\langle\frac{\tilde{\boldsymbol{u}}^{n+1}-\boldsymbol{u}^n}{\Delta t},\boldsymbol{\phi}\right\rangle\mathrm{d}t\right|}{\|\boldsymbol{\phi}\|_{L^2(0,T;V)}}\le C, \tag{3.21}$$

and so $\partial_t\boldsymbol{u}_{\Delta t}\in L^2(0,T;V')$ uniformly in Δt. □

Next we show a uniform estimate in Δt for $\partial_t \boldsymbol{Q}_{\Delta t}$.

Lemma 3.10. *For every $\Delta t > 0$, we have*

$$\partial_t \boldsymbol{Q}_{\Delta t} \in L^2\Big(0, T; L^{\frac{6}{5}}\Big).$$

Proof. For any function $\boldsymbol{\varphi} \in L^2(0, T; L^6)$,

$$\left\langle \frac{\boldsymbol{Q}^{n+1} - \boldsymbol{Q}^n}{\Delta t}, \boldsymbol{\varphi} \right\rangle = -\big\langle \tilde{\boldsymbol{u}}^{n+1} \cdot \nabla \boldsymbol{Q}^n, \boldsymbol{\varphi} \big\rangle + \big\langle \boldsymbol{s}^{n+1}, \boldsymbol{\varphi} \big\rangle + M \big\langle \boldsymbol{H}^{n+1}, \boldsymbol{\varphi} \big\rangle \coloneqq \sum_{k=1}^{3} J_k^n.$$

Using energy estimate (3.18), the first term can be bounded as follows

$$\begin{aligned}
\left| \sum_{n=0}^{N-1} \int_{n\Delta t}^{(n+1)\Delta t} J_1^n \, \mathrm{d}t \right| &= \left| \sum_{n=0}^{N-1} \int_{n\Delta t}^{(n+1)\Delta t} \int_\Omega \tilde{\boldsymbol{u}}^{n+1} \cdot \nabla \boldsymbol{Q}^n : \boldsymbol{\varphi} \, \mathrm{d}x \, \mathrm{d}t \right| \\
&\le \sum_{n=0}^{N-1} \int_{n\Delta t}^{(n+1)\Delta t} \big\| \tilde{\boldsymbol{u}}^{n+1} \big\|_{L^4} \| \nabla \boldsymbol{Q}^n \| \| \boldsymbol{\varphi}(\cdot, t) \|_{L^4} \, \mathrm{d}t \\
&\overset{(3.18)}{\le} C \sum_{n=0}^{N-1} \int_{n\Delta t}^{(n+1)\Delta t} \big\| \nabla \tilde{\boldsymbol{u}}^{n+1} \big\| \| \boldsymbol{\varphi}(\cdot, t) \|_{L^6} \, \mathrm{d}t \\
&\le C \left(\sum_{n=0}^{N-1} \big\| \nabla \tilde{\boldsymbol{u}}^{n+1} \big\|^2 \Delta t \right)^{\frac{1}{2}} \left(\int_0^T \| \boldsymbol{\varphi}(\cdot, t) \|_{L^6}^2 \, \mathrm{d}t \right)^{\frac{1}{2}} \overset{(3.18)}{\le} C \| \boldsymbol{\varphi} \|_{L^2(0,T;L^6)}.
\end{aligned}$$

Using the Sobolev inequality and definitions (1.3), (3.2), we have

$$\begin{aligned}
\left| \sum_{n=0}^{N-1} \int_{n\Delta t}^{(n+1)\Delta t} J_2^n \, \mathrm{d}t \right| &= \Bigg| \sum_{n=0}^{N-1} \int_{n\Delta t}^{(n+1)\Delta t} \Big\langle \tilde{\boldsymbol{W}}^{n+1} \boldsymbol{Q}^n - \boldsymbol{Q}^n \tilde{\boldsymbol{W}}^{n+1} + \xi \Big(\boldsymbol{Q}^n \tilde{\boldsymbol{D}}^{n+1} + \tilde{\boldsymbol{D}}^{n+1} \boldsymbol{Q}^n \Big) \\
&\quad + \frac{2\xi}{d} \tilde{\boldsymbol{D}}^{n+1} - \frac{2\xi}{d^2} \nabla \cdot \tilde{\boldsymbol{u}}^{n+1} \boldsymbol{I} - 2\xi \Big(\tilde{\boldsymbol{D}}^{n+1} : \boldsymbol{Q}^n \Big) \Big(\boldsymbol{Q}^n + \frac{1}{d} \boldsymbol{I} \Big), \boldsymbol{\varphi} \Big\rangle \mathrm{d}t \Bigg| \\
&\le \sum_{n=0}^{N-1} \int_{n\Delta t}^{(n+1)\Delta t} \Big(\big\| \nabla \tilde{\boldsymbol{u}}^{n+1} \big\| \| \boldsymbol{Q}^n \|_{L^4} \| \boldsymbol{\varphi}(\cdot, t) \|_{L^4} + \big\| \nabla \tilde{\boldsymbol{u}}^{n+1} \big\| \| \boldsymbol{\varphi}(\cdot, t) \| \\
&\quad + \big\| \nabla \tilde{\boldsymbol{u}}^{n+1} \big\| \| \boldsymbol{Q}^n \|_{L^6}^2 \| \boldsymbol{\varphi}(\cdot, t) \|_{L^6} \Big) \, \mathrm{d}t \\
&\le C \sum_{n=0}^{N-1} \int_{n\Delta t}^{(n+1)\Delta t} \Big(\big\| \nabla \tilde{\boldsymbol{u}}^{n+1} \big\| \| \nabla \boldsymbol{Q}^n \| \| \boldsymbol{\varphi}(\cdot, t) \|_{L^6} + \big\| \nabla \tilde{\boldsymbol{u}}^{n+1} \big\| \| \boldsymbol{\varphi}(\cdot, t) \|_{L^6} \\
&\quad + \big\| \nabla \tilde{\boldsymbol{u}}^{n+1} \big\| \| \nabla \boldsymbol{Q}^n \|^2 \| \boldsymbol{\varphi}(\cdot, t) \|_{L^6} \Big) \, \mathrm{d}t \\
&\overset{(3.18)}{\le} C \sum_{n=0}^{N-1} \int_{n\Delta t}^{(n+1)\Delta t} \big(\big\| \nabla \tilde{\boldsymbol{u}}^{n+1} \big\| \| \boldsymbol{\varphi}(\cdot, t) \|_{L^6} + \big\| \nabla \tilde{\boldsymbol{u}}^{n+1} \big\| \| \boldsymbol{\varphi}(\cdot, t) \|_{L^6} + \big\| \nabla \tilde{\boldsymbol{u}}^{n+1} \big\| \| \boldsymbol{\varphi}(\cdot, t) \|_{L^6} \big) \, \mathrm{d}t \\
&\le C \left(\sum_{n=0}^{N-1} \big\| \nabla \tilde{\boldsymbol{u}}^{n+1} \big\|^2 \Delta t \right)^{\frac{1}{2}} \left(\int_0^T \| \boldsymbol{\varphi}(\cdot, t) \|_{L^6}^2 \, \mathrm{d}t \right)^{\frac{1}{2}} \overset{(3.18)}{\le} C \| \boldsymbol{\varphi} \|_{L^2(0,T;L^6)}.
\end{aligned}$$

The last term J_3^n satisfies

$$\left|\sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t} J_3^n\,\mathrm{d}t\right| = \left|\sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t}\int_\Omega \boldsymbol{H}^{n+1}:\boldsymbol{\varphi}\,\mathrm{d}x\,\mathrm{d}t\right| \le \sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t}\|\boldsymbol{H}^{n+1}\|\|\boldsymbol{\varphi}(\cdot,t)\|\,\mathrm{d}t$$
$$\le C\left(\sum_{n=0}^{N-1}\|\boldsymbol{H}^{n+1}\|^2\,\Delta t\right)^{\frac{1}{2}}\left(\int_0^T\|\boldsymbol{\varphi}(\cdot,t)\|_{L^2}^2\,\mathrm{d}t\right)^{\frac{1}{2}} \overset{(3.18)}{\le} C\|\boldsymbol{\varphi}\|_{L^2(0,T;L^2)}.$$

Combining these estimates for J_1, J_2 and J_3, we have shown $\partial_t\boldsymbol{Q}_{\Delta t}\in L^2(0,T;L^{\frac{6}{5}})$. □

This estimate naturally leads to the following corollary:

Corollary 3.11. *We have*

$$\partial_t r_{\Delta t}\in L^2\big(0,T;L^1(\Omega)\big)\cap L^{6/5}([0,T]\times\Omega),$$

uniformly in Δt.

Proof. We obtain from (3.1c) that

$$\int_0^T\left(\int_\Omega|\partial_t r_{\Delta t}(x,t)|\mathrm{d}x\right)^2\mathrm{d}t = \sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t}\|\boldsymbol{P}^n:\partial_t\boldsymbol{Q}_{\Delta t}(\cdot,t)\|_{L^1}^2\,\mathrm{d}t$$
$$\le \sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t}\|\boldsymbol{P}^n\|_{L^6}^2\|\partial_t\boldsymbol{Q}_{\Delta t}(\cdot,t)\|_{L^{\frac{6}{5}}}^2\,\mathrm{d}t$$
$$\overset{\text{Lemma 2.9}}{\le} C\sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t}\|\boldsymbol{Q}^n\|_{L^6}^2\|\partial_t\boldsymbol{Q}_{\Delta t}(\cdot,t)\|_{L^{\frac{6}{5}}}^2\,\mathrm{d}t$$
$$\le C\sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t}\|\nabla\boldsymbol{Q}^n\|^2\|\partial_t\boldsymbol{Q}_{\Delta t}(\cdot,t)\|_{L^{\frac{6}{5}}}^2\,\mathrm{d}t$$
$$\overset{(3.18)}{\le} C\sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t}\|\partial_t\boldsymbol{Q}_{\Delta t}(\cdot,t)\|_{L^{\frac{6}{5}}}^2\,\mathrm{d}t = C\|\partial_t\boldsymbol{Q}_{\Delta t}\|_{L^2\left(0,T;L^{\frac{6}{5}}\right)}^2<\infty.$$

To obtain the second estimate, we instead compute

$$\left(\int_0^T\int_\Omega|\partial_t r_{\Delta t}(x,t)|^{\frac{6}{5}}\mathrm{d}x\,\mathrm{d}t\right)^{\frac{5}{6}} = \left(\sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t}\|\boldsymbol{P}^n:\partial_t\boldsymbol{Q}_{\Delta t}(\cdot,t)\|_{L^{6/5}}^{\frac{6}{5}}\mathrm{d}t\right)^{\frac{5}{6}}$$
$$\le\left(\sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t}\|\boldsymbol{P}^n\|_{L^\infty}^3\mathrm{d}t\right)^{\frac{1}{3}}\left(\sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t}\|\partial_t\boldsymbol{Q}_{\Delta t}(\cdot,t)\|_{L^{\frac{6}{5}}}^2\mathrm{d}t\right)^{\frac{1}{2}}$$
$$\overset{\text{Lemma 2.9}}{\le} C\left(\sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t}\|\boldsymbol{Q}_{\Delta t}\|_{L^\infty}^3\mathrm{d}t\right)^{\frac{1}{3}}\|\partial_t\boldsymbol{Q}_{\Delta t}(\cdot,t)\|_{L^2\left(0,T;L^{\frac{6}{5}}\right)}$$
$$\le C\left(\sum_{n=0}^{N-1}\int_{n\Delta t}^{(n+1)\Delta t}\|\boldsymbol{Q}_{\Delta t}\|_{W^{1,\frac{18}{5}}}^3\mathrm{d}t\right)^{\frac{1}{3}}\|\partial_t\boldsymbol{Q}_{\Delta t}(\cdot,t)\|_{L^2\left(0,T;L^{\frac{6}{5}}\right)}$$
$$\overset{\text{Remark 3.8, (3.18)}}{\le} C\|\partial_t\boldsymbol{Q}_{\Delta t}(\cdot,t)\|_{L^2\left(0,T;L^{\frac{6}{5}}\right)}<\infty.$$

□

4. Convergence analysis

In this section, we will prove convergence of the semi-discrete numerical scheme constructed in the previous section as the time step Δt tends to zero. We will show that a subsequence of $\{\boldsymbol{Q}_{\Delta t}, \boldsymbol{u}^*_{\Delta t}, \boldsymbol{H}_{\Delta t}, r_{\Delta t}\}_{\Delta t}$ converges to a weak solution of system (1.10a)–(1.10e). This leads to the following main theorem:

Theorem 4.1. *The piece-wise linear interpolations* (3.19a)–(3.19g) *computed using scheme* (3.1a)–(3.4) *converge up to a subsequence to a weak solution of* (1.10a)–(1.10e) *(as in Def. 2.5) as* $\Delta t \to 0$.

Proof. Our proof utilizes the energy estimates derived in the last section for the linear interpolations defined in (3.19a)–(3.19g). Then we will use compactness theorems, such as Lemma 2.3, to extract a convergent subsequence and pass the limit, obtaining a weak solution of system (1.10a)–(1.10e). We split the proof into several steps as follows.

Step 1: Smoothing the initial data. In order for Lemma 3.7 to be useful, we need $\Delta t\big\|\Delta \boldsymbol{Q}^0\big\|^2$ to be uniformly bounded in Δt. However, the initial data $\boldsymbol{Q}_{\text{in}}$ may be less regular, for example, in $H^1(\Omega)$ only. In order to approximate $\boldsymbol{Q}_{\text{in}}$ with a sufficiently regular initial approximation $\boldsymbol{Q}^0$, we proceed as follows: Given $\boldsymbol{Q}_{\text{in}} \in H^1_0$, we determine $\boldsymbol{Q}^0 \in H^1_0 \cap H^2$ by solving the equation

$$(\boldsymbol{I} - \Delta t \Delta)\, \boldsymbol{Q}^0 = \boldsymbol{Q}_{\text{in}}.$$

We obtain from an energy estimate that

$$\big\|\nabla \boldsymbol{Q}^0\big\|^2 + \Delta t\big\|\Delta \boldsymbol{Q}^0\big\|^2 \le \|\nabla \boldsymbol{Q}_{\text{in}}\|\, \|\nabla \boldsymbol{Q}^0\| \le \frac{1}{2}\|\nabla \boldsymbol{Q}_{\text{in}}\|^2 + \frac{1}{2}\big\|\nabla \boldsymbol{Q}^0\big\|^2. \tag{4.1}$$

This implies that $\Delta t\|\Delta \boldsymbol{Q}^0\|^2$ is bounded and, therefore, $\|\Delta t \Delta \boldsymbol{Q}^0\|^2 = O(\Delta t)$. As Δt tends to 0, $\|\Delta t \Delta \boldsymbol{Q}^0\|^2$ tends to 0. Then we can conclude that $\boldsymbol{Q}^0 \to \boldsymbol{Q}_{\text{in}}$ strongly in L^2 and weakly in H^1.

Step 2: Compactness. The *a priori* estimates from the previous section can be summarized as follows: For any fixed $T > 0$,

$$\begin{aligned}
&\sup_{\Delta t} \|\boldsymbol{Q}_{\Delta t}\|_{L^2(0,T;H^2)\cap L^\infty(0,T;H^1)} < \infty, \qquad \sup_{\Delta t} \|\boldsymbol{Q}^*_{\Delta t}\|_{L^2(0,T;H^2)\cap L^\infty(0,T;H^1)} < \infty,\\
&\sup_{\Delta t} \|\boldsymbol{u}_{\Delta t}\|_{L^2(0,T;H^1_\sigma)\cap L^\infty(0,T;L^2_\sigma)} < \infty, \qquad \sup_{\Delta t} \|\boldsymbol{u}^*_{\Delta t}\|_{L^2(0,T;H^1)\cap L^\infty(0,T;L^2)} < \infty\\
&\sup_{\Delta t} \|r_{\Delta t}\|_{L^\infty(0,T;L^2(\Omega))} < \infty.
\end{aligned} \tag{4.2}$$

Lemmas 3.9 and 3.10 imply

$$\sup_{\Delta t}\|\partial_t \boldsymbol{u}_{\Delta t}\|_{L^2(0,T;V')} < \infty, \qquad \sup_{\Delta t}\|\partial_t \boldsymbol{Q}_{\Delta t}\|_{L^2(0,T;H^{-1})} < \infty. \tag{4.3}$$

Noting that $L^2_\sigma(\Omega)$ is continuously embedded into $V' = \big(W^{1,p}(\Omega) \cap H^1_{0,\sigma}(\Omega)\big)'$, we can apply Lemma 2.3 to obtain that there exists $\boldsymbol{u} \in L^2(0,T;H^1_{0,\sigma}) \cap L^\infty(0,T;L^2)$ and a subsequence of $\{\boldsymbol{u}_{\Delta t}\}_{\Delta t}$, which will be denoted as $\{\boldsymbol{u}_{\Delta t_m}\}_m$, such that

$$\boldsymbol{u}_{\Delta t_m} \rightharpoonup \boldsymbol{u} \text{ in } L^2\big(0,T;H^1_{0,\sigma}\big), \quad \boldsymbol{u}_{\Delta t_m} \to \boldsymbol{u} \text{ in } L^2\big(0,T;L^2_\sigma\big), \quad \boldsymbol{u}_{\Delta t_m}(t) \overset{*}{\rightharpoonup} \boldsymbol{u}(t) \text{ in } L^2 \text{ for a.e. } t \in [0,T]. \tag{4.4}$$

Similarly, for the Q-tensor, H^1 is continuously embedded into $H^{-1}(\Omega)$ and so we apply Lemma 2.3 again, to obtain $\boldsymbol{Q}, \boldsymbol{Q}^* \in L^2(0,T;H^2) \cap L^\infty(0,T;H^1)$ and subsequences of $\{\boldsymbol{Q}_{\Delta t}\}_{\Delta t}$ and $\{\boldsymbol{Q}^*_{\Delta t}\}_{\Delta t}$ which will be denoted by $\boldsymbol{Q}_{\Delta t_m}$ and $\boldsymbol{Q}^*_{\Delta t_m}$, such that

$$\boldsymbol{Q}_{\Delta t_m} \rightharpoonup \boldsymbol{Q} \text{ in } L^2(0,T;H^2), \quad \boldsymbol{Q}_{\Delta t_m} \to \boldsymbol{Q} \text{ in } L^2(0,T;H^1), \quad \boldsymbol{Q}_{\Delta t_m}(t) \to \boldsymbol{Q}(t) \text{ in } L^2,\ \forall\, t \in [0,T], \tag{4.5}$$

$$\boldsymbol{Q}^*_{\Delta t_m} \rightharpoonup \boldsymbol{Q}^* \text{ in } L^2(0,T;H^2), \quad \boldsymbol{Q}^*_{\Delta t_m} \to \boldsymbol{Q}^* \text{ in } L^2(0,T;H^1), \quad \boldsymbol{Q}^*_{\Delta t_m}(t) \to \boldsymbol{Q}^*(t) \text{ in } L^2, \forall\, t \in [0,T]. \quad (4.6)$$

Since $\boldsymbol{Q}_{\Delta t_m}$, $\boldsymbol{Q}^*_{\Delta t_m}$ are symmetric and trace-free for every Δt, it follows that the limits $\boldsymbol{Q}$ and $\boldsymbol{Q}^*$ are also symmetric and trace-free, since these are linear properties. According to Lemma 2.9, the Lipschitz continuity of P guarantees the strong convergence properties of subsequence $\{\boldsymbol{Q}^*_{\Delta t_m}\}_m$ hold as well for the sequence $\{P(\boldsymbol{Q}_{\Delta t_m})\}_m$, that is,

$$\boldsymbol{P}_{\Delta t_m} \to P(\boldsymbol{Q}^*) \text{ in } L^2([0,T) \times \Omega). \quad (4.7)$$

In view of the Banach–Alaoglu theorem [18] and Lemma 3.10, we can extract a weakly convergent subsequence $\{\partial_t \boldsymbol{Q}_{\Delta t_m}\}_m$ such that

$$\partial_t \boldsymbol{Q}_{\Delta t_m} \rightharpoonup \partial_t \boldsymbol{Q} \text{ in } L^2\big(0,T;H^{-1}\big), \quad (4.8)$$

and a weakly convergent subsequence of $\{r_{\Delta t_m}\}_m$ from $\{r_{\Delta t}\}_{\Delta t}$ such that

$$r_{\Delta t_m} \overset{*}{\rightharpoonup} r \text{ in } L^\infty\big(0,T;L^2\big). \quad (4.9)$$

Step 3: Equivalence between $\boldsymbol{Q}$ and $\boldsymbol{Q}^*$ and convergence of $\boldsymbol{u}^*_{\Delta t}$. This step's primary purpose is to show that the limit functions of the various subsequences coincide. Noting that $\boldsymbol{Q}_{\Delta t_m}$ differs from $\boldsymbol{Q}^*_{\Delta t_m}$ since they are interpolations of numerical solutions obtained at consecutive time steps, we can make use of the upper bound of the term $\sum_{n=0}^N \|\nabla \boldsymbol{Q}^{n+1} - \nabla \boldsymbol{Q}^n\|^2$ obtained in Lemma 3.6 to deduce that

$$\begin{aligned}
&\|\boldsymbol{Q} - \boldsymbol{Q}^*\|_{L^2(0,T;H^1)} \\
&\quad \le \|\boldsymbol{Q} - \boldsymbol{Q}_{\Delta t_m}\|_{L^2(0,T;H^1)} + \big\|\boldsymbol{Q}_{\Delta t_m} - \boldsymbol{Q}^*_{\Delta t_m}\big\|_{L^2(0,T;H^1)} + \big\|\boldsymbol{Q}^* - \boldsymbol{Q}^*_{\Delta t_m}\big\|_{L^2(0,T;H^1)} \\
&\quad = \|\boldsymbol{Q} - \boldsymbol{Q}_{\Delta t_m}\|_{L^2(0,T;H^1)} + \sum_{n=0}^N \left\| \frac{(n+1)\Delta t - t}{\Delta t}\big(\boldsymbol{Q}^n - \boldsymbol{Q}^{n-1}\big) + \frac{t - n\Delta t}{\Delta t}\big(\boldsymbol{Q}^{n+1} - \boldsymbol{Q}^n\big)\right\|_{L^2(S_n;H^1)} \\
&\qquad + \big\|\boldsymbol{Q}^* - \boldsymbol{Q}^*_{\Delta t_m}\big\|_{L^2(0,T;H^1)} \\
&\quad = \|\boldsymbol{Q} - \boldsymbol{Q}_{\Delta t_m}\|_{L^2(0,T;H^1)} + \sum_{n=0}^N \big[\big\|\boldsymbol{Q}^n - \boldsymbol{Q}^{n-1}\big\|_{H^1} + \big\|\boldsymbol{Q}^{n+1} - \boldsymbol{Q}^n\big\|_{H^1}\big]\Delta t \\
&\qquad + \big\|\boldsymbol{Q}^* - \boldsymbol{Q}^*_{\Delta t_m}\big\|_{L^2(0,T;H^1)} \\
&\quad \le \|\boldsymbol{Q} - \boldsymbol{Q}_{\Delta t_m}\|_{L^2(0,T;H^1)} + C\left(\sum_{n=0}^N \big\|\nabla \boldsymbol{Q}^{n+1} - \nabla \boldsymbol{Q}^n\big\|^2 \Delta t\right)^{\frac{1}{2}} + \big\|\boldsymbol{Q}^* - \boldsymbol{Q}^*_{\Delta t_m}\big\|_{L^2(0,T;H^1)}.
\end{aligned} \quad (4.10)$$

As $\Delta t \to 0$, the convergence results (4.5) and (4.6) imply that the first and third will go to 0 as Δt tends to 0 while the second is $O(\sqrt{\Delta t})$ by energy estimate (3.16), and so it goes to 0, too. So we conclude that $\boldsymbol{Q}$ is equal to $\boldsymbol{Q}^*$ in $L^2(0,T;H^1)$.

For the velocity field, though the sequence $\{\boldsymbol{u}^*_{\Delta t}\}_m$ does not preserve the divergence-free property on each step, we will show that the limit of its subsequence $\boldsymbol{u}^*_{\Delta t_m}$ agrees with $\boldsymbol{u}$. To see this, we infer from definitions (3.19a) and (3.19b) that

$$\begin{aligned}
\big\|\boldsymbol{u} - \boldsymbol{u}^*_{\Delta t_m}\big\|_{L^2([0,T)\times\Omega)} &\le \|\boldsymbol{u} - \boldsymbol{u}_{\Delta t_m}\|_{L^2([0,T)\times\Omega)} + \big\|\boldsymbol{u}_{\Delta t_m} - \boldsymbol{u}^*_{\Delta t_m}\big\|_{L^2([0,T)\times\Omega)} \\
&\le \|\boldsymbol{u} - \boldsymbol{u}_{\Delta t_m}\|_{L^2([0,T)\times\Omega)} + C\left(\sum_{n=0}^N \big\|\tilde{\boldsymbol{u}}^{n+1} - \boldsymbol{u}^{n+1}\big\|^2 \Delta t\right)^{\frac{1}{2}}.
\end{aligned} \quad (4.11)$$

As $\Delta t \to 0$, the convergence result (4.4) implies that the first term will go to 0 while the second is $O(\sqrt{\Delta t})$ by energy estimate (3.16), and so it goes to 0 as well. In this way, we have shown that $\boldsymbol{u}^*_{\Delta t_m} \to \boldsymbol{u}$ strongly in $L^2([0,T)\times\Omega)$. For each Δt, we note that $\boldsymbol{u}_{\Delta t}$ is divergence-free and therefore, by the weak convergence in (4.4), we obtain that for almost every $t\in[0,T]$ and any smooth function $\phi\in C_c^\infty(\Omega)$,

$$\begin{aligned}0=\lim_{m\to\infty}\int_\Omega \phi(x)\nabla\cdot\boldsymbol{u}_{\Delta t_m}(t,x)\,\mathrm{d}x &= -\lim_{m\to\infty}\int \nabla\phi(x)\cdot\boldsymbol{u}_{\Delta t_m}(t,x)\,\mathrm{d}x\\ &= \int_\Omega \nabla\phi(x)\cdot\boldsymbol{u}(t,x)\,\mathrm{d}x=\int_\Omega \phi(x)\nabla\cdot\boldsymbol{u}(t,x)\,\mathrm{d}x. \end{aligned}\tag{4.12}$$

This implies that $\boldsymbol{u}$ is weakly divergence-free which implies that it is divergence free almost everywhere in $[0,T)\times\Omega$.

Step 4: Weak convergence to $\boldsymbol{H}$, $\boldsymbol{S}$, $\boldsymbol{\Sigma}$. We let $\boldsymbol{H}=L\Delta\boldsymbol{Q}-rP(\boldsymbol{Q})$. This is well-defined thanks to the regularity estimates we obtained for $\boldsymbol{Q}$ in the previous steps. To obtain a representation of $\boldsymbol{H}_{\Delta t}$ in terms of r^n and $\boldsymbol{P}^n$, we introduce the following piece-wise linear function $\widetilde{r\boldsymbol{P}}_{\Delta t}$ to approximate $r\boldsymbol{P}$,

$$\widetilde{r\boldsymbol{P}}_{\Delta t}=\sum_{n=0}^{N-1}\left[\frac{(n+1)\Delta t-t}{\Delta t}\,r^n\boldsymbol{P}^{n-1}+\frac{t-n\Delta t}{\Delta t}\,r^{n+1}\boldsymbol{P}^n\right]\chi_{S_n}. \tag{4.13}$$

Recalling definitions (3.19f) and (3.1d), the interpolation $\boldsymbol{H}_{\Delta t}$ satisfies the following weak form

$$\langle\boldsymbol{H}_{\Delta t},\boldsymbol{\phi}\rangle=-L\langle\nabla\boldsymbol{Q}_{\Delta t},\nabla\boldsymbol{\phi}\rangle-\left\langle\widetilde{r\boldsymbol{P}}_{\Delta t},\boldsymbol{\phi}\right\rangle$$

for any smooth matrix-valued test function $\boldsymbol{\phi}$ with compact support in $[0,T)\times\Omega$. Accordingly, the subsequence $\boldsymbol{H}_{\Delta t_m}$ satisfies

$$\langle\boldsymbol{H}_{\Delta t_m},\boldsymbol{\phi}\rangle=-L\langle\nabla\boldsymbol{Q}_{\Delta t_m},\nabla\boldsymbol{\phi}\rangle-\left\langle\widetilde{r\boldsymbol{P}}_{\Delta t_m},\boldsymbol{\phi}\right\rangle.$$

To show that $\widetilde{r\boldsymbol{P}}_{\Delta t_m}$ converges weakly to $rP(\boldsymbol{Q})$, we introduce a piece-wise constant interpolation $\boldsymbol{P}^*_{\Delta t}$ to approximate $\boldsymbol{P}$ as

$$\boldsymbol{P}^*_{\Delta t}=\sum_{n=0}^{N-1}\boldsymbol{P}^{n-1}\chi_{S_n}. \tag{4.14}$$

Then for any smooth test function $\boldsymbol{\phi}$, we have

$$\begin{aligned}&\int_0^T\int_\Omega\left(\widetilde{r\boldsymbol{P}}_{\Delta t_m}-rP(\boldsymbol{Q})\right):\boldsymbol{\phi}\,\mathrm{d}x\,\mathrm{d}t\\ &\quad=\underbrace{\int_0^T\int_\Omega\left(\widetilde{r\boldsymbol{P}}_{\Delta t_m}-r_{\Delta t_m}\boldsymbol{P}^*_{\Delta t_m}\right):\boldsymbol{\phi}\,\mathrm{d}x\,\mathrm{d}t}_{K_1}+\underbrace{\int_0^T\int_\Omega r_{\Delta t_m}\left(\boldsymbol{P}^*_{\Delta t_m}-\boldsymbol{P}_{\Delta t_m}\right):\boldsymbol{\phi}\,\mathrm{d}x\,\mathrm{d}t}_{K_2}\\ &\qquad+\underbrace{\int_0^T\int_\Omega r_{\Delta t_m}(\boldsymbol{P}_{\Delta t_m}-P(\boldsymbol{Q})):\boldsymbol{\phi}\,\mathrm{d}x\,\mathrm{d}t}_{K_3}+\underbrace{\int_0^T\int_\Omega(r_{\Delta t_m}-r)P(\boldsymbol{Q}):\boldsymbol{\phi}\,\mathrm{d}x\,\mathrm{d}t}_{K_4}.\end{aligned}$$

Our goal is to show that when $m \to \infty$, each $K_i, i = 1,2,3,4$ tends to 0. With (3.19g), (4.13), (4.14) and using Lemmas 2.9, 3.6, we can estimate K_1 as

$$
\begin{aligned}
|K_1| &= \Bigg| \int_0^T \int_\Omega \sum_{n=0}^{N-1} \left[\frac{(n+1)\Delta t_m - t}{\Delta t_m} r^n \boldsymbol{P}^{n-1} + \frac{t - n\Delta t_m}{\Delta t_m} r^{n+1} \boldsymbol{P}^n \right] \chi_{S_n} : \boldsymbol{\phi} \, \mathrm{d}x \, \mathrm{d}t \\
&\quad - \int_0^T \int_\Omega \sum_{n=0}^{N-1} \left[\frac{(n+1)\Delta t_m - t}{\Delta t_m} r^n \boldsymbol{P}^{n-1} + \frac{t - n\Delta t_m}{\Delta t_m} r^{n+1} \boldsymbol{P}^{n-1} \right] \chi_{S_n} : \boldsymbol{\phi} \, \mathrm{d}x \, \mathrm{d}t \Bigg| \\
&= \left| \int_0^T \int_\Omega \sum_{n=0}^{N-1} \frac{t - n\Delta t_m}{\Delta t_m} r^{n+1} \big(\boldsymbol{P}^n - \boldsymbol{P}^{n-1} \big) \chi_{S_n} : \boldsymbol{\phi} \, \mathrm{d}x \, \mathrm{d}t \right| \\
&\le \Delta t_m \|\boldsymbol{\phi}\|_{L^\infty([0,T)\times\Omega)} \sum_{n=0}^{N-1} \int_\Omega |r^{n+1}| \left| \boldsymbol{P}^n - \boldsymbol{P}^{n-1} \right| \mathrm{d}x \\
&\le \tilde{L} \Delta t_m \|\boldsymbol{\phi}\|_{L^\infty([0,T)\times\Omega)} \sum_{n=0}^{N-1} \int_\Omega |r^{n+1}| \left| \boldsymbol{Q}^n - \boldsymbol{Q}^{n-1} \right| \mathrm{d}x \\
&\le \tilde{L} \Delta t_m \left(\max_{0 \le n \le N-1} \|r^{n+1}\| \right) \|\boldsymbol{\phi}\|_{L^\infty([0,T)\times\Omega)} \sum_{n=0}^{N-1} \left\| \boldsymbol{Q}^n - \boldsymbol{Q}^{n-1} \right\| \\
&\le \tilde{L} T^{\frac{1}{2}} \Delta t_m^{\frac{1}{2}} \left(\max_{0 \le n \le N-1} \|r^{n+1}\| \right) \|\boldsymbol{\phi}\|_{L^\infty([0,T)\times\Omega)} \left(\sum_{n=0}^{N-1} \left\| \boldsymbol{Q}^n - \boldsymbol{Q}^{n-1} \right\|^2 \right)^{\frac{1}{2}} \\
&\le C \Delta t_m^{\frac{1}{2}} \left(\max_{0 \le n \le N-1} \|r^{n+1}\| \right) \|\boldsymbol{\phi}\|_{L^\infty([0,T)\times\Omega)} \left(\sum_{n=0}^{N-1} \left\| \nabla\boldsymbol{Q}^n - \nabla\boldsymbol{Q}^{n-1} \right\|^2 \right)^{\frac{1}{2}} \to 0.
\end{aligned}
$$

The estimate for K_2 is similar. Specifically, we have

$$
\begin{aligned}
|K_2| &= \left| \int_0^T \int_\Omega r_{\Delta t_m} \left\{ \sum_{n=0}^{N-1} \boldsymbol{P}^{n-1} \chi_{S_n} - \sum_{n=0}^{N-1} \left[\frac{(n+1)\Delta t_m - t}{\Delta t_m} \boldsymbol{P}^{n-1} + \frac{t - n\Delta t_m}{\Delta t_m} \boldsymbol{P}^n \right] \chi_{S_n} \right\} : \boldsymbol{\phi} \, \mathrm{d}x \, \mathrm{d}t \right| \\
&= \left| \int_0^T \int_\Omega r_{\Delta t_m} \sum_{n=0}^{N-1} \left[\frac{t - n\Delta t_m}{\Delta t_m} \big(\boldsymbol{P}^{n-1} - \boldsymbol{P}^n \big) \chi_{S_n} \right] : \boldsymbol{\phi} \, \mathrm{d}x \, \mathrm{d}t \right| \\
&\le C \Delta t_m \|r_{\Delta t_m}\|_{L^\infty([0,T);L^2(\Omega))} \|\boldsymbol{\phi}\|_{L^\infty([0,T)\times\Omega)} \sum_{n=0}^{N-1} \left\| \boldsymbol{Q}^n - \boldsymbol{Q}^{n-1} \right\| \\
&\le C \Delta t_m^{\frac{1}{2}} \|r_{\Delta t_m}\|_{L^\infty([0,T);L^2(\Omega))} \|\boldsymbol{\phi}\|_{L^\infty([0,T)\times\Omega)} \left(\sum_{n=0}^{N-1} \left\| \nabla\boldsymbol{Q}^n - \nabla\boldsymbol{Q}^{n-1} \right\|^2 \right)^{\frac{1}{2}} \to 0.
\end{aligned}
$$

K_3 tends to 0 as well thanks to the strong convergence of $\boldsymbol{P}_{\Delta t_m}$ to $P(\boldsymbol{Q})$, see (4.7), (4.10). The last term K_4 goes to 0 as m tends to infinity by the weak convergence of $r_{\Delta t_m}$ towards r. Thus, $\widetilde{r\boldsymbol{P}}_{\Delta t_m} \rightharpoonup rP(\boldsymbol{Q})$. Using this, we prove $\boldsymbol{H}_{\Delta t_m} \rightharpoonup \boldsymbol{H}$ in $L^2([0,T) \times \Omega)$. Indeed, we have

$$
\begin{aligned}
&\int_0^T \int_\Omega \boldsymbol{H}_{\Delta t_m} : \boldsymbol{\phi} \, \mathrm{d}x \, \mathrm{d}t - \int_0^T \int_\Omega \boldsymbol{H} : \boldsymbol{\phi} \, \mathrm{d}x \, \mathrm{d}t \\
&\quad = - \int_0^T \int_\Omega L(\nabla \boldsymbol{Q}_{\Delta t_m} - \nabla \boldsymbol{Q}) : \nabla \boldsymbol{\phi} - \int_0^T \int_\Omega \Big(\widetilde{r\boldsymbol{P}}_{\Delta t_m} - rP(\boldsymbol{Q}) \Big) : \boldsymbol{\phi} \, \mathrm{d}x \, \mathrm{d}t \to 0, \qquad (4.15)
\end{aligned}
$$

as m tends to infinity since $\nabla \boldsymbol{Q}_{\Delta t_m} \to \boldsymbol{Q}$ in L^2. This shows that $\boldsymbol{H}_{\Delta t_m} \rightharpoonup \boldsymbol{H}$ in $L^2([0,T)\times\Omega)$. Since $\boldsymbol{H}_{\Delta t_m}$ are trace-free and symmetric for every Δt, by Lemma 3.3, it follows that the limit $\boldsymbol{H}$ is also trace-free and symmetric since these are linear properties.

According to (3.2), we can define

$$\boldsymbol{s}_{\Delta t} = \boldsymbol{W}_{\Delta t}\boldsymbol{Q}^*_{\Delta t} - \boldsymbol{Q}^*_{\Delta t}\boldsymbol{W}_{\Delta t} + \xi(\boldsymbol{Q}^*_{\Delta t}\boldsymbol{D}_{\Delta t} + \boldsymbol{D}_{\Delta t}\boldsymbol{Q}^*_{\Delta t}) + \frac{2\xi}{d}\boldsymbol{D}_{\Delta t} - 2\xi(\boldsymbol{D}_{\Delta t} : \boldsymbol{Q}^*_{\Delta t})\left(\boldsymbol{Q}^*_{\Delta t} + \frac{1}{d}\boldsymbol{I}\right),$$

$$\boldsymbol{\Sigma}_{\Delta t} = \boldsymbol{Q}^*_{\Delta t}\boldsymbol{H}_{\Delta t} - \boldsymbol{H}_{\Delta t}\boldsymbol{Q}^*_{\Delta t} - \xi(\boldsymbol{H}_{\Delta t}\boldsymbol{Q}^*_{\Delta t} + \boldsymbol{Q}^*_{\Delta t}\boldsymbol{H}_{\Delta t}) - \frac{2\xi}{d}\boldsymbol{H}_{\Delta t} + 2\xi(\boldsymbol{Q}^*_{\Delta t} : \boldsymbol{H}_{\Delta t})\left(\boldsymbol{Q}^*_{\Delta t} + \frac{1}{d}\boldsymbol{I}\right),$$

where

$$\boldsymbol{D}^*_{\Delta t} = \frac{1}{2}(\nabla \boldsymbol{u}^*_{\Delta t} + \nabla \boldsymbol{u}^{*\intercal}_{\Delta t}), \qquad \boldsymbol{W}^*_{\Delta t} = \frac{1}{2}(\nabla \boldsymbol{u}^*_{\Delta t} - \nabla \boldsymbol{u}^{*\intercal}_{\Delta t}).$$

Taking $\boldsymbol{S} = S(\nabla \boldsymbol{u}, \boldsymbol{Q})$, $\boldsymbol{\Sigma} = \Sigma(\boldsymbol{Q}, \boldsymbol{H})$ and $\boldsymbol{D} = \frac{1}{2}(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^\intercal)$, $\boldsymbol{W} = \frac{1}{2}(\nabla \boldsymbol{u} - \nabla \boldsymbol{u}^\intercal)$, we claim that $\boldsymbol{s}_{\Delta t_m} \rightharpoonup \boldsymbol{S}$ and $\boldsymbol{\Sigma}_{\Delta t_m} \rightharpoonup \boldsymbol{\Sigma}$. Using formula (3.5), we can rewrite $\boldsymbol{s}_{\Delta t_m}$ as

$$\boldsymbol{s}_{\Delta t_m} = S\big(\boldsymbol{u}^*_{\Delta t_m}, \boldsymbol{Q}^*_{\Delta t_m}\big) - \frac{2\xi}{d^2}\,(\nabla \cdot \boldsymbol{u}^*_{\Delta t_m})\boldsymbol{I}.$$

As it is shown in (4.4), (4.11) and (4.12), $\nabla \cdot \boldsymbol{u}^*_{\Delta t_m} \rightharpoonup \nabla \cdot \boldsymbol{u} = 0$, and so we only need to show $S(\boldsymbol{u}^*_{\Delta t_m}, \boldsymbol{Q}^*_{\Delta t_m}) \rightharpoonup \boldsymbol{S}$. The most challenging term to treat within $S(\boldsymbol{u}^*_{\Delta t_m}, \boldsymbol{Q}^*_{\Delta t_m})$ is $(\boldsymbol{D}_{\Delta t_m} : \boldsymbol{Q}^*_{\Delta t_m})\boldsymbol{Q}^*_{\Delta t_m}$. The weak convergence of other terms follows in a similar way. Applying the generalized Hölder's inequality and Sobolev inequality, for any smooth function $\boldsymbol{\varphi}$ with compact support in $[0,T)\times\Omega$, we obtain,

$$\begin{aligned}
&\left|\int_0^T \int_\Omega \big(\boldsymbol{D}_{\Delta t_m} : \boldsymbol{Q}^*_{\Delta t_m}\big)\,\boldsymbol{Q}^*_{\Delta t_m} : \boldsymbol{\varphi}\,\mathrm{d}x\,\mathrm{d}t - \int_0^T \int_\Omega (\boldsymbol{D} : \boldsymbol{Q})\,\boldsymbol{Q} : \boldsymbol{\varphi}\,\mathrm{d}x\,\mathrm{d}t\right| \\
&\quad = \left|\int_0^T \int_\Omega \big(\boldsymbol{D}_{\Delta t_m} : \boldsymbol{Q}^*_{\Delta t_m}\big)\,\big(\boldsymbol{Q}^*_{\Delta t_m} - \boldsymbol{Q}\big) : \boldsymbol{\varphi}\,\mathrm{d}x\,\mathrm{d}t + \int_0^T \int_\Omega \big(\boldsymbol{D}_{\Delta t_m} : \big(\boldsymbol{Q}^*_{\Delta t_m} - \boldsymbol{Q}\big)\big)\,\boldsymbol{Q} : \boldsymbol{\varphi}\,\mathrm{d}x\,\mathrm{d}t \right.\\
&\qquad \left. + \int_0^T \int_\Omega ((\boldsymbol{D}_{\Delta t_m} - \boldsymbol{D}) : \boldsymbol{Q})\,\boldsymbol{Q} : \boldsymbol{\varphi}\,\mathrm{d}x\,\mathrm{d}t\right| \\
&\quad \le C\|\boldsymbol{\varphi}\|_{L^\infty([0,T)\times\Omega)}\|\boldsymbol{D}_{\Delta t_m}\|_{L^2([0,T)\times\Omega)}\big\|\boldsymbol{Q}^*_{\Delta t_m}\big\|_{L^\infty(0,T;L^4)}\big\|\boldsymbol{Q}^*_{\Delta t_m} - \boldsymbol{Q}\big\|_{L^2([0,T);L^4)} \\
&\qquad + C\|\boldsymbol{\varphi}\|_{L^\infty([0,T)\times\Omega)}\|\boldsymbol{D}_{\Delta t_m}\|_{L^2([0,T)\times\Omega)}\|\boldsymbol{Q}\|_{L^\infty([0,T);L^4)}\big\|\boldsymbol{Q}^*_{\Delta t_m} - \boldsymbol{Q}\big\|_{L^2([0,T);L^4)} \\
&\qquad + \left|\int_0^T \int_\Omega ((\boldsymbol{D}_{\Delta t_m} - \boldsymbol{D}) : \boldsymbol{Q})\,\boldsymbol{Q} : \boldsymbol{\varphi}\,\mathrm{d}x\,\mathrm{d}t\right| \\
&\quad \le C\Big(\big\|\boldsymbol{Q}^*_{\Delta t_m}\big\|_{L^\infty(0,T;H^1)} + \|\boldsymbol{Q}\|_{L^\infty(0,T;H^1)}\Big)\big\|\boldsymbol{Q}^*_{\Delta t_m} - \boldsymbol{Q}\big\|_{L^2(0,T;H^1)} \\
&\qquad + \left|\int_0^T \int_\Omega ((\boldsymbol{D}_{\Delta t_m} - \boldsymbol{D}) : \boldsymbol{Q})\,\boldsymbol{Q} : \boldsymbol{\varphi}\,\mathrm{d}x\,\mathrm{d}t\right|.
\end{aligned} \tag{4.16}$$

As m tends to infinity, the first term goes to 0 since $\boldsymbol{Q}^*_{\Delta t_m} \to \boldsymbol{Q}$ in $L^2(0,T;H^1)$. While the second term tends to 0 because $\boldsymbol{D}^*_{\Delta t_m} \rightharpoonup \boldsymbol{D}$ in L^2, and $(\boldsymbol{Q} : \boldsymbol{\varphi})\boldsymbol{Q} \in L^2([0,T)\times\Omega)$.

To show $\boldsymbol{\Sigma}_{\Delta t_m} \rightharpoonup \Sigma$ in $L^2([0,T)\times\Omega)$ is similar, therefore, we will only present the treatment of the most challenging term within $\boldsymbol{\Sigma}_{\Delta t_m}$, which is $(\boldsymbol{Q}^*_{\Delta t_m} : \boldsymbol{H}_{\Delta t_m})\boldsymbol{Q}^*_{\Delta t_m}$. For any smooth function $\boldsymbol{\varphi}$ with compact support in $[0,T)\times\Omega$, we have

$$\begin{aligned}
&\left|\int_0^T\int_\Omega \left(\boldsymbol{Q}^*_{\Delta t_m}:\boldsymbol{H}_{\Delta t_m}\right)\boldsymbol{Q}^*_{\Delta t_m}:\boldsymbol{\varphi}\,\mathrm{d}x\,\mathrm{d}t-\int_0^T\int_\Omega(\boldsymbol{Q}:\boldsymbol{H})\boldsymbol{Q}:\boldsymbol{\varphi}\,\mathrm{d}x\,\mathrm{d}t\right|\\
&\quad=\left|\int_0^T\int_\Omega\left(\boldsymbol{Q}^*_{\Delta t_m}:\boldsymbol{H}_{\Delta t_m}\right)\left(\boldsymbol{Q}^*_{\Delta t_m}-\boldsymbol{Q}\right):\boldsymbol{\varphi}\,\mathrm{d}x\,\mathrm{d}t+\int_0^T\int_\Omega\left(\left(\boldsymbol{Q}^*_{\Delta t_m}-\boldsymbol{Q}\right):\boldsymbol{H}_{\Delta t_m}\right)\boldsymbol{Q}:\boldsymbol{\varphi}\,\mathrm{d}x\,\mathrm{d}t\right.\\
&\qquad\left.+\int_0^T\int_\Omega\left(\boldsymbol{Q}:\left(\boldsymbol{H}_{\Delta t_m}-\boldsymbol{H}\right)\right)\boldsymbol{Q}:\boldsymbol{\varphi}\,\mathrm{d}x\,\mathrm{d}t\right|\\
&\quad\le C\|\boldsymbol{\varphi}\|_{L^\infty([0,T)\times\Omega)}\left(\left\|\boldsymbol{Q}^*_{\Delta t_m}\right\|_{L^\infty(0,T;L^4)}+\|\boldsymbol{Q}\|_{L^\infty(0,T;L^4)}\right)\|\boldsymbol{H}_{\Delta t_m}\|_{L^2([0,T)\times\Omega)}\\
&\qquad\times\left\|\boldsymbol{Q}^*_{\Delta t_m}-\boldsymbol{Q}\right\|_{L^2(0,T;L^4)}+\left|\int_0^T\int_\Omega\left(\boldsymbol{Q}:\left(\boldsymbol{H}_{\Delta t_m}-\boldsymbol{H}\right)\right)\boldsymbol{Q}:\boldsymbol{\varphi}\,\mathrm{d}x\,\mathrm{d}t\right|\\
&\quad\le C\left\|\boldsymbol{Q}^*_{\Delta t_m}-\boldsymbol{Q}\right\|_{L^2(0,T;H^1)}+\left|\int_0^T\int_\Omega\left(\boldsymbol{Q}:\left(\boldsymbol{H}_{\Delta t_m}-\boldsymbol{H}\right)\right)\boldsymbol{Q}:\boldsymbol{\varphi}\,\mathrm{d}x\,\mathrm{d}t\right|.
\end{aligned}\tag{4.17}$$

As m tends to infinity, the first term goes to 0 since $\boldsymbol{Q}^*_{\Delta t_m}\to\boldsymbol{Q}$ in $L^2(0,T;H^1)$. The second term tends to 0 because $\boldsymbol{H}_{\Delta t_m}\rightharpoonup\boldsymbol{H}$ in $L^2([0,T)\times\Omega)$, and $(\boldsymbol{Q}:\boldsymbol{\varphi})\boldsymbol{Q}\in L^2([0,T)\times\Omega)$.

Step 5: Passing the limit. Using the results from the previous steps, we can pass to the limit in most terms in weak formulation (3.1a), and (3.1b) after integrating over $[0,T)$. The convergence of the terms in the equation for $r_{\Delta t}$ follows by combining the weak convergence of $\partial_t\boldsymbol{Q}_{\Delta t}$ with the Lipschitz continuity of P and the strong convergence of $\boldsymbol{Q}_{\Delta t}$ in $L^2([0,T]\times\Omega)$ (see also [20] for details). The only two remaining terms remaining are $\int_0^T\int_\Omega\boldsymbol{H}_{\Delta t_m}\nabla\boldsymbol{Q}^*_{\Delta t_m}\cdot\boldsymbol{\psi}\,\mathrm{d}x\,\mathrm{d}t$ and $\int_0^T\int_\Omega(\boldsymbol{u}^*_{\Delta t_m}\cdot\nabla\boldsymbol{Q}^*_{\Delta t_m}):\boldsymbol{\varphi}\,\mathrm{d}x\,\mathrm{d}t$. Combining weak and strong convergence as in Step 4, it follows that

$$\begin{aligned}
\int_0^T\int_\Omega\boldsymbol{H}_{\Delta t_m}\nabla\boldsymbol{Q}^*_{\Delta t_m}\cdot\boldsymbol{\psi}\,\mathrm{d}x\,\mathrm{d}t&\rightharpoonup\int_0^T\int_\Omega\boldsymbol{H}\nabla\boldsymbol{Q}\cdot\boldsymbol{\psi}\,\mathrm{d}x\,\mathrm{d}t,\\
\int_0^T\int_\Omega\left(\boldsymbol{u}^*_{\Delta t_m}\cdot\nabla\boldsymbol{Q}^*_{\Delta t_m}\right):\boldsymbol{\varphi}\,\mathrm{d}x\,\mathrm{d}t&\rightharpoonup\int_0^T\int_\Omega(\boldsymbol{u}\cdot\nabla\boldsymbol{Q}):\boldsymbol{\varphi}\,\mathrm{d}x\,\mathrm{d}t.
\end{aligned}\tag{4.18}$$

This shows that $(\boldsymbol{u},\boldsymbol{Q},\boldsymbol{H},r)$ is a weak solution satisfying Definition 2.5. □

In order to conclude, we need to show that the reformulated system (1.10a)–(1.10e) and the original hydrodynamics system (1.1a)–(1.1c) are equivalent in the weak sense. This follows from the following lemma that was proved in Lemma 5.2 of [20]:

Lemma 4.2. *Assume that* $(\boldsymbol{u},\boldsymbol{Q},\boldsymbol{H},r)$ *is a weak solution in the sense of Definition 2.5. Then for any smooth function* ϕ *with compact support in* $(0,T)\times\Omega$ *(compactly supported in both time and space), we have*

$$\int_0^T\int_\Omega r\phi\,\mathrm{d}x\,\mathrm{d}t=\int_0^T\int_\Omega r(\boldsymbol{Q})\phi\,\mathrm{d}x\,\mathrm{d}t\tag{4.19}$$

where $r(\boldsymbol{Q})$ *is defined in* (1.8).

Proof. We only provide a sketch of the proof here since this result follows in a similar way as in Lemma 5.2 of [20]. Firstly, in Corollary 3.11, we have shown that $\partial_t r_{\Delta t}\in L^2(0,T;L^1(\Omega))$, uniformly in Δt, from which it follows that the weak limit r satisfies the same regularity estimate. Thus, it follows from Lemma 1.1, p. 250 of [38] that r is absolutely continuous in time with values in $L^1(\Omega)$. Moreover, from the *a priori* estimates, we have that the limit $\boldsymbol{Q} \in L^2(0,T;H^2(\Omega))$ which implies that $\boldsymbol{Q} \in L^2(0,T;L^\infty(\Omega))$ (and also $\boldsymbol{Q} \in L^\infty(0,T;H^1)$ which implies $\boldsymbol{Q} \in L^\infty(0,T;L^6(\Omega))$). With the Lipschitz continuity of $P(\boldsymbol{Q})$, this implies that $P(\boldsymbol{Q}) \in L^2(0,T;L^\infty(\Omega))$ (and $P(\boldsymbol{Q}) \in L^\infty(0,T;L^6(\Omega))$). Combining this with $\boldsymbol{Q}_t \in L^2(0,T;L^{6/5}(\Omega))$ from Lemma 3.10, we obtain that the product $P(\boldsymbol{Q}) : \boldsymbol{Q}_t \in L^1([0,T]\times\Omega)$ (or better) as in Lemma 5.2 of [20]. Thus, the rest of the proof follows in the same way as in Lemma 5.2 of [20]. □

Remark 4.3. For a similar reason as Remark 2.6, it is also valid to choose L^2 functions as test functions in (4.19) since r is bounded in L^2.

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References

[1] H. Abels, G. Dolzmann and Y. Liu, Well-posedness of a fully coupled Navier–Stokes/Q-tensor system with inhomogeneous boundary data. *SIAM J. Math. Anal.* **46** (2014) 3050–3077.

[2] H. Abels, G. Dolzmann and Y. Liu, Strong solutions for the Beris-Edwards model for nematic liquid crystals with homogeneous Dirichlet boundary conditions. *Adv. Differ. Equ.* **21** (2016) 109–152.

[3] D. Andrienko, Introduction to liquid crystals. *J. Mol. Liq.* **267** (2018) 520–541. Special Issue Dedicated to the Memory of Professor Y. Reznikov.

[4] I. Bajc, F. Hecht and S. Zumer, A mesh adaptivity scheme on the Landau–de Gennes functional minimization case in 3D, and its driving efficiency. *J. Comput. Phys.* **321** (2016) 981–996.

[5] J.M. Ball, Mathematics and liquid crystals. *Mol. Cryst. Liq. Cryst.* **647** (2017) 1–27.

[6] S. Bartels and A. Raisch, Simulation of Q-tensor fields with constant orientational order parameter in the theory of uniaxial nematic liquid crystals, in Singular Phenomena and Scaling in Mathematical Models. Springer International Publishing, Cham (2013) 383–412.

[7] A. Beris and B. Edwards, Thermodynamics of Flowing Systems: With Internal Microstructure. *Oxford Engineering Science Series.* Oxford University Press (1994).

[8] J.P. Borthagaray, R.H. Nochetto and S.W. Walker, A structure-preserving FEM for the uniaxially constrained Q-tensor model of nematic liquid crystals. *Numer. Math.* **145** (2020) 837–881.

[9] F. Boyer and P. Fabrie, Mathematical Tools for the Study of the Incompressible Navier–Stokes Equations and Related Models. Vol. 183. Springer Science & Business Media (2012).

[10] C. Cavaterra, E. Rocca, H. Wu and X. Xu, Global strong solutions of the full Navier–Stokes and Q-tensor system for nematic liquid crystal flows in two dimensions. *SIAM J. Math. Anal.* **48** (2016) 1368–1399.

[11] A.J. Chorin, The numerical solution of the Navier–Stokes equations for an incompressible fluid. *Bull. Am. Math. Soc.* **73** (1967) 928–931.

[12] P. Constantin and C. Foias, Navier–Stokes Equations. University of Chicago Press, Chicago (2022).

[13] K.R. Daly, G. D'Alessandro and M. Kaczmarek, An efficient $\mathcal{Q}$-tensor-based algorithm for liquid crystal alignment away from defects. *SIAM J. Appl. Math.* **70** (2010) 2844–2860.

[14] T.A. Davis and E.C. Gartland, Finite element analysis of the Landau–de Gennes minimization problem for liquid crystals. *SIAM J. Numer. Anal.* **35** (1998) 336–362.

[15] P. de Gennes and J. Prost, The Physics of Liquid Crystals. *International Series of Monographs on Physics*. Clarendon Press, Oxford (1993).

[16] J.L. Ericksen, Hydrostatic theory of liquid crystals. *Arch. Ration. Mech. Anal.* **9** (1962) 371–378.

[17] L.C. Evans, Partial Differential Equations. American Mathematical Society, Providence, RI (2010).

[18] G.B. Folland, Real Analysis: Modern Techniques and Their Applications. Wiley, New York (1984).

[19] P. Grisvard, Elliptic Problems in Nonsmooth Domains. Society for Industrial and Applied Mathematics (2011).

[20] V.M. Gudibanda, F. Weber and Y. Yue, Convergence analysis of a fully discrete energy-stable numerical scheme for the Q-tensor flow of liquid crystals. *SIAM J. Numer. Anal.* **60** (2022) 2150–2181.

[21] F. Guillén-González and M. Ángeles Rodríguez-Bellido, Weak time regularity and uniqueness for a Q-tensor model. *SIAM J. Math. Anal.* **46** (2014) 3540–3567.

[22] F. Guillén-González and M.Á. Rodríguez-Bellido, Weak solutions for an initial–boundary Q-tensor problem related to liquid crystals. *Nonlinear Anal. Theory Methods App.* **112** (2015) 84–104.

[23] F. Guillén-González and G. Tierra, On linear schemes for a Cahn–Hilliard diffuse interface model. *J. Comput. Phys.* **234** (2013) 140–171.

[24] C. Jiang, W. Cai and Y. Wang, A linearly implicit and local energy-preserving scheme for the sine-Gordon equation based on the invariant energy quadratization approach. *J. Sci. Comput.* **80** (2019) 1629–1655.

[25] F.M. Leslie, Some constitutive equations for anisotropic fluids. *Q. J. Mech. Appl. Math.* **19** (1966) 357–370.

[26] F.M. Leslie, Some constitutive equations for liquid crystals. *Arch. Ration. Mech. Anal.* **28** (1968) 265–283.

[27] F. Lin and C. Liu, Static and dynamic theories of liquid crystals. *J. Part. Differ. Equ.* **14** (2001) 289–330.

[28] C.S. MacDonald, J.A. Mackenzie, A. Ramage and C.J.P. Newton, Efficient moving mesh methods for Q-tensor models of nematic liquid crystals. *SIAM J. Sci. Comput.* **37** (2015) B215–B238.

[29] A. Majumdar, Equilibrium order parameters of nematic liquid crystals in the Landau–de Gennes theory. *Eur. J. Appl. Math.* **21** (2010) 181–203.

[30] A. Majumdar and A. Zarnescu, Landau–de Gennes theory of nematic liquid crystals: the Oseen–Frank limit and beyond. *Arch. Ration. Mech. Anal.* **196** (2010) 227–280.

[31] R.H. Nochetto and J.-H. Pyo, The Gauge–Uzawa finite element method. Part I: the Navier–Stokes equations. *SIAM J. Numer. Anal.* **43** (2005) 1043–1068.

[32] M. Paicu and A. Zarnescu, Global existence and regularity for the full coupled Navier–Stokes and Q-tensor system. *SIAM J. Math. Anal.* **43** (2011) 2009–2049.

[33] M. Paicu and A. Zarnescu, Energy dissipation and regularity for a coupled Navier–Stokes and Q-tensor system. *Arch. Rat. Mech. Anal.* **203** (2012) 45–67.

[34] J. Shen, On error estimates of projection methods for Navier–Stokes equations: first-order schemes. *SIAM J. Numer. Anal.* **29** (1992) 57–77.

[35] J. Simon, Compact sets in the space $L_p(0,T;B)$. *Ann. Mat. App.* **146** (1986) 65–96.

[36] A.M. Sonnet and E. Virga, Dissipative Ordered Fluids, Theories for Liquid Crystals. Springer US (2012).

[37] M.J. Stephen and J.P. Straley, Physics of liquid crystals. *Rev. Mod. Phys.* **46** (1974) 617–704.

[38] R. Temam and A. Chorin, Navier–Stokes Equations: Theory and Numerical Analysis. Vol. 45. (1978).

[39] X. Yang and L. Ju, Efficient linear schemes with unconditional energy stability for the phase field elastic bending energy model. *Comput. Methods Appl. Mech. Eng.* **315** (2017) 691–712.

[40] X. Yang and J. Zhao, On linear and unconditionally energy stable algorithms for variable mobility Cahn–Hilliard type equation with logarithmic Flory–Huggins potential. *Commun. Comput. Phys.* **25** (2018) 703–728.

[41] X. Yang, J. Zhao and Q. Wang, Numerical approximations for the molecular beam epitaxial growth model based on the invariant energy quadratization method. *J. Comput. Phys.* **333** (2017) 104–127.

[42] X. Yang, J. Zhao and X. He, Linear, second order and unconditionally energy stable schemes for the viscous Cahn–Hilliard equation with hyperbolic relaxation using the invariant energy quadratization method. *J. Comput. Appl. Math.* **343** (2018) 80–97.

[43] J. Zhao and Q. Wang, Semi-discrete energy-stable schemes for a tensor-based hydrodynamic model of nematic liquid crystal flows. *J. Sci. Comput.* **68** (2016) 1241–1266.

[44] J. Zhao, X. Yang, Y. Gong and Q. Wang, A novel linear second order unconditionally energy stable scheme for a hydrodynamic Q-tensor model of liquid crystals. *Comput. Methods Appl. Mech. Eng.* **318** (2017) 803–825.