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A Second Order Accurate in Time, Energy Stable Finite Element Scheme for a Liquid Thin Film Coarsening Model

Maoqin Yuan¹, Lixiu Dong^{2,*} and Juan Zhang³

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Abstract. In this paper, we propose and analyze a second order accurate (in time) mass lumped mixed finite element numerical scheme for the liquid thin film coarsening model with a singular Leonard-Jones energy potential. The backward differentiation formula (BDF) stencil is applied in the temporal discretization, and a convex-concave decomposition is derived, so that the concave part corresponds to a quadratic energy. In turn, the Leonard-Jones potential term is treated implicitly and the concave part is approximated by a second order Adams-Bashforth explicit extrapolation. An artificial Douglas-Dupont regularization term is added to ensure the energy stability. Furthermore, we provide a theoretical justification that this numerical algorithm has a unique solution, such that the positivity property is always preserved for the phase variable at a point-wise level, so that a singularity is avoided in the scheme. In fact, the singular nature of the Leonard-Jones potential term around the value of 0 and the mass lumped FEM approach play an essential role in the positivity-preserving property in the discrete level. In addition, an optimal rate convergence estimate in the $\ell^{\infty}(0,T;H_h^{-1})\cap\ell^2(0,T;H_h^1)$ norm is presented. Finally, two numerical experiments are carried out to verify the theoretical properties.

AMS subject classifications: 60F10, 60J75, 62P10, 92C37

Key words: Liquid thin film model, second order accuracy, mass lumped mixed FEM, positivity preserving, energy stability, optimal rate convergence analysis.

*Corresponding author. *Email addresses*: (L. Dong), jzhang@lut.edu.cn (J. Zhang)

 $\verb"mqyuan@cupk.edu.cn" (M. Yuan), lxdong@bnu.edu.cn"$

¹ Department of Mathematics, School of Science and Art, China University of Petroleum-Beijing at Karamay, Karamay 834000, P.R.China

Department of Mathematics, Faculty of Arts and Sciences, Beijing Normal University, Zhuhai 519087, P.R. China
 School of Sciences, Lanzhou University of Technology, Lanzhou 730050, P.R. China

1. Introduction

Certain liquids on a solid, chemo-attractive substrate spontaneously form a droplet structure connected by a very thin precursor (or wetting) layer. After the droplets appear, coarsening will occur, whereby smaller droplets will shrink and larger droplets will grow. The coarsening behavior, especially the rate of coarsening, of droplets has been of great scientific interest [38]. The average droplet size increases with the decrease of the number of droplets and the increase of the characteristic distance. The droplet coarsening model with a singular Lennard-Jones energy potential involved mainly describes the coarsening phenomenon of droplets. The related content of liquid thin film coarsening phenomenon and some numerical simulation results can be found in [7,8,14,20,24,30].

Under the assumption that the liquid film does not evaporates, lubrication theory leads to a single equation for the height function, $\phi = \phi(\mathbf{x}, t) > 0$, of a time-dependent film [20], in the form of an H^{-1} gradient flow

$$\partial_t \phi = \nabla \cdot (\mathcal{M}(\phi) \nabla \delta_\phi F).$$

Here F is the free energy of the film/substrate system and is given by

$$F(\phi) = \int_{\Omega} \left(\mathcal{U}(\phi) + \frac{\varepsilon^2}{2} |\nabla \phi|^2 \right) d\mathbf{x}, \tag{1.1}$$

where $\phi:\Omega\to\mathbb{R}$ is a periodic height function, $\varepsilon>0$ is the surface diffusion coefficient, and

$$\mathcal{U}(\phi) = \frac{1}{3}\phi^{-8} - \frac{4}{3}\phi^{-2}$$

is the well-known Lennard-Jones-type potential [12]. The H^{-1} gradient flow associated with the given free energy functional (1.1) with constant mobility $\mathcal{M}(\phi) \equiv 1$ (non-constant mobility case could be handled in a similar way) is

$$\partial_t \phi = \Delta \mu, \quad \mu := \delta_\phi F = -\frac{8}{3} (\phi^{-9} - \phi^{-3}) - \varepsilon^2 \Delta \phi. \tag{1.2}$$

Obviously, this problem is mass conservation. Due to the gradient structure, the following energy dissipation law is formally available:

$$\frac{d}{dt}F(\phi(t)) = -\int_{\Omega} |\nabla \mu|^2 d\mathbf{x} \le 0.$$

In addition, from the mathematical expression, the structure of the potential function requires that the phase variable has to maintain a fixed sign, that is, being either positive or negative, to avoid a singularity. A positivity-preserving structure is required for the numerical scheme and for physical reality [38]. For simplicity of presentation, we assume periodic boundary conditions hold over the rectangular domain Ω . Other types of boundary conditions, such as homogeneous Neumann, can also be handled.

There are various time discretization methods for gradient flows to ensure energy stability. For example, convex splitting method proposed in [6], stabilization method [31], exponential time differencing approach in [29], invariant energy quadratization method proposed in [33], scalar auxiliary variable approach proposed in [15] and Lagrange multiplier approaches. Recently, by introducing a supplementary variable to reformulate the original problem into a constrained optimization problem, Hong *et al.* [9] proposed a novel energy-stable scheme which satisfies the original energy dissipation.

However, the positivity-preserving property of numerical solutions is very important for gradient flows with singular energy functionals. Chen et al. [2] presented a positivity-preserving theoretical framework for the convex splitting method. In detail, it transforms numerical scheme into Euler-Lagrange equation of a convex discrete functional, thereby transforming the computation of numerical scheme into the problem of finding the minimum value of a convex discrete functional. Then the positivitypreserving property of the numerical solution can be obtained by utilizing the singularity of the energy functional. In recent years, based on above framework for convex splitting method, there are many works to analyze the positivity of numerical solutions by finite difference method for gradient flows with singular energy potential. See the related works for the MMC-TDGL equation [5], ternary MMC system [4], binary fluidsurfactant system [23], Poisson-Nernst-Planck (PNP) system [17], and droplet liquid film model [38], etc. Here, we would like to extend the theoretical framework of positivity preserving scheme to the fully discrete finite element scheme for a droplet liquid film model. Based on the finite element approximations in space, Karthik et al. [13] have adopted a robust staggered algorithm to solve a phase field fracture model. The standard mixed FEM leads to a theoretical difficulty to justify the positivity-preserving property because of the non-diagonal mass matrix. To overcome this subtle difficulty, we apply a mass lumped FEM instead, which is a modification of standard FEM and the diagonal elements are the row sums of the original mass matrix [26]. There are also a few works using the mass lumped FEM to justify the positivity-preserving property for gradient flows with logarithmic singularity potential [18,34]. At present, most high-order schemes in temporal discretization have been constructed for polynomial phase-field gradient flows without singularity, such as extrapolated Runge-Kutta with scalar auxiliary variable (RK-SAV) method in time [1, 25, 27, 28], exponential scalar auxiliary variable approaches with relaxation (RE-SAV) method [11, 19] or the k-th backward differentiation formula (BDFk) method [3, 16].

In [22], the author proposed and analyzed a finite element approximation of the relaxed Cahn-Hilliard equation with singular single-well potential of Lennard-Jones type and degenerate mobility that is energy stable and nonnegativity preserving. Recently, Zhang *et al.* [36, 37] analyzed two linear and efficiency schemes by using the (S)SAV approach to solve the liquid thin film coarsening model. However, the SAV method incorporates nonlinear energy functionals into the scalar auxiliary variable, making it difficult to theoretically obtain the positivity-preserving property of numerical solution. Furthermore, the coarsening dynamics problem usually is a long time process.

To improve the computational efficiency, some adaptive time stepping strategies has also become a popular issue for a class of PDEs which is relatively more difficult than the uniform temporal mesh in theoretical analysis. There are also some works on the variable-steps BDF2 schemes combining SAV method [10, 11] or convex splitting method [18]. Recently, comparing to the preconditional gradient descent method, Park *et al.* [21] also proposed a preconditioned Nesterov's accelerated gradient descentfast solver for the phase field crystal and functionalized Cahn-Hilliard equations.

In this paper, we propose and analyze a second order accurate in time mass lumped mixed finite element numerical scheme for a droplet liquid coarsening model for singular energy functional with negative powers, which is a fourth-order partial differential system. Compared with the finite difference method, the finite element method has more flexible mesh, so we consider the finite element method in the spatial discretization. In more details, the BDF2 stencil is applied in the temporal discretization, and a convex-concave decomposition is formulated so that the concave part corresponds to a quadratic energy. The combined Leonard-Jones potential term is treated implicitly, and the concave part is approximated by a second order Adams-Bashforth explicit extrapolation. An artificial Douglas-Dupont regularization term is added to ensure the energy stability. Furthermore, the unique solvability and the positivity-preserving property for the second order scheme is established, in which the singular nature of the Leonard-Jones potential term around the value of 0 and the mass lumped approach play an essential role in the positivity-preserving property. In addition, an optimal rate convergence estimate in the $\ell^\infty(0,T;H_h^{-1})\cap\ell^2(0,T;H_h^1)$ norm is presented, in which the convexity property of the nonlinear potential term and the surface diffusion term play an important role.

The rest of the paper is organized as follows. In Section 2, the mass lumped method and the fully discrete BDF2 scheme is proposed. In Section 3, the unique solvability and positivity-preserving property for the proposed scheme is derived. Then the modified energy dissipation laws will be obtained in Section 4. In Section 5, the optimal rate convergence analysis is provided. The numerical simulation results are presented in Section 6. Finally, some concluding remarks are given in Section 7.

2. Preliminary and the fully discrete numerical scheme

In this section, we present some definitions and lemmas which will be utilized next, and the fully discrete scheme based on the mass lumped FEM for the droplet liquid thin film coarsening equation is proposed.

2.1. The mass lumped finite element method

Let \mathcal{T}_h be a shape-regular triangulation of Ω , with mesh size h, denote h_e the diameter of each triangle $e \in \mathcal{T}_h$ and \triangle_e the area of e. Note that the element is shape regular, we can assume that h_e^2/\triangle_e is uniformly bounded by one constant $C_{\mathcal{T}}: h_e^2/\triangle_e \leq C_{\mathcal{T}}$. Based on the quasi-uniform triangulated mesh \mathcal{T}_h , the finite element space is defined

as

$$\begin{split} S_h &:= \left\{ v \in H^1_{per}(\Omega) \mid \ v \text{ is piecewise linear on each } e \in \mathcal{T}_h \right\} \\ &= \operatorname{span} \left\{ \chi_j \mid j = 1, \dots, N_p \right\}, \end{split}$$

where $\chi_j \in S_h$ is the *j*-th Lagrange nodal basis function, which has the property $\chi_j(P_i) = \delta_{ij}$. Define

$$\overset{\circ}{S}_h := S_h \cap L_0^2(\Omega),$$

where

$$L_0^2(\Omega) = \{ v \in L^2(\Omega) \mid (v, 1) = 0 \}$$

is the function space with the zero mean in $L^2(\Omega)$.

The mass lumped FEM can simplify the computation for the inverse of mass matrix and overcome the shortage of the standard FEM (2.2) that can not preserve the maximum principle for homogeneous parabolic equations. In more details, let $P_{e,k}$ (k=1,2,3) be the three vertices of triangle. The generation of the mass lumped matrix can be regarded as introducing the following quadrature formula:

$$Q_h(f) = \sum_{e \in \mathcal{T}_h} Q_e(f), \quad \forall f \in C(\Omega; \mathbb{R}),$$

where

$$Q_e(f) = \frac{\triangle_e}{3} \sum_{k=1}^3 f(P_{e,k}) \approx \int_e f d\mathbf{x}.$$

By the above quadrature formula, it is easy to derive $Q_h(\chi_j \chi_k) = 0$ for $k \neq j$, so that

$$Q_h(\chi_j \chi_k) = \delta_{jk} Q_h(\chi_j^2), \quad j, k = 1, \dots, N_p.$$

It is obvious that

$$Q_h(\chi_j^2) = \sum_{e \in \mathcal{T}_h} Q_e(\chi_j^2) = \frac{1}{3} \operatorname{area}(D_j), \quad D_j := \operatorname{supp}(\chi_j).$$

We define an approximation of the canonical inner product on S_h by

$$(\psi, \eta)_Q := Q_h(\psi \eta), \quad \forall \psi, \eta \in S_h. \tag{2.1}$$

We define $\|\eta\|_Q := \sqrt{(\eta, \eta)_Q}$ for any $\eta \in S_h$. This norm is observed to be equivalent to the standard $\|\cdot\|_{L^2}$ norm by considering each triangle separately.

To facilitate the analysis below, we have to modify the definition of the discrete Laplacian operator and the discrete H^{-1} norm. In fact, the primary difference is in the integral definition.

Definition 2.1. The discrete Laplacian operator $\Delta_h: S_h \to \overset{\circ}{S}_h$ is defined as follows: For any $v_h \in S_h$, $\Delta_h v_h \in \overset{\circ}{S}_h$ denote the unique solution to the problem

$$(\Delta_h v_h, \chi)_Q = -(\nabla v_h, \nabla \chi), \quad \forall \chi \in S_h.$$

It is straightforward to show that by restricting the domain, $\Delta_h: \overset{\circ}{S}_h \to \overset{\circ}{S}_h$ is invertible, and for any $v_h \in \overset{\circ}{S}_h$, we have

$$(\nabla (-\Delta_h)^{-1} v_h, \nabla \chi) = (v_h, \chi)_O, \quad \forall \chi \in S_h.$$

Definition 2.2. The discrete H^{-1} norm $\|\cdot\|_{-1,Q}$, is defined as follows:

$$||v_h||_{-1,Q} := \sqrt{\left(v_h, (-\Delta_h)^{-1}v_h\right)_Q}, \quad \forall v_h \in \overset{\circ}{S}_h.$$

2.2. The fully discrete numerical scheme

We recall a convex-concave decomposition of the energy (1.1). The detailed proof of the following preliminary and lemma results could be found in the work [38].

Lemma 2.1. For x > 0, the function

$$f(x) = \frac{1}{3}x^{-8} - \frac{4}{3}x^{-2} + \frac{4}{3}A_0x^2$$

is convex, provided that

$$A_0 \ge A_0^* := \frac{9}{5} \left(\frac{2}{15}\right)^{\frac{2}{3}}.$$

As a result, we obtain the following decomposition of $F(\phi)$:

$$F(\phi) = F_c(\phi) - F_e(\phi),$$

where

$$F_c(\phi) = \int_{\Omega} \left(\frac{1}{3} \phi^{-8} - \frac{4}{3} \phi^{-2} + \frac{4}{3} A_0 \phi^2 + \frac{\varepsilon^2}{2} |\nabla \phi|^2 \right) d\mathbf{x}, \quad F_e(\phi) = \int_{\Omega} \frac{4}{3} A_0 \phi^2 d\mathbf{x},$$

and

$$g(\phi) := -\frac{8}{3}(\phi^{-9} - \phi^{-3}) + \frac{8}{3}A_0\phi, \quad \delta_{\phi}F_c = g(\phi) - \varepsilon^2\Delta\phi, \quad \delta_{\phi}F_e = \frac{8}{3}A_0\phi.$$

The mixed weak formulation of the droplet liquid film equation (1.2) is to find $(\phi, \mu) \in L^2(0, T; H^1_{per}(\Omega))$, with $\phi_t \in L^2(0, T; H^{-1}_{per}(\Omega))$, satisfying

$$\begin{cases} (\phi_t, v) + (\nabla \mu, \nabla v) = 0, & \forall v \in H^1_{per}(\Omega), \\ (\mu, w) = \left(g(\phi) - \frac{8}{3}A_0\phi, w\right) + \varepsilon^2(\nabla \phi, \nabla w), & \forall w \in H^1_{per}(\Omega) \end{cases}$$
(2.2)

for almost every $t \in [0, T]$.

Using the idea of the convex splitting and the mass lumped FEM, we consider the following semi-implicit, fully discrete scheme: For $n \geq 1$, given $\phi_h^n, \phi_h^{n-1} \in S_h$, find $\phi_h^{n+1}, \mu_h^{n+1} \in S_h$, such that

$$\begin{cases}
\left(\frac{3\phi_{h}^{n+1} - 4\phi_{h}^{n} + \phi_{h}^{n-1}}{2\tau}, v_{h}\right)_{Q} + \left(\nabla\mu_{h}^{n+1}, \nabla v_{h}\right) = 0, & \forall v_{h} \in S_{h}, \\
\left(\mu_{h}^{n+1}, w_{h}\right)_{Q} = \left(g(\phi_{h}^{n+1}) - \frac{8}{3}A_{0}\check{\phi}_{h}^{n+1}, w_{h}\right)_{Q} + \varepsilon^{2}(\nabla\phi_{h}^{n+1}, \nabla w_{h}) \\
+ A\tau\left(\nabla(\phi_{h}^{n+1} - \phi_{h}^{n}), \nabla w_{h}\right), & \forall w_{h} \in S_{h},
\end{cases}$$
(2.3)

where $\check{\phi}_h^{n+1}:=2\phi_h^n-\phi_h^{n-1}$ and $A\geq 0$ is a stabilization parameter to be determined. The initialization step comes from the first-order convex splitting method and the mass lumped FEM, as follows:

$$\begin{cases}
\left(\frac{\phi_h^1 - \phi_h^0}{\tau}, v_h\right)_Q + \left(\nabla \mu_h^1, \nabla v_h\right) = 0, & \forall v_h \in S_h, \\
\left(\mu_h^1, w_h\right)_Q = \left(g(\phi_h^1) - \frac{8}{3}A_0\phi_h^0, w_h\right)_Q + \varepsilon^2 \left(\nabla \phi_h^1, \nabla w_h\right), & \forall w_h \in S_h.
\end{cases}$$
(2.4)

The initial data is chosen $\phi_h^0 := R_h \phi^0$, where the Ritz projection operator $R_h : H^1_{per}(\Omega) \to S_h$, satisfying

$$(\nabla(R_h u - u), \nabla \chi) = 0, \quad \forall \chi \in S_h, \quad (R_h u - u, 1) = 0.$$

3. Unique solvability analysis

In this section, the unique existence and positivity-preserving property of the solution for the second order fully discrete numerical scheme is verified. If the solution exists, they will hold the mass conservative property at a discrete level

$$\bar{\phi}_h^0 := |\Omega|^{-1} \left(\phi_h^0, 1 \right)_Q = \bar{\phi}_h^1 = \dots = \bar{\phi}_h^n := |\Omega|^{-1} (\phi_h^n, 1)_Q, \quad \forall n \in \mathbb{N}.$$

The following lemmas are needed to prove the desired result, the detailed proof could be found in the work [35].

Lemma 3.1. Given $u_1, u_2 \in S_h$, with $u_2 - u_1 \in \overset{\circ}{S}_h$. Suppose that $||u_1||_{\infty} < 1, ||u_2||_{\infty} \le M$. Then, we have the following estimate:

$$\|(-\Delta_h)^{-1}(u_2-u_1)\|_{\infty} \le C_1,$$

where $C_1 > 0$ depends only upon M and Ω . In particular, C_1 is independent of the mesh spacing h.

Lemma 3.2. For any $\phi \in S_h$, and any piecewise linear Lagrange nodal basis element χ_j , we have

$$(\nabla \phi, \nabla \chi_j) \le \sum_{e \in D_j} \frac{h_e^2}{2\Delta_e} \sum_{i=1}^3 \phi(P_{e,i})$$

on \mathcal{T}_h with mesh size h_e .

Theorem 3.1. Assume that $\mathcal{M}(\phi) \equiv 1$. Given $\phi_h^k \in S_h$, with $\delta_0 \leq \phi_h^k \leq M_h$, k = n, n-1, for some $\delta_0 > 0$, $M_h > 0$, and $\bar{\phi}_h^n = \bar{\phi}_h^{n-1} = \bar{\phi}_h^0$, there exists a unique solution $\phi_h^{n+1} \in S_h$ to (2.3), with $\phi_h^{n+1} - \bar{\phi}_h^n \in \overset{\circ}{S}_h$ and $\phi_h^{n+1} > 0$ at a point-wise level.

Proof. The numerical scheme is a minimizer of the following discrete energy functional:

$$\begin{split} \mathcal{J}(\phi) &= \frac{1}{3\tau} \left\| \frac{3}{2} \phi - 2\phi_h^n + \frac{1}{2} \phi_h^{n-1} \right\|_{-1,Q}^2 + \frac{1}{3} (\phi^{-8} - 4\phi^{-2}, 1)_Q \\ &+ \frac{4}{3} A_0(\phi^2, 1)_Q + \frac{\varepsilon^2 + A\tau}{2} \|\nabla \phi\|_2^2 - (\nabla \phi, A\tau \nabla \phi_h^n) - \frac{8}{3} A_0(\check{\phi}_h^{n+1}, \phi)_Q, \end{split}$$

over an admissible set

$$A_h := \{ \phi \in S_h \mid 0 < \phi \le M_h, (\phi - \bar{\phi}_h^0, 1)_O = 0 \},$$

where $M_h = 3\bar{\phi}_h^0 |\Omega|/\mathrm{area}(D), D := \min_{1 \leq j \leq N_p} |\mathrm{supp}(\chi_j)|$. Details, we have

$$\bar{\phi}_h^0 = \frac{1}{|\Omega|} (\phi_h, 1)_Q = \frac{1}{|\Omega|} \sum_{e \in \mathcal{T}_h} \frac{\Delta_e}{3} \sum_{k=1}^3 \phi_h(P_{e,k})$$
$$\geq \frac{1}{3|\Omega|} \operatorname{area}(D_j) \phi_h(P_j), \quad j = 1, 2, \dots, N_p,$$

this means that $\phi \leq M_h$. To facilitate the analysis below and use Lemma 3.1, we transform the minimization problem into an equivalent one. Consider the functional

$$\begin{split} \mathcal{F}(\varphi) &:= \mathcal{J} \left(\varphi + \bar{\phi}_h^0 \right) \\ &= \frac{1}{3\tau} \left\| \frac{3}{2} \left(\varphi + \bar{\phi}_h^0 \right) - 2 \phi_h^n + \frac{1}{2} \phi_h^{n-1} \right\|_{-1,Q}^2 \\ &+ \frac{1}{3} \left((\varphi + \bar{\phi}_h^0)^{-8} - 4 (\varphi + \bar{\phi}_h^0)^{-2}, 1 \right)_Q \\ &+ \frac{4}{3} A_0 \left((\varphi + \bar{\phi}_h^0)^2, 1 \right)_Q + \frac{\varepsilon^2 + A\tau}{2} \|\nabla \varphi\|_2^2 \\ &- \left(\nabla (\varphi + \bar{\phi}_h^0), A\tau \nabla \phi_h^n \right) - \frac{8}{3} A_0 \left(\check{\phi}_h^{n+1}, \varphi + \bar{\phi}_h^0 \right)_Q, \end{split}$$

where φ lies in the following admissible set:

$$\mathring{A}_h := \left\{ \varphi \in \overset{\circ}{S}_h \mid -\bar{\phi}_h^0 < \varphi \le M_h - \bar{\phi}_h^0 \right\}$$

Observe that \mathcal{F} is a strictly convex functional on an bounded, compact and convex set \mathring{A}_h . In order to show that the minimizer can not reach the left boundary of \mathring{A}_h , we introduce the following set with a sufficiently small δ , for $\delta \in (0, 1/2)$:

$$\mathring{A}_{h,\delta} := \left\{ \varphi \in \overset{\circ}{S}_h \mid \delta - \bar{\phi}_h^0 \le \varphi \le M_h - \bar{\phi}_h^0 \right\}.$$

Since $\mathring{A}_{h,\delta}$ is a bounded, compact, and convex set in the subspace \mathring{S}_h , there exists a minimizer of \mathcal{F} over $\mathring{A}_{h,\delta}$. The key point of the positivity analysis is that such a minimizer could not occur on the left boundary, when δ is sufficiently small.

To get a contradiction, assume that the minimizer of \mathcal{F} , call it φ^* occurs at the left boundary of $\mathring{A}_{h,\delta}$. There is at least one grid $P_{\vec{\alpha}_0}=(i_0,j_0)$ such that $\varphi^*|_{\vec{\alpha}_0}=\delta-\bar{\phi}_h^0$. Thus, the numerical function φ^* has a global minimum at $\vec{\alpha}_0$. Suppose that $P_{\vec{\alpha}_1}=(i_1,j_1)$ is a grid point at which φ^* achieves its maximum. By the fact that $\bar{\varphi}^*=0$, it is obvious that $0\leq \varphi^*|_{\vec{\alpha}_1}\leq M_h-\bar{\phi}_h^0$. Since \mathcal{F} is smooth over $\mathring{A}_{h,\delta}$, for all $\varphi\in \mathring{S}_h$, the directional derivative becomes

$$d_{s}\mathcal{F}(\varphi^{*} + s\psi)|_{s=0} = \frac{1}{\tau} \left((-\Delta_{h})^{-1} \left(\frac{3}{2} (\varphi^{*} + \bar{\phi}_{h}^{0}) - 2\phi_{h}^{n} + \frac{1}{2} \phi_{h}^{n-1} \right), \psi \right)_{Q}$$

$$+ \frac{8}{3} \left((-\varphi^{*} + \bar{\phi}_{h}^{0})^{-9} + (\varphi^{*} + \bar{\phi}_{h}^{0})^{-3} + A_{0} (\varphi^{*} + \bar{\phi}_{h}^{0}), \psi \right)_{Q}$$

$$+ (\varepsilon^{2} + A\tau) (\nabla \varphi^{*}, \nabla \psi) - (A\tau \nabla \phi_{h}^{n}, \nabla \psi)$$

$$- \frac{8}{3} A_{0} (\check{\phi}_{h}^{n+1}, \psi)_{Q} =: \sum_{i=1}^{5} I_{i}.$$

$$(3.1)$$

For simplicity, we write $\phi^* := \varphi^* + \bar{\phi}_h^0$. Let us choose $\psi \in \overset{\circ}{S}_h$ as

$$\psi = \chi_{\vec{\alpha}_0} - \frac{\operatorname{area}(D_{\vec{\alpha}_0})}{\operatorname{area}(D_{\vec{\alpha}_1})} \chi_{\vec{\alpha}_1},$$

where $D_{\vec{\alpha}_0}$, $D_{\vec{\alpha}_1}$ are the compact support of the basis functions $\chi_{\vec{\alpha}_0}$, $\chi_{\vec{\alpha}_1}$, respectively. Next we will estimate each term on the right-hand side of (3.1). For I_1 , using the definition of $(\cdot, \cdot)_Q$ and Lemma 3.1, we have

$$I_{1} = \frac{1}{\tau} \left((-\Delta_{h})^{-1} \left(\frac{3}{2} \phi^{*} - 2\phi_{h}^{n} + \frac{1}{2} \phi_{h}^{n-1} \right), \psi \right)_{Q}$$

$$= \frac{1}{\tau} \sum_{e \in \mathcal{T}_{h}} \frac{\Delta_{e}}{3} \sum_{j=1}^{3} (-\Delta_{h})^{-1} \left(\frac{3}{2} \phi^{*} - 2\phi_{h}^{n} + \frac{1}{2} \phi_{h}^{n-1} \right) \psi(P_{e,j})$$

$$= \frac{\operatorname{area}(D_{\vec{\alpha}_{0}})}{3\tau} \left((-\Delta_{h})^{-1} \left(\frac{3}{2} \phi^{*} - 2\phi_{h}^{n} + \frac{1}{2} \phi_{h}^{n-1} \right) |_{\vec{\alpha}_{0}} \right)$$

$$- (-\Delta_{h})^{-1} \left(\frac{3}{2} \phi^{*} - 2\phi_{h}^{n} + \frac{1}{2} \phi_{h}^{n-1} \right) |_{\vec{\alpha}_{1}}$$

$$\leq \frac{\operatorname{area}(D_{\vec{\alpha}_{0}})}{3\tau} 4C_{1}. \tag{3.2}$$

For I_2 , using $\phi^{\star}|_{\vec{\alpha}_0} = \delta$, $\phi^{\star}|_{\vec{\alpha}_1} \geq \bar{\phi}_h^0$ and the monotonicity of function $g(\phi)$, we have

$$I_{2} = \frac{8}{3} \left(-(\phi^{\star})^{-9} + (\phi^{\star})^{-3} + A_{0}\phi^{\star}, \psi \right)_{Q}$$

$$= \frac{8}{3} \sum_{e \in \mathcal{T}_{h}} \frac{\Delta_{e}}{3} \sum_{j=1}^{3} \left(-(\phi^{\star})^{-9} + (\phi^{\star})^{-3} + A_{0}\phi^{\star} \right) \psi(P_{e,j})$$

$$= \frac{8}{3} \frac{\operatorname{area}(D_{\vec{\alpha}_{0}})}{3} \left((-(\phi^{\star})^{-9} + (\phi^{\star})^{-3} + A_{0}\phi^{\star})|_{\vec{\alpha}_{0}} - (-(\phi^{\star})^{-9} + (\phi^{\star})^{-3} + A_{0}\phi^{\star})|_{\vec{\alpha}_{1}} \right)$$

$$\leq \frac{8 \operatorname{area}(D_{\vec{\alpha}_{0}})}{9} \left(-\delta^{-9} + \delta^{-3} + (\bar{\phi}_{h}^{0})^{-9} - (\bar{\phi}_{h}^{0})^{-3} + A_{0}(\delta - \bar{\phi}_{h}^{0}) \right). \tag{3.3}$$

For I_3 , we have

$$I_{3} = (\varepsilon^{2} + A\tau) (\nabla \phi^{*}, \nabla \psi)$$

$$= (\varepsilon^{2} + A\tau) \left((\nabla \phi^{*}, \nabla \chi_{\vec{\alpha}_{0}}) - \frac{\operatorname{area}(D_{\vec{\alpha}_{0}})}{\operatorname{area}(D_{\vec{\alpha}_{1}})} (\nabla \phi^{*}, \nabla \chi_{\vec{\alpha}_{1}}) \right) \leq 0.$$
(3.4)

For I_4 , using the Lemma 3.2, we have

$$I_{4} = -A\tau \left(\nabla \phi_{h}^{n}, \nabla \psi \right)$$

$$= -A\tau \left(\left(\nabla \phi_{h}^{n}, \nabla \chi_{\vec{\alpha}_{0}} \right) - \frac{\operatorname{area}(D_{\vec{\alpha}_{0}})}{\operatorname{area}(D_{\vec{\alpha}_{1}})} \left(\nabla \phi_{h}^{n}, \nabla \chi_{\vec{\alpha}_{1}} \right) \right)$$

$$\leq A\tau \left(\sum_{e \in D_{\vec{\alpha}_{0}}} \frac{h_{e}^{2}}{2\Delta_{e}} \sum_{j=1}^{3} \phi_{h}^{n}(P_{e,j}) + \frac{\operatorname{area}(D_{\vec{\alpha}_{0}})}{\operatorname{area}(D_{\vec{\alpha}_{1}})} \sum_{e \in D_{\vec{\alpha}_{1}}} \frac{h_{e}^{2}}{2\Delta_{e}} \sum_{j=1}^{3} \phi_{h}^{n}(P_{e,j}) \right)$$

$$\leq A\tau \left(\sum_{e \in D_{\vec{\alpha}_{0}}} \frac{h_{e}^{2}}{2\Delta_{e}} 3M_{h} + \frac{\operatorname{area}(D_{\vec{\alpha}_{0}})}{\operatorname{area}(D_{\vec{\alpha}_{1}})} \sum_{e \in D_{\vec{\alpha}_{1}}} \frac{h_{e}^{2}}{2\Delta_{e}} 3M_{h} \right)$$

$$\leq \frac{3M_{h}A\tau C\tau}{2} \left(\sum_{e \in D_{\vec{\alpha}_{0}}} 1|_{e} + \frac{\operatorname{area}(D_{\vec{\alpha}_{0}})}{\operatorname{area}(D_{\vec{\alpha}_{1}})} \sum_{e \in D_{\vec{\alpha}_{1}}} 1|_{e} \right)$$

$$= \frac{3M_{h}A\tau}{2} \tilde{C}\tau, \tag{3.5}$$

where

$$\tilde{C}_{\mathcal{T}} := C_{\mathcal{T}} \left(\sum_{e \in D_{\vec{\alpha}_0}} 1|_e + \frac{\operatorname{area}(D_{\vec{\alpha}_0})}{\operatorname{area}(D_{\vec{\alpha}_1})} \sum_{e \in D_{\vec{\alpha}_1}} 1|_e \right).$$

For the numerical solution ϕ_h^k , k=n,n-1 at the previous time steps, the a-priori assumption $\delta_0 \leq \|\phi_h^k\|_{\infty} \leq M_h$ yields

$$\delta_0 - M_h \le \phi_h^k|_{\vec{\alpha}_0} - \phi_h^k|_{\vec{\alpha}_1} \le M_h - \delta_0,$$

then, we have

$$3(\delta_0 - M_h) \le \check{\phi}_h^{n+1}|_{\vec{\alpha}_0} - \check{\phi}_h^{n+1}|_{\vec{\alpha}_1} \le 3(M_h - \delta_0). \tag{3.6}$$

For I_5 , we have

$$I_{5} = -\frac{8}{3}A_{0} \left(\check{\phi}_{h}^{n+1}, \psi\right)_{Q}$$

$$= -\frac{8}{3}A_{0} \sum_{e \in \mathcal{T}_{h}} \frac{\Delta_{e}}{3} \sum_{j=1}^{3} \left(\check{\phi}_{h}^{n+1}\psi\right) \left(P_{e,j}\right)$$

$$= -\frac{8}{3}A_{0} \frac{\operatorname{area}(D_{\vec{\alpha}_{0}})}{3} \left(\check{\phi}_{h}^{n+1}|_{\vec{\alpha}_{0}} - \check{\phi}_{h}^{n+1}|_{\vec{\alpha}_{1}}\right)$$

$$\leq \frac{8}{3}A_{0} \operatorname{area}(D_{\vec{\alpha}_{0}})(M_{h} - \delta_{0})$$

$$\leq \frac{8}{3}A_{0} \operatorname{area}(D_{\vec{\alpha}_{0}})M_{h}, \tag{3.7}$$

in which the next-to-last comes from the a priori assumption (3.6) at the previous time steps.

Substituting (3.2)-(3.7) into (3.1), we derive that

$$d_{s}\mathcal{F}(\varphi^{*} + s\psi)|_{s=0} \leq \operatorname{area}(D_{\vec{\alpha}_{0}}) \left(\frac{8}{9} \left(-\delta^{-9} + \delta^{-3} + (\bar{\phi}_{h}^{0})^{-9} - (\bar{\phi}_{h}^{0})^{-3} + A(\delta - \bar{\phi}_{h}^{0})\right) + \frac{4C_{1}}{3\tau} + \frac{8A_{0}}{3}M_{h}\right) + \frac{3M_{h}A\tau}{2}\tilde{C}_{\mathcal{T}}$$

$$= \frac{8}{9}\operatorname{area}(D_{\vec{\alpha}_{0}}) \left(-\delta^{-9} + \delta^{-3} + A\delta + r_{1}\right),$$

where

$$r_1 = (\bar{\phi}_h^0)^{-9} - (\bar{\phi}_h^0)^{-3} - A\bar{\phi}_h^0 + \frac{3C_1}{2\tau} + 3A_0M_h + \frac{27M_hA\tau\tilde{C}_T}{16\operatorname{area}(D_{\vec{\alpha}_0})}.$$

Notice that r_1 is a constant depending on $\bar{\phi}_h^0$, $\operatorname{area}(D_{\vec{\alpha}_0})$ and τ . For any fixed τ , we can choose $\delta \in (0, 1/2)$ sufficiently small such that

$$-\delta^{-9} + \delta^{-3} + A\delta + r_1 < 0. {(3.8)}$$

This in turn shows that, provided δ satisfies (3.8) such that

$$|d_s \mathcal{F}(\varphi^* + s\psi)|_{s=0} < 0.$$

Then the desired contradiction is obtained since the directional derivative is always nonnegative at the minimum point. This contradicts the assumption that \mathcal{F} has a minimum at φ^* . Therefore, the global minimum of \mathcal{F} over $\mathring{A}_{h,\delta}$ could only possibly occur at interior point. We conclude that there must be a solution $\phi \in A_h$ that minimizers \mathcal{J} over A_h , which is equivalent to the numerical solution of (2.3). The existence of the numerical solution is established. In addition, since \mathcal{J} is a strictly convex function over A_h , the uniqueness analysis for this numerical solution is straightforward. Using similar argument, the positivity-preserving property is established for the initialization step (2.4), the details are left to the interested readers.

4. Energy dissipation law

In the following theorem, we could prove that a modified energy stability is available for the second order BDF scheme (2.3), provided that $A \ge (4/9)A_0^2$.

Theorem 4.1. The full discrete numerical scheme (2.3) preserves the modified energy dissipation law

$$\bar{E}_h\left(\phi_h^{n+1}, \phi_h^n\right) \le \bar{E}_h\left(\phi_h^n, \phi_h^{n-1}\right), \quad \text{if} \quad A \ge \frac{4}{9}A_0^2$$
(4.1)

with

$$\bar{E}_h\left(\phi_h^{n+1}, \phi_h^n\right) = E_h\left(\phi_h^{n+1}\right) + \frac{1}{4\tau} \|\phi_h^{n+1} - \phi_h^n\|_{-1,Q}^2 + \frac{4}{3} A_0 \|\phi_h^{n+1} - \phi_h^n\|_Q^2, \tag{4.2}$$

where

$$E_h(\phi) = \frac{1}{3}(\phi^{-8}, 1)_Q + \frac{\varepsilon^2}{2} \|\nabla \phi\|^2 - \frac{4}{3}(\phi^{-2}, 1)_Q.$$

Proof. In (2.3), by choosing

$$v_h = (-\Delta_h)^{-1} \left(\phi_h^{n+1} - \phi_h^n\right), \quad w_h = \phi_h^{n+1} - \phi_h^n$$

we could derive the following expression:

$$\left(\frac{3\phi_h^{n+1} - 4\phi_h^n + \phi_h^{n-1}}{2\tau}, (-\Delta_h)^{-1}(\phi_h^{n+1} - \phi_h^n)\right)_Q + (g(\phi_h^{n+1}), \phi_h^{n+1} - \phi_h^n)_Q - \frac{8}{3}A_0\left(\check{\phi}_h^{n+1}, \phi_h^{n+1} - \phi_h^n\right)_Q + \varepsilon^2\left(\nabla\phi_h^{n+1}, \nabla(\phi_h^{n+1} - \phi_h^n)\right) + A\tau \|\nabla(\phi_h^{n+1} - \phi_h^n)\|^2 = 0.$$
(4.3)

For the first term of the left-hand side of (4.3), we have

$$\left(\frac{3\phi_h^{n+1} - 4\phi_h^n + \phi_h^{n-1}}{2\tau}, (-\Delta_h)^{-1}(\phi_h^{n+1} - \phi_h^n)\right)_Q$$

$$\geq \frac{5}{4\tau} \|\phi_h^{n+1} - \phi_h^n\|_{-1,Q}^2 - \frac{1}{4\tau} \|\phi_h^n - \phi_h^{n-1}\|_{-1,Q}^2. \tag{4.4}$$

For the second term of the left-hand side of (4.3), we have

$$\begin{aligned}
&\left(g(\phi_h^{n+1}), \phi_h^{n+1} - \phi_h^n\right)_Q \\
&= \left(-\frac{8}{3}((\phi_h^{n+1})^{-9} - (\phi_h^{n+1})^{-3}) + \frac{8}{3}A_0\phi_h^{n+1}, \phi_h^{n+1} - \phi_h^n\right)_Q \\
&\geq \frac{1}{3}\left((\phi_h^{n+1})^{-8} - 4(\phi_h^{n+1})^{-2} + 4A_0(\phi_h^{n+1})^2, 1\right)_Q \\
&- \frac{1}{3}\left((\phi_h^n)^{-8} - 4(\phi_h^n)^{-2} + 4A_0(\phi_h^n)^2, 1\right)_Q,
\end{aligned} \tag{4.5}$$

in which the last step comes from the convexity of the function

$$y = \frac{1}{3} \left(x^{-8} - 4x^{-2} + 4A_0^2 \right).$$

For the third term of the left-hand side of (4.3), we have

$$-\frac{8}{3}A_{0}\left(\check{\phi}_{h}^{n+1},\phi_{h}^{n+1}-\phi_{h}^{n}\right)_{Q}$$

$$=-\frac{8}{3}A_{0}\left(2\phi_{h}^{n}-\phi_{h}^{n-1},\phi_{h}^{n+1}-\phi_{h}^{n}\right)_{Q}$$

$$\geq -\frac{4A_{0}}{3}\left(\|\phi_{h}^{n+1}\|_{Q}^{2}-\|\phi_{h}^{n}\|_{Q}^{2}\right)-\frac{4A_{0}}{3}\|\phi_{h}^{n}-\phi_{h}^{n-1}\|_{Q}^{2}.$$

$$(4.6)$$

For the fourth term of the left-hand side of (4.3), we have

$$\varepsilon^{2} \left(\nabla \phi_{h}^{n+1}, \nabla (\phi_{h}^{n+1} - \phi_{h}^{n}) \right)$$

$$= \frac{\varepsilon^{2}}{2} \left(\| \nabla \phi_{h}^{n+1} \|^{2} - \| \nabla \phi_{h}^{n} \|^{2} + \| \nabla (\phi_{h}^{n+1} - \phi_{h}^{n}) \|^{2} \right). \tag{4.7}$$

Meanwhile, an application of Cauchy inequality yields

$$\frac{1}{\tau} \|\phi_h^{n+1} - \phi_h^n\|_{-1,Q}^2 + A\tau \|\nabla(\phi_h^{n+1} - \phi_h^n)\|^2 \ge 2A^{\frac{1}{2}} \|\phi_h^{n+1} - \phi_h^n\|_Q^2. \tag{4.8}$$

A combination of (4.4)-(4.8) yields

$$E_{h}\left(\phi_{h}^{n+1}\right) - E_{h}\left(\phi_{h}^{n}\right) + \frac{1}{4\tau}\left(\|\phi_{h}^{n+1} - \phi_{h}^{n}\|_{-1,Q}^{2} - \|\phi_{h}^{n} - \phi_{h}^{n-1}\|_{-1,Q}^{2}\right) + \frac{4A_{0}}{3}\left(\|\phi_{h}^{n+1} - \phi_{h}^{n}\|_{Q}^{2} - \|\phi_{h}^{n} - \phi_{h}^{n-1}\|_{Q}^{2}\right) \\ \leq \left(\frac{4}{3}A_{0} - 2A^{\frac{1}{2}}\right)\|\phi_{h}^{n+1} - \phi_{h}^{n}\|_{Q}^{2} \leq 0,$$

provided that $A \ge (4/9)A_0^2$. Therefore, by denoting a modified energy as given by (4.2), we get the energy estimate (4.1). This completes the proof of Theorem 4.1.

5. Optimal rate convergence analysis in $\ell^{\infty}(0,T;H_h^{-1})\cap\ell^2(0,T;H_h^1)$

Next, we will provide a convergence analysis for the proposed numerical scheme (2.3)-(2.4), in the $\ell^\infty(0,T;H_h^{-1})\cap\ell^2(0,T;H_h^1)$ norm. We denote the exact solution as $\phi^n=\phi(x,t_n)$ at $t=t_n$. As usual, a regularity assumption has to be made in the error analysis. The following estimates hold for Ritz projection:

$$||R_{h}\varphi||_{1,p} \le C_{2}||\varphi||_{1,p}, \qquad \forall 1 ||\varphi - R_{h}\varphi||_{0,p} + h ||\varphi - R_{h}\varphi||_{1,p} \le C_{2}h^{q+1}||\varphi||_{q+1,p}, \quad \forall 1
(5.1)$$

Suppose that $\phi \in L^{\infty}(0,T;W^{1,p})$. Combining (5.1) and the Sobolev imbedding theorem $W^{1,p}(\Omega) \hookrightarrow L^{\infty}(\Omega)$, for 2 <math>(d=2), 3 <math>(d=3), there are constants $C_3, C_4 > 0$ such that

$$\|\phi^{n}\|_{\infty} \leq C \|\phi^{n}\|_{1,p} \leq C_{3},$$

$$\|R_{h}\phi^{n}\|_{\infty} \leq C \|R_{h}\phi^{n}\|_{1,p} \leq CC_{2} \|\phi^{n}\|_{1,p} \leq C_{4}.$$
(5.2)

By (ϕ, μ) we denote the exact solution to the weak formulation (2.2). We say that the solution pair belongs to regularity of class C if and only if

$$\begin{split} \phi \in W^{2,\infty}\left(0,T;L^2_{per}(\Omega)\right) \cap W^{1,\infty}\left(0,T;H^2_{per}(\Omega)\right) \cap L^2\left(0,T;H^2_{per}(\Omega)\right),\\ \mu \in L^2\left(0,T;H^2_{per}(\Omega)\right). \end{split}$$

The following lemma is the similar version of [35, Lemma 4.1] where the Ritz projection solution only has the upper bound, here it has the lower and upper bound.

Lemma 5.1. If $\phi \in H^2(\Omega)$, where $\Omega \in \mathbb{R}^d$, and $\delta \leq \|\phi\|_{\infty} \leq M$, $\delta > 0$, then there exists $0 < h_0 < 1$ such that for any $h \leq h_0$,

$$\frac{\delta}{2} \le \|R_h \phi\|_{L^{\infty}} \le M + \frac{\delta}{2}.\tag{5.3}$$

Lemma 5.2 ([26]). Let $\kappa_h(v,w) = (v,w) - (v,w)_Q$ denote the quadrature error in (2.1). Then we have

$$|\kappa_h(\psi,\chi)| \le C_5 h^2 ||\nabla \psi|| \cdot ||\nabla \chi||, \quad \forall \psi, \chi \in S_h.$$

Lemma 5.3 ([35]). Suppose $g(\cdot) \in W^{2,\infty}(\mathbb{R})$ and $\kappa_h(g(\cdot),\cdot) = (g(\cdot),\cdot) - (g(\cdot),\cdot)_Q$, then we have

$$|\kappa_h(g(\psi),\chi)| \le C_6 h^2 \left(\|\nabla \psi\|_{L^4}^2 \cdot \|\chi\| + \|\nabla \psi\| \cdot \|\nabla \chi\| \right), \quad \forall \psi, \chi \in S_h,$$

where $C_6 = C \max\{\|g''\|_{L^{\infty}}, \|g'\|_{L^{\infty}}\}$ is independent of h.

Lemma 5.4 ([32]). For a fixed $T = \tau \cdot N$ is a positive integer, and $\tau > 0$, assume that $\{a^n\}_{n=1}^N$, $\{b^n\}_{n=1}^N$ and $\{c^n\}_{n=1}^{N-1}$ are all non-negative sequences, with $\tau \sum_{n=1}^{N-1} c^n \leq C_7$, where $C_7 > 0$ is independent of τ and N, but possibly dependent on T. If for all $\tau > 0$, there is some $C_8 > 0$, which is independent of τ and N, such that

$$a^{N} + \tau \sum_{n=1}^{N} b^{n} \le C_{8} + \tau \sum_{n=1}^{N-1} a^{n} c^{n},$$

then

$$a^{N} + \tau \sum_{n=1}^{N} b^{n} \le (C_{8} + \tau a^{0}c^{0}) \exp\left(\tau \sum_{n=1}^{N-1} c^{n}\right) \le (C_{8} + \tau a^{0}c^{0}) \exp\left(C_{7}\right).$$

Before proceeding into the convergence analysis, we introduce a new norm. Let Ω be an arbitrary bounded domain and $\mathbf{p}=[u,v]^T\in [L^2(\Omega)]^2$. We define $\|\cdot\|_G$ to be a weighted inner product

$$\|\mathbf{p}\|_{G}^{2} = (\mathbf{p}, G(-\Delta_{h})^{-1}\mathbf{p})_{Q}, \quad G = \begin{pmatrix} \frac{1}{2} & -1\\ -1 & \frac{5}{2} \end{pmatrix}.$$

Since G is symmetric positive definite, the norm is well-defined. Moreover,

$$G = \begin{pmatrix} \frac{1}{2} & -1 \\ -1 & \frac{5}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & -1 \\ -1 & 2 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{2} \end{pmatrix} =: G_1 + G_2.$$

By the positive semi-definiteness of G_1 , we immediately have

$$\|\mathbf{p}\|_{G}^{2} = (\mathbf{p}, (G_{1} + G_{2})(-\Delta_{h})^{-1}\mathbf{p})_{Q} \ge (\mathbf{p}, G_{2}(-\Delta_{h})^{-1}\mathbf{p})_{Q} = \frac{1}{2}\|v\|_{-1,Q}^{2}.$$

In addition, for any $v_i \in L^2(\Omega)$, i = 0, 1, 2, the following equality is valid:

$$\left(\frac{3}{2}v_2 - 2v_1 + \frac{1}{2}v_0, (-\Delta_h)^{-1}v_2\right)_C = \frac{1}{2}\left(\|\mathbf{p_2}\|_G^2 - \|\mathbf{p_1}\|_G^2\right) + \frac{\|v_2 - 2v_1 + v_0\|_{-1,Q}^2}{4}$$

with
$$\mathbf{p_1} = [v_0, v_1]^T, \mathbf{p_2} = [v_1, v_2]^T$$
.

Theorem 5.1. Suppose that the exact solution pair (ϕ, μ) is the regularity class \mathcal{C} for the fixed time T>0. Let ϕ_h^n be the solution at $t=t_n$ to the fully discrete numerical scheme (2.3)-(2.4), for $1 \leq n \leq N$, with $N \cdot \tau = T$, provided that τ and h are sufficiently small, then we have the error estimate

$$\|\phi^{n+1} - \phi_h^{n+1}\|_{-1,Q} + \left(2\tau\varepsilon^2 \sum_{k=0}^n \|\nabla(\phi^{k+1} - \phi_h^{k+1})\|^2\right)^{\frac{1}{2}} \le C(T,\varepsilon)(\tau^2 + h^2),$$

for some constant $C(T,\varepsilon) > 0$ that is independent of τ and h.

Proof. First we define

$$\begin{split} \xi_{\phi}^{n+1} &= \phi^{n+1} - \phi_h^{n+1}, \quad \rho_{\phi}^{n+1} = \phi^{n+1} - R_h \phi^{n+1}, \quad \sigma_{\phi}^{n+1} = R_h \phi^{n+1} - \phi_h^{n+1}, \\ \xi_{\mu}^{n+1} &= \mu^{n+1} - \mu_h^{n+1}, \quad \rho_{\mu}^{n+1} = \mu^{n+1} - R_h \mu^{n+1}, \quad \sigma_{\mu}^{n+1} = R_h \mu^{n+1} - \mu_h^{n+1}. \end{split}$$

Obviously, $\xi_{\phi}^{n+1}=\rho_{\phi}^{n+1}+\sigma_{\phi}^{n+1},\ \xi_{\mu}^{n+1}=\rho_{\mu}^{n+1}+\sigma_{\mu}^{n+1}.$ Similar to Chapter 15 of Thomée's classical book [26], by careful calculation, the following error evolutionary equation

could be derived:

where

$$\delta_{\tau}v^{n+1} := \begin{cases} \frac{3v^{n+1} - 4v^n + v^{n-1}}{2\tau}, & n \ge 1, \\ \frac{v^1 - v^0}{\tau}, & n = 0, \end{cases}$$

$$R_1^{n+1} := \partial_t \phi^{n+1} - \delta_{\tau} \phi^{n+1},$$

$$R_2^{n+1} := \phi^{n+1} - \begin{cases} 2\phi^n - \phi^{n-1}, & n \ge 1, \\ \phi^0, & n = 0, \end{cases}$$

$$R_3^{n+1} := \begin{cases} A\Delta \left(\phi^{n+1} - \phi^n\right), & n \ge 1, \\ 0, & n = 0, \end{cases}$$

$$T_1^{n+1} := \begin{cases} 2\sigma_{\phi}^n - \sigma_{\phi}^{n-1}, & n \ge 1, \\ \sigma_{\phi}^0, & n = 0, \end{cases}$$

$$T_2^{n+1} := \begin{cases} A\left(\sigma_{\phi}^{n+1} - \sigma_{\phi}^n\right), & n \ge 1, \\ 0, & n = 0. \end{cases}$$

$$T_2^{n+1} := \begin{cases} A\left(\sigma_{\phi}^{n+1} - \sigma_{\phi}^n\right), & n \ge 1, \\ 0, & n = 0. \end{cases}$$

Taking $w_h = \Delta_h v_h$ in (5.4), we have

$$(\delta_{\tau}\sigma_{\phi}^{n+1}, v_{h})_{Q} - \varepsilon^{2} \left(\nabla\sigma_{\phi}^{n+1}, \nabla\Delta_{h}v_{h}\right) - \tau \left(\nabla T_{2}^{n+1}, \nabla\Delta_{h}v_{h}\right)$$

$$= -\left(R_{1}^{n+1}, v_{h}\right) - \kappa_{h} \left(\delta_{\tau}R_{h}\phi^{n+1}, v_{h}\right) - \left(\delta_{\tau}\rho_{\phi}^{n+1}, v_{h}\right) + \left(g(\phi^{n+1}) - g(R_{h}\phi^{n+1}), \Delta_{h}v_{h}\right)$$

$$+ \left(g(R_{h}\phi^{n+1}) - g(\phi_{h}^{n+1}), \Delta_{h}v_{h}\right)_{Q} + \kappa_{h} \left(g(R_{h}\phi^{n+1}), \Delta_{h}v_{h}\right) - \frac{8A_{0}}{3} \left(\rho_{\phi}^{n+1}, \Delta_{h}v_{h}\right)$$

$$- \frac{8A_{0}}{3} \left(T_{1}^{n+1}, \Delta_{h}v_{h}\right)_{Q} - \frac{8A_{0}}{3} \left(R_{h}R_{2}^{n+1}, \Delta_{h}v_{h}\right)_{Q} - \frac{8A_{0}}{3} \kappa_{h} \left(R_{h}\phi^{n+1}, \Delta_{h}v_{h}\right)$$

$$+ \tau \left(R_{3}^{n+1}, \Delta_{h}v_{h}\right) - \left(\rho_{\mu}^{n+1}, \Delta_{h}v_{h}\right) - \kappa_{h} \left(R_{h}\mu^{n+1}, \Delta_{h}v_{h}\right).$$

$$(5.6)$$

In turn, taking $v_h = (-\Delta_h)^{-1} \sigma_\phi^{n+1}$, we write Eq. (5.6) as follows:

$$\left(\delta_{\tau}\sigma_{\phi}^{n+1}, (-\Delta_{h})^{-1}\sigma_{\phi}^{n+1}\right)_{Q} + \varepsilon^{2} \|\nabla\sigma_{\phi}^{n+1}\|^{2} + \tau \left(\nabla T_{2}^{n+1}, \nabla\sigma_{\phi}^{n+1}\right)$$

$$= -\left(R_{1}^{n+1}, (-\Delta_{h})^{-1}\sigma_{\phi}^{n+1}\right) - \kappa_{h}\left(\delta_{\tau}R_{h}\phi^{n+1}, (-\Delta_{h})^{-1}\sigma_{\phi}^{n+1}\right) - \left(\delta_{\tau}\rho_{\phi}^{n+1}, (-\Delta_{h})^{-1}\sigma_{\phi}^{n+1}\right)$$

$$- \left(g(\phi^{n+1}) - g(R_{h}\phi^{n+1}), \sigma_{\phi}^{n+1}\right) - \left(g(R_{h}\phi^{n+1}) - g(\phi_{h}^{n+1}), \sigma_{\phi}^{n+1}\right)_{Q}$$

$$- \kappa_{h}\left(g(R_{h}\phi^{n+1}), \sigma_{\phi}^{n+1}\right) + \frac{8A_{0}}{3}\left(\rho_{\phi}^{n+1}, \sigma_{\phi}^{n+1}\right) + \frac{8A_{0}}{3}\left(T_{1}^{n+1}, \sigma_{\phi}^{n+1}\right)_{Q}$$

$$+ \frac{8A_{0}}{3}\left(R_{h}R_{2}^{n+1}, \sigma_{\phi}^{n+1}\right)_{Q} + \frac{8A_{0}}{3}\kappa_{h}\left(R_{h}\phi^{n+1}, \sigma_{\phi}^{n+1}\right) - \tau\left(R_{3}^{n+1}, \sigma_{\phi}^{n+1}\right)$$

$$+ \left(\rho_{\mu}^{n+1}, \sigma_{\phi}^{n+1}\right) + \kappa_{h}\left(R_{h}\mu^{n+1}, \sigma_{\phi}^{n+1}\right) = \sum_{i=1}^{13}Q_{i} =: Q.$$

$$(5.7)$$

For the first term of left-hand side of (5.7), we have

$$\begin{split} & \left(\delta_{\tau}\sigma_{\phi}^{n+1}, (-\Delta_{h})^{-1}\sigma_{\phi}^{n+1}\right)_{Q} \\ & = \begin{cases} \frac{1}{2\tau} \left(\|\mathbf{p}^{n+1}\|_{G}^{2} - \|\mathbf{p}^{n}\|_{G}^{2}\right) + \frac{1}{4\tau} \|\sigma_{\phi}^{n+1} - 2\sigma_{\phi}^{n} + \sigma_{\phi}^{n-1}\|_{-1,Q}^{2}, & n \geq 1, \\ \frac{1}{2\tau} \left(\|\sigma_{\phi}^{1}\|_{-1,Q}^{2} - \|\sigma_{\phi}^{0}\|_{-1,Q}^{2}\right) + \frac{1}{2\tau} \|\sigma_{\phi}^{1} - \sigma_{\phi}^{0}\|_{-1,Q}^{2}, & n = 0, \end{cases} \end{split}$$

where $\mathbf{p}^{k+1}=(\sigma_\phi^k,\sigma_\phi^{k+1})^T.$ For the third term of left-hand side of (5.7), we have

$$\tau\left(\nabla T_2^{n+1}, \nabla \sigma_{\phi}^{n+1}\right) = \begin{cases} A\tau\left(\nabla(\sigma_{\phi}^{n+1} - \sigma_{\phi}^n), \nabla \sigma_{\phi}^{n+1}\right) \ge \frac{1}{2}A\tau\left(\|\nabla \sigma_{\phi}^{n+1}\|^2 - \|\nabla \sigma_{\phi}^n\|^2\right), & n \ge 1, \\ 0, & n = 0, \end{cases}$$

in which the last step comes from

$$2(a-b)a = a^2 - b^2 + (a-b)^2,$$

and A = 0 used for n = 0.

A combination of (5.7) reveals that, the right-hand side of (5.7) is bounded from below

$$Q \ge \begin{cases} \frac{1}{2\tau} \left(\|\mathbf{p}^{n+1}\|_{G}^{2} - \|\mathbf{p}^{n}\|_{G}^{2} \right) + \frac{1}{2} A \tau \left(\|\nabla \sigma_{\phi}^{n+1}\|^{2} - \|\nabla \sigma_{\phi}^{n}\|^{2} \right) \\ + \varepsilon^{2} \|\nabla \sigma_{\phi}^{n+1}\|^{2}, & n \ge 1, \\ \frac{1}{2\tau} \|\sigma_{\phi}^{1}\|_{-1,Q}^{2} + \varepsilon^{2} \|\nabla \sigma_{\phi}^{1}\|^{2}, & n = 0, \end{cases}$$

$$(5.8)$$

in which $\sigma_{\phi}^0 \equiv 0$.

For Q_1 , we have

$$Q_{1} = -\left(R_{1}^{n+1}, (-\Delta_{h})^{-1}\sigma_{\phi}^{n+1}\right)$$

$$= -\left(\nabla(-\Delta)^{-1}R_{1}^{n+1}, \nabla(-\Delta_{h})^{-1}\sigma_{\phi}^{n+1}\right)$$

$$\leq \|\nabla(-\Delta)^{-1}R_{1}^{n+1}\| \cdot \|\nabla(-\Delta_{h})^{-1}\sigma_{\phi}^{n+1}\|$$

$$= \|R_{1}^{n+1}\|_{H^{-1}} \cdot \|\sigma_{\phi}^{n+1}\|_{-1,Q}$$

$$\leq C\|R_{1}^{n+1}\|_{2} \cdot \|\sigma_{\phi}^{n+1}\|_{-1,Q}$$

$$\leq \begin{cases} 2C^{2}\|R_{1}^{n+1}\|_{2}^{2} + \frac{1}{8}\|\sigma_{\phi}^{n+1}\|_{-1,Q}^{2}, & n \geq 1, \\ 2C^{2}\tau\|R_{1}^{1}\|_{2}^{2} + \frac{1}{8\tau}\|\sigma_{\phi}^{n+1}\|_{-1,Q}^{2}, & n = 0, \end{cases}$$

$$(5.9)$$

in which the first step comes from the integral by parts formula, the second step is based on the Hölder inequality, and the fourth step is based on the fact that $\|f\|_{H^{-1}} \leq C\|f\|_{L^2}$. Similarly, for Q_3 , we have

$$Q_{3} = C \|\delta_{\tau} \rho_{\phi}^{n+1}\|_{2} \cdot \|\sigma_{\phi}^{n+1}\|_{-1,Q}$$

$$\leq C C_{2} h^{2} \|\delta_{\tau} \phi^{n+1}\|_{H^{2}} \cdot \|\sigma_{\phi}^{n+1}\|_{-1,Q}$$

$$\leq 2 C^{2} C_{2}^{2} h^{4} \|\delta_{\tau} \phi^{n+1}\|_{H^{2}}^{2} + \frac{1}{8} \|\sigma_{\phi}^{n+1}\|_{-1,Q}^{2},$$
(5.10)

in which the next-to-last step is based on the Ritz projection estimate (5.1). For Q_2 , we have

$$-\kappa_{h} \left(\delta_{\tau} R_{h} \phi^{n+1}, (-\Delta_{h})^{-1} \sigma_{\phi}^{n+1} \right)$$

$$\leq C_{5} h^{2} \| \nabla \delta_{\tau} R_{h} \phi^{n+1} \| \cdot \| \nabla (-\Delta_{h})^{-1} \sigma_{\phi}^{n+1} \|$$

$$= C_{5} h^{2} \| \nabla \delta_{\tau} R_{h} \phi^{n+1} \| \cdot \| \sigma_{\phi}^{n+1} \|_{-1,Q}$$

$$\leq C_{2} C_{5} h^{2} \| \nabla \delta_{\tau} \phi^{n+1} \| \cdot \| \sigma_{\phi}^{n+1} \|_{-1,Q}$$

$$\leq 2 \left(C_{2} C_{5} h^{2} \right)^{2} \| \nabla \delta_{\tau} \phi^{n+1} \|^{2} + \frac{1}{8} \| \sigma_{\phi}^{n+1} \|_{-1,Q}^{2}, \tag{5.11}$$

in which the first step is based on the Lemma 5.2, the second step comes from the definition of $\|\cdot\|_{-1,Q}$ and the third step comes from the Ritz projection estimate (5.1). Similarly, for Q_{10} , we have

$$\frac{8A_0}{3} \kappa_h \left(R_h \phi^{n+1}, \sigma_{\phi}^{n+1} \right)
\leq \frac{4C_5^2 h^4}{\varepsilon^2} \left(\frac{8A_0}{3} \right)^2 \|\nabla R_h \phi^{n+1}\|^2 + \frac{\varepsilon^2}{16} \|\nabla \sigma_{\phi}^{n+1}\|^2
\leq \frac{4C_2^2 C_5^2 h^4}{\varepsilon^2} \left(\frac{8A_0}{3} \right)^2 \|\nabla \phi^{n+1}\|^2 + \frac{\varepsilon^2}{16} \|\nabla \sigma_{\phi}^{n+1}\|^2.$$
(5.12)

Similarly, for Q_{13} , we have

$$\kappa_h(R_h\mu^{n+1}, \sigma_\phi^{n+1}) \le \frac{4C_2^2C_5^2h^4}{\varepsilon^2} \|\nabla\mu^{n+1}\|^2 + \frac{\varepsilon^2}{16} \|\nabla\sigma_\phi^{n+1}\|^2.$$
 (5.13)

Suppose that $\delta \leq \phi^{n+1}$. Based on the Lemma 5.1, we have $\delta/2 \leq \|R_h\phi^{n+1}\|_{L^{\infty}}$. For Q_4 , we have

$$-\left(g(\phi^{n+1}) - g(R_h\phi^{n+1}), \sigma_{\phi}^{n+1}\right)$$

$$= -\left(g'(\lambda^{n+1})\rho_{\phi}^{n+1}, \sigma_{\phi}^{n+1}\right)$$

$$\leq \|g'\|_{\infty} \cdot \|\rho_{\phi}^{n+1}\|_{L^2} \cdot \|\sigma_{\phi}^{n+1}\|_{L^2}$$

$$\leq C_8 C \|\rho_{\phi}^{n+1}\|_{L^2} \cdot \|\nabla\sigma_{\phi}^{n+1}\|_{L^2}$$

$$\leq \frac{2(C_8 C h^2)^2}{\varepsilon^2} \|\phi^{n+1}\|_{H^2}^2 + \frac{\varepsilon^2}{8} \|\nabla\sigma_{\phi}^{n+1}\|_{L^2}^2, \tag{5.14}$$

in which λ^{n+1} is between ϕ^{n+1} and $R_h\phi^{n+1}$, the third step is based on Lemma 5.1 and Poincaré inequality, and the last step comes from the Ritz projection estimate (5.1).

For Q_5 , based on the monotonicity of function $g(\phi)$, we have

$$-(g(R_h\phi^{n+1}) - g(\phi_h^{n+1}), \sigma_\phi^{n+1})_Q \le 0.$$
 (5.15)

For Q_6 , the following bounds could be derived:

$$-\kappa_{h}(g(R_{h}\phi^{n+1}), \sigma_{\phi}^{n+1})$$

$$\leq C_{6}h^{2}\left(\|\nabla R_{h}\phi^{n+1}\|_{L^{4}}^{2} \cdot \|\sigma_{\phi}^{n+1}\| + \|\nabla R_{h}\phi^{n+1}\| \cdot \|\nabla \sigma_{\phi}^{n+1}\|\right)$$

$$\leq CC_{2}^{2}C_{6}h^{2}\|\nabla \phi^{n+1}\|_{L^{4}}^{2} \cdot \|\nabla \sigma_{\phi}^{n+1}\| + C_{2}C_{6}h^{2}\|\nabla \phi^{n+1}\| \cdot \|\nabla \sigma_{\phi}^{n+1}\|$$

$$\leq \frac{8(CC_{2}^{2}C_{6}h^{2})^{2}}{\varepsilon^{2}}\|\nabla \phi^{n+1}\|_{L^{4}}^{4} + \frac{8(C_{2}C_{6}h^{2})^{2}}{\varepsilon^{2}}\|\nabla \phi^{n+1}\|^{2} + \frac{\varepsilon^{2}}{16}\|\nabla \sigma_{\phi}^{n+1}\|^{2}, \qquad (5.16)$$

in which the first step comes from the Lemma 5.3, the second step is based on the Poincare's inequality and the Ritz projection estimate (5.1).

For Q_7 , we have

$$\frac{8A_0}{3} \left(\rho_{\phi}^{n+1}, \sigma_{\phi}^{n+1} \right) \leq \frac{8A_0}{3} \| \rho_{\phi}^{n+1} \|_{H^{-1}} \cdot \| \nabla \sigma_{\phi}^{n+1} \| \leq \frac{8A_0C}{3} \| \rho_{\phi}^{n+1} \| \cdot \| \nabla \sigma_{\phi}^{n+1} \| \\
\leq \frac{8A_0C}{3} C_2 h^2 \| \phi^{n+1} \|_{H^2} \cdot \| \nabla \sigma_{\phi}^{n+1} \| \\
\leq 2 \left(\frac{8A_0CC_2}{3\varepsilon} \right)^2 h^4 \| \phi^{n+1} \|_{H^2}^2 + \frac{\varepsilon^2}{8} \| \nabla \sigma_{\phi}^{n+1} \|^2, \tag{5.17}$$

in which the second step comes from $||f||_{H^{-1}} \le C||f||_{L^2}$ and the third step comes from the Ritz projection estimate (5.1).

Similarly, for Q_{12} , we have

$$(\rho_{\mu}^{n+1}, \sigma_{\phi}^{n+1}) \leq \|\rho_{\mu}^{n+1}\|_{H^{-1}} \cdot \|\nabla \sigma_{\phi}^{n+1}\|$$

$$\leq \frac{4C^{2}C_{2}^{2}h^{4}}{\varepsilon^{2}} \|\mu^{n+1}\|_{H^{2}}^{2} + \frac{\varepsilon^{2}}{16} \|\nabla \sigma_{\phi}^{n+1}\|^{2}.$$
(5.18)

For Q_8 , we have

$$\frac{8A_0}{3} \left(T_1^{n+1}, \sigma_{\phi}^{n+1} \right)_Q = \frac{8A_0}{3} \left(\nabla (-\Delta_h)^{-1} T_1^{n+1}, \nabla \sigma_{\phi}^{n+1} \right) \\
\leq \frac{8A_0}{3} \| \nabla (-\Delta_h)^{-1} T_1^{n+1} \| \cdot \| \nabla \sigma_{\phi}^{n+1} \| \\
= \frac{8A_0}{3} \| T_1^{n+1} \|_{-1,Q} \cdot \| \nabla \sigma_{\phi}^{n+1} \| \\
\leq \left(\frac{8A_0}{3} \right)^2 \frac{2}{\varepsilon^2} \| T_1^{n+1} \|_{-1,Q}^2 + \frac{\varepsilon^2}{8} \| \nabla \sigma_{\phi}^{n+1} \|^2 \\
\left(\left(\frac{8A_0}{3} \right)^2 \frac{2}{\varepsilon^2} (6 \| \sigma_{\phi}^n \|_{-1,Q}^2 + 3 \| \sigma_{\phi}^{n-1} \|_{-1,Q}^2) \\
\leq \left\{ \frac{\varepsilon^2}{8} \| \nabla \sigma_{\phi}^{n+1} \|^2, \qquad n \geq 1, \quad (5.19) \\
\left(\frac{8A_0}{3} \right)^2 \frac{2}{\varepsilon^2} \| \sigma_{\phi}^0 \|_{-1,Q}^2 + \frac{\varepsilon^2}{8} \| \nabla \sigma_{\phi}^1 \|^2, \qquad n = 0, \\
\end{cases}$$

in which the first and the third step comes from the definition of $(\cdot,\cdot)_Q$ inner product and $\|\cdot\|_{-1,Q}$.

For Q_9 , we have

$$\frac{8A_0}{3} (R_h R_2^{n+1}, \sigma_{\phi}^{n+1})_Q = \frac{8A_0}{3} (\nabla R_h R_2^{n+1}, \nabla (-\Delta_h)^{-1} \sigma_{\phi}^{n+1}) \\
\leq \frac{8A_0}{3} \|\nabla R_h R_2^{n+1}\|_{L^2} \cdot \|\nabla (-\Delta_h)^{-1} \sigma_{\phi}^{n+1}\|_{L^2} \\
= \frac{8A_0}{3} \|\nabla R_h R_2^{n+1}\|_{L^2} \cdot \|\sigma_{\phi}^{n+1}\|_{-1,Q} \\
\leq \frac{8A_0C_2}{3} \|\nabla R_2^{n+1}\|_{L^2} \cdot \|\sigma_{\phi}^{n+1}\|_{-1,Q} \\
\leq \left\{ \frac{2\left(\frac{8A_0C_2}{3}\right)^2 \|\nabla R_2^{n+1}\|_{L^2} + \frac{1}{8} \|\sigma_{\phi}^{n+1}\|_{-1,Q}^2, \quad n \geq 1, \\
2\left(\frac{8A_0C_2}{3}\right)^2 C\tau^3 + \frac{1}{8\tau} \|\sigma_{\phi}^1\|_{-1,Q}^2, \quad n = 0, \\
\end{cases} (5.20)$$

in which the first step comes from the definition of discrete Laplacian operator and the fourth step comes from the Ritz projection estimate (5.1).

For Q_{11} , we have

$$-\tau (R_{3}^{n+1}, \sigma_{\phi}^{n+1}) = -A\tau (\Delta(\phi^{n+1} - \phi^{n}), \sigma_{\phi}^{n+1})$$

$$= A\tau (\nabla(\phi^{n+1} - \phi^{n}), \nabla\sigma_{\phi}^{n+1})$$

$$\leq A\tau \|\nabla(\phi^{n+1} - \phi^{n})\| \cdot \|\nabla\sigma_{\phi}^{n+1}\|$$

$$\leq \begin{cases} \frac{2(A\tau)^{2}}{\varepsilon^{2}} \|\nabla(\phi^{n+1} - \phi^{n})\|^{2} + \frac{\varepsilon^{2}}{8} \|\nabla\sigma_{\phi}^{n+1}\|^{2}, & n \geq 1, \\ 0, & n = 0. \end{cases}$$
(5.21)

Substituting above estimates (5.9)-(5.21) into the left-hand side of (5.7), we have, for $n \ge 1$,

$$Q \leq 2C^{2} \|R_{1}^{n+1}\|_{2}^{2} + 2C^{2}C_{2}^{2}h^{4}\|\delta_{\tau}\phi^{n+1}\|_{H^{2}}^{2} + 2\left(\frac{8A_{0}C_{2}}{3}\right)^{2} \|\nabla R_{2}^{n+1}\|_{L^{2}}^{2}$$

$$+ 2(C_{2}C_{5}h^{2})^{2} \|\nabla\delta_{\tau}\phi^{n+1}\|^{2} + \frac{8(CC_{2}^{2}C_{6}h^{2})^{2}}{\varepsilon^{2}} \|\nabla\phi^{n+1}\|_{L^{4}}^{4} + \frac{8(C_{2}C_{6}h^{2})^{2}}{\varepsilon^{2}} \|\nabla\phi^{n+1}\|^{2}$$

$$+ \frac{4C_{2}^{2}C_{5}^{2}h^{4}}{\varepsilon^{2}} \left(\frac{8A_{0}}{3}\right)^{2} \|\nabla\phi^{n+1}\|^{2} + \frac{4C_{2}^{2}C_{5}^{2}h^{4}}{\varepsilon^{2}} \|\nabla\mu^{n+1}\|^{2} + \frac{2(A\tau)^{2}}{\varepsilon^{2}} \|\nabla(\phi^{n+1} - \phi^{n})\|^{2}$$

$$+ 2\left(\frac{8A_{0}CC_{2}}{3\varepsilon}\right)^{2} h^{4} \|\phi^{n+1}\|_{H^{2}}^{2} + \frac{4C^{2}C_{2}^{2}h^{4}}{\varepsilon^{2}} \|\mu^{n+1}\|_{H^{2}}^{2}$$

$$+ \left(\frac{8A_{0}}{3}\right)^{2} \frac{2}{\varepsilon^{2}} (6\|\sigma_{\phi}^{n}\|_{-1,Q}^{2} + 3\|\sigma_{\phi}^{n-1}\|_{-1,Q}^{2}) + \frac{2(C_{8}Ch^{2})^{2}}{\varepsilon^{2}} \|\phi^{n+1}\|_{H^{2}}^{2}$$

$$+ \frac{3\varepsilon^{2}}{4} \|\nabla\sigma_{\phi}^{n+1}\|^{2} + \frac{1}{2} \|\sigma_{\phi}^{n+1}\|_{-1,Q}^{2}. \tag{5.22}$$

For n = 0, a similar inequality could be derived

$$Q \leq 2C^{2}\tau \|R_{1}^{1}\|_{2}^{2} + 2C^{2}C_{2}^{2}h^{4}\|\delta_{\tau}\phi^{1}\|_{H^{2}}^{2} + 2\left(\frac{8A_{0}C_{2}}{3}\right)^{2}C\tau^{3}$$

$$+ 2(C_{2}C_{5}h^{2})^{2}\|\nabla\delta_{\tau}\phi^{1}\|^{2} + \frac{8(CC_{2}^{2}C_{6}h^{2})^{2}}{\varepsilon^{2}}\|\nabla\phi^{1}\|_{L^{4}}^{4} + \frac{8(C_{2}C_{6}h^{2})^{2}}{\varepsilon^{2}}\|\nabla\phi^{1}\|^{2}$$

$$+ \frac{4C_{2}^{2}C_{5}^{2}h^{4}}{\varepsilon^{2}}\left(\frac{8A_{0}}{3}\right)^{2}\|\nabla\phi^{1}\|^{2} + \frac{4C_{2}^{2}C_{5}^{2}h^{4}}{\varepsilon^{2}}\|\nabla\mu^{1}\|^{2}$$

$$+ 2\left(\frac{8A_{0}CC_{2}}{3\varepsilon}\right)^{2}h^{4}\|\phi^{1}\|_{H^{2}}^{2} + \frac{4C^{2}C_{2}^{2}h^{4}}{\varepsilon^{2}}\|\mu^{1}\|_{H^{2}}^{2}$$

$$+ \frac{2(C_{8}Ch^{2})^{2}}{\varepsilon^{2}}\|\phi^{1}\|_{H^{2}}^{2} + \frac{3\varepsilon^{2}}{4}\|\nabla\sigma_{\phi}^{1}\|^{2} + \frac{1}{8\tau}\|\sigma_{\phi}^{n+1}\|_{-1,Q}^{2} + \frac{3}{8}\|\sigma_{\phi}^{1}\|_{-1,Q}^{2}. \tag{5.23}$$

By the Cauchy-Schwarz inequality, we have the following estimate:

$$||R_1^{n+1}||^2 \le \begin{cases} 32\tau^3 \int_{t_{n-1}}^{t_{n+1}} ||\partial_{ttt}\phi||^2 dt = C\tau^4, & n \ge 1, \\ \frac{\tau}{3} \int_0^{t_1} ||\partial_{tt}\phi||^2 dt \le \frac{\tau^2}{3} ||\phi||_{W^{2,\infty}(0,T;L^2)} = C\tau^2, & n = 0. \end{cases}$$

An analogous estimate is available for the second remainder term

$$||R_2^{n+1}||^2 \le \begin{cases} 32\tau^3 \int_{t_{n-1}}^{t_{n+1}} ||\partial_{tt}\phi||^2 dt = C\tau^4, & n \ge 1, \\ \tau \int_0^{t_1} ||\partial_t\phi||^2 dt \le \tau^2 ||\phi||_{W^{1,\infty}(0,T;L^2)} = C\tau^2, & n = 0, \end{cases}$$

$$||\nabla R_2^{n+1}||^2 \le \begin{cases} 32\tau^3 \int_{t_{n-1}}^{t_{n+1}} ||\partial_{tt}\nabla\phi||^2 dt = C\tau^4, & n \ge 1, \\ \tau \int_0^{t_1} ||\partial_t\nabla\phi||^2 dt \le \tau^2 ||\phi||_{W^{1,\infty}(0,T;H^1_{per}(\Omega))} = C\tau^2, & n = 0. \end{cases}$$

For the third remainder term, we obtain the estimate

$$\|\nabla(\phi^{n+1} - \phi^n)\|^2 \le \begin{cases} \tau \int_{t_n}^{t_{n+1}} \|\partial_t \nabla \phi\|^2 dt \le \tau^2 \|\phi\|_{W^{1,\infty}(0,T;H^1_{\mathrm{per}}(\Omega))} = C\tau^2, & n \ge 1, \\ 0, & n = 0. \end{cases}$$

Combining (5.8) and (5.22), for $n \ge 1$, we have

$$\frac{1}{2\tau} \left(\|\mathbf{p}^{n+1}\|_{G}^{2} - \|\mathbf{p}^{n}\|_{G}^{2} \right) + \frac{1}{2} A \tau \left(\|\nabla \sigma_{\phi}^{n+1}\|^{2} - \|\nabla \sigma_{\phi}^{n}\|^{2} \right) + \frac{\varepsilon^{2}}{4} \|\nabla \sigma_{\phi}^{n+1}\|^{2}
\leq 2C^{2} \|R_{1}^{n+1}\|_{2}^{2} + 2C^{2} C_{2}^{2} h^{4} \|\delta_{\tau} \phi^{n+1}\|_{H^{2}}^{2} + 2 \left(\frac{8A_{0}C_{2}}{3} \right)^{2} \|\nabla R_{2}^{n+1}\|_{L^{2}}^{2}
+ 2(C_{2}C_{5}h^{2})^{2} \|\nabla \delta_{\tau} \phi^{n+1}\|^{2} + \frac{8(CC_{2}^{2}C_{6}h^{2})^{2}}{\varepsilon^{2}} \|\nabla \phi^{n+1}\|_{L^{4}}^{4} + \frac{8(C_{2}C_{6}h^{2})^{2}}{\varepsilon^{2}} \|\nabla \phi^{n+1}\|^{2}
+ \frac{4C_{2}^{2}C_{5}^{2}h^{4}}{\varepsilon^{2}} \left(\frac{8A_{0}}{3} \right)^{2} \|\nabla \phi^{n+1}\|^{2} + \frac{4C_{2}^{2}C_{5}^{2}h^{4}}{\varepsilon^{2}} \|\nabla \mu^{n+1}\|^{2} + \frac{2(A\tau)^{2}}{\varepsilon^{2}} \|\nabla (\phi^{n+1} - \phi^{n})\|^{2}
+ \left(2\left(\frac{8A_{0}CC_{2}}{3\varepsilon} \right)^{2} + \frac{2(C_{8}C)^{2}}{\varepsilon^{2}} \right) h^{4} \|\phi^{n+1}\|_{H^{2}}^{2} + \frac{4C^{2}C_{2}^{2}h^{4}}{\varepsilon^{2}} \|\mu^{n+1}\|_{H^{2}}^{2}
+ \left(\frac{8A_{0}}{3} \right)^{2} \frac{2}{\varepsilon^{2}} \left(6\|\sigma_{\phi}^{n}\|_{-1,Q}^{2} + 3\|\sigma_{\phi}^{n-1}\|_{-1,Q}^{2} \right) + \frac{1}{2}\|\sigma_{\phi}^{n+1}\|_{-1,Q}^{2}, \tag{5.24}$$

in which

$$\|\mathbf{p}^1\|_G^2 = \frac{5}{2} \|\sigma_\phi^1\|_{-1,Q}^2, \quad \|\mathbf{p}^{n+1}\|_G^2 \ge \frac{1}{2} \|\sigma_\phi^{n+1}\|_{-1,Q}^2.$$

Combining (5.8) and (5.23), for n = 0, a similar inequality could be derived

$$\begin{split} \frac{3}{8\tau} \|\sigma_{\phi}^{1}\|_{-1,Q}^{2} + \frac{\varepsilon^{2}}{4} \|\nabla\sigma_{\phi}^{1}\|^{2} \\ &\leq 2C^{2}\tau \|R_{1}^{1}\|_{2}^{2} + 2C^{2}C_{2}^{2}h^{4} \|\delta_{\tau}\phi^{1}\|_{H^{2}}^{2} \\ &+ 2\left(\frac{8A_{0}C_{2}}{3}\right)^{2}C\tau^{3} + 2(C_{2}C_{5}h^{2})^{2} \|\nabla\delta_{\tau}\phi^{1}\|^{2} \end{split}$$

$$+ \frac{4C_{2}^{2}C_{5}^{2}h^{4}}{\varepsilon^{2}} \|\nabla\mu^{1}\|^{2} + \frac{8(CC_{2}^{2}C_{6}h^{2})^{2}}{\varepsilon^{2}} \|\nabla\phi^{1}\|_{L^{4}}^{4}$$

$$+ \left(\frac{8(C_{2}C_{6})^{2}}{\varepsilon^{2}} + \frac{4C_{2}^{2}C_{5}^{2}}{\varepsilon^{2}} (\frac{8A_{0}}{3})^{2}\right) h^{4} \|\nabla\phi^{1}\|^{2}$$

$$+ \left(2\left(\frac{8A_{0}CC_{2}}{3\varepsilon}\right)^{2} + \frac{2(C_{8}C)^{2}}{\varepsilon^{2}}\right) h^{4} \|\phi^{1}\|_{H^{2}}^{2}$$

$$+ \frac{4C^{2}C_{2}^{2}h^{4}}{\varepsilon^{2}} \|\mu^{1}\|_{H^{2}}^{2} + \frac{3}{8} \|\sigma_{\phi}^{1}\|_{-1,Q}^{2}. \tag{5.25}$$

Equivalently, multiplying by $20\tau/3$ on both sides of (5.25), we have

$$\frac{5}{2} \|\sigma_{\phi}^{1}\|_{-1,Q}^{2} + \frac{5\varepsilon^{2}\tau}{3} \|\nabla\sigma_{\phi}^{1}\|^{2} \le \frac{5\tau}{2} \|\sigma_{\phi}^{1}\|_{-1,Q}^{2} + \mathcal{R}^{0}, \tag{5.26}$$

in which

$$\mathcal{R}^{0} = \frac{40\tau}{3} C^{2} \tau \|R_{1}^{1}\|_{2}^{2} + \frac{40\tau}{3} C^{2} C_{2}^{2} h^{4} \|\delta_{\tau} \phi^{1}\|_{H^{2}}^{2} + \frac{40\tau}{3} \left(\frac{8A_{0}C_{2}}{3}\right)^{2} C \tau^{3}$$

$$+ \frac{40\tau}{3} (C_{2}C_{5}h^{2})^{2} \|\nabla\delta_{\tau} \phi^{1}\|^{2} + \frac{160(CC_{2}^{2}C_{6}h^{2})^{2}\tau}{3\varepsilon^{2}} \|\nabla\phi^{1}\|_{L^{4}}^{4}$$

$$+ \frac{160(C_{2}C_{6}h^{2})^{2}\tau}{3\varepsilon^{2}} \|\nabla\phi^{1}\|^{2} + \frac{80C_{2}^{2}C_{5}^{2}h^{4}\tau}{3\varepsilon^{2}} \left(\frac{8A_{0}}{3}\right)^{2} \|\nabla\phi^{1}\|^{2}$$

$$+ \frac{80C_{2}^{2}C_{5}^{2}h^{4}\tau}{3\varepsilon^{2}} \|\nabla\mu^{1}\|^{2} + \frac{40\tau}{3} \left(\frac{8A_{0}CC_{2}}{3\varepsilon}\right)^{2} h^{4} \|\phi^{1}\|_{H^{2}}^{2}$$

$$+ \frac{80C^{2}C_{2}^{2}h^{4}\tau}{3\varepsilon^{2}} \|\mu^{1}\|_{H^{2}}^{2} + \frac{40(C_{8}Ch^{2})^{2}\tau}{3\varepsilon^{2}} \|\phi^{1}\|_{H^{2}}^{2}$$

$$\leq C(\varepsilon)(\tau^{4} + h^{4})$$

Summing (5.24) from k = 1 to k = n + 1, multiplying by 2τ on both sides, we arrive at the following estimate:

$$\frac{1}{2} \|\sigma_{\phi}^{n+1}\|_{-1,Q}^{2} - \frac{5}{2} \|\sigma_{\phi}^{1}\|_{-1,Q}^{2} + A\tau^{2} (\|\nabla\sigma_{\phi}^{n+1}\|^{2} - \|\nabla\sigma_{\phi}^{1}\|^{2}) + \frac{\varepsilon^{2}\tau}{2} \sum_{k=1}^{n} \|\nabla\sigma_{\phi}^{k+1}\|^{2} \\
\leq \left(\frac{8A_{0}}{3}\right)^{2} \frac{4\tau}{\varepsilon^{2}} \sum_{k=1}^{n} \left(6 \|\sigma_{\phi}^{k}\|_{-1,Q}^{2} + 3 \|\sigma_{\phi}^{k-1}\|_{-1,Q}^{2}\right) + \tau \sum_{k=1}^{n} \|\sigma_{\phi}^{k+1}\|_{-1,Q}^{2} + \sum_{k=1}^{n} \mathcal{R}^{k}, \quad (5.27)$$

in which

$$\mathcal{R}^{k} = 4C^{2}\tau \|R_{1}^{k+1}\|_{2}^{2} + 4C^{2}C_{2}^{2}h^{4}\tau \|\delta_{\tau}\phi^{k+1}\|_{H^{2}}^{2} + 4\left(\frac{8A_{0}C_{2}}{3}\right)^{2}\tau \|\nabla R_{2}^{k+1}\|_{L^{2}}^{2} + 4(C_{2}C_{5}h^{2})^{2}\tau \|\nabla \delta_{\tau}\phi^{k+1}\|^{2} + \frac{16(CC_{2}^{2}C_{6}h^{2})^{2}\tau}{\varepsilon^{2}} \|\nabla \phi^{k+1}\|_{L^{4}}^{4}$$

$$\begin{split} &+ \frac{16(C_{2}C_{6}h^{2})^{2}\tau}{\varepsilon^{2}} \|\nabla\phi^{k+1}\|^{2} + \frac{8C_{2}^{2}C_{5}^{2}h^{4}\tau}{\varepsilon^{2}} \left(\frac{8A_{0}}{3}\right)^{2} \|\nabla\phi^{k+1}\|^{2} \\ &+ \frac{8C_{2}^{2}C_{5}^{2}h^{4}\tau}{\varepsilon^{2}} \|\nabla\mu^{k+1}\|^{2} + \frac{4A^{2}\tau^{3}}{\varepsilon^{2}} \|\nabla(\phi^{k+1} - \phi^{k})\|^{2} \\ &+ 4\left(\frac{8A_{0}CC_{2}}{3\varepsilon}\right)^{2} h^{4}\tau \|\phi^{k+1}\|_{H^{2}}^{2} + \frac{8C^{2}C_{2}^{2}h^{4}\tau}{\varepsilon^{2}} \|\mu^{k+1}\|_{H^{2}}^{2} + \frac{4(C_{8}Ch^{2})^{2}\tau}{\varepsilon^{2}} \|\phi^{k+1}\|_{H^{2}}^{2} \\ &\leq C(T, \varepsilon)(\tau^{4} + h^{4}), \end{split}$$

and $C(T, \varepsilon)$ is independent of τ and h.

Combining (5.26) and (5.27), we have

$$\frac{1}{2} \|\sigma_{\phi}^{n+1}\|_{-1,Q}^{2} + \frac{5\varepsilon^{2}\tau}{3} \|\nabla\sigma_{\phi}^{1}\|^{2} + A\tau^{2} (\|\nabla\sigma_{\phi}^{n+1}\|^{2} - \|\nabla\sigma_{\phi}^{1}\|^{2}) + \frac{\varepsilon^{2}\tau}{2} \sum_{k=1}^{n} \|\nabla\sigma_{\phi}^{k+1}\|^{2} \\
\leq \left(\frac{8A_{0}}{3}\right)^{2} \frac{4\tau}{\varepsilon^{2}} \sum_{k=1}^{n} \left(6 \|\sigma_{\phi}^{k}\|_{-1,Q}^{2} + 3 \|\sigma_{\phi}^{k-1}\|_{-1,Q}^{2}\right) + \tau \sum_{k=1}^{n} \|\sigma_{\phi}^{k+1}\|_{-1,Q}^{2} \\
+ \sum_{k=0}^{n} \mathcal{R}^{k} + \frac{5\tau}{2} \|\sigma_{\phi}^{1}\|_{-1,Q}^{2}. \tag{5.28}$$

Let $\tau \leq \min\{7\varepsilon^2/6A, 1/4\}$, we have

$$\frac{1}{4} \|\sigma_{\phi}^{n+1}\|_{-1,Q}^{2} + \frac{\varepsilon^{2}\tau}{2} \sum_{k=1}^{n} \|\nabla\sigma_{\phi}^{k+1}\|^{2}$$

$$\leq \left(\frac{256A_{0}^{2}}{\varepsilon^{2}} + \frac{7}{2}\right) \tau \sum_{k=1}^{n} \|\sigma_{\phi}^{k}\|_{-1,Q}^{2} + \sum_{k=0}^{n} \mathcal{R}^{k}.$$
(5.29)

An application of the discrete Gronwall inequality of Lemma 5.4 leads to the desired convergence result

$$\|\sigma_{\phi}^{n+1}\|_{-1,Q}^2 + 2\varepsilon^2 \tau \sum_{k=0}^n \|\nabla \sigma_{\phi}^{k+1}\|^2 \le C(T,\varepsilon)(\tau^4 + h^4).$$

The proof is complete.

6. Numerical results

In this section, we provide two numerical examples to illustrate the presented scheme satisfies the properties of mass conservation, energy dissipation and positivity-preserving. The first example demonstrates the convergence order of the proposed scheme (2.3). The second example aims to test the properties of the numerical solution and demonstrates the coarsening phenomenon for the droplet liquid film model. We consistently apply periodic boundary conditions across all experiments, and the surface diffusion coefficient is set as $\varepsilon=0.08$, the stabilization parameter A=1, and the concave term coefficient $A_0=1$.

6.1. Accuracy test

We first perform numerical simulations to test the convergence rates of the scheme. Considered computational domain $\Omega = [0, 1]^2$, the initial data is chosen as

$$\phi(x, y, t) = 2 + \frac{1}{2\pi} \sin(2\pi x) \cos(2\pi y) \cos(t).$$

First, we fix the spatial resolution as $N_s=256$ (with h=1/256), so that the spatial numerical error is negligible, the final time is set as T=1. Naturally, a sequence of time step sizes are taken as $\tau=T/N_t$, with $N_t=100,200,400,800,1600,3200,6400,12800$. The expected temporal numerical accuracy assumption $e=C\tau^2$ indicates that $\ln|e|=\ln(CT^2)-2\ln N_t$, so that we plot $\ln|e|$ vs. $\ln N_t$ to demonstrate the temporal convergence order. In Fig. 1, we quantify our calculation error using the differences between adjacent time steps at the same node, measured in both the L^∞ norm and L^2 norm. We observe that our scheme almost perfect matches the second-order accuracy in time. For the spatial convergence test, we fix the temporal resolution at $N_t=12800$ (with $\tau=1/12800$), and set the final time as T=1. Naturally, a sequence of spatial step sizes is taken as $h=1/N_s$, where $N_s=4,8,16,32,64,128,256,512$. Similarly, we plot $\ln|e|$ vs. $\ln N_s$ as shown in Fig. 2, which verifies a consistent second-order convergence in space.

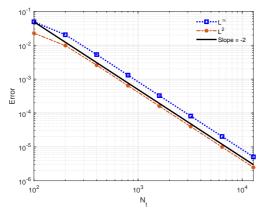


Figure 1: Errors and convergence rates of the fully discrete scheme, where h=1/256 and T=1.

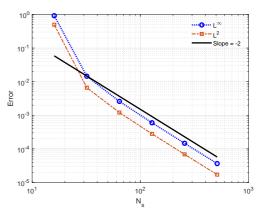


Figure 2: Errors and convergence rates of the fully discrete scheme, where $\tau=7.8125e^{-5}$ and T=1.

6.2. Coarsening process

In this subsection, we perform a two-dimensional numerical simulation showing the coarsening process. The computational domain is set as $\Omega=(0,L)^2$, with L=12.8. The initial data is given by

$$\phi(x, y, 0) = 2 + 0.1(2r_{i,j} - 1),$$

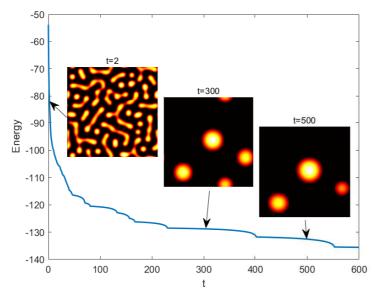


Figure 3: Evolution of the discrete energy of the fully discrete scheme, where h=1/128 and T=600.

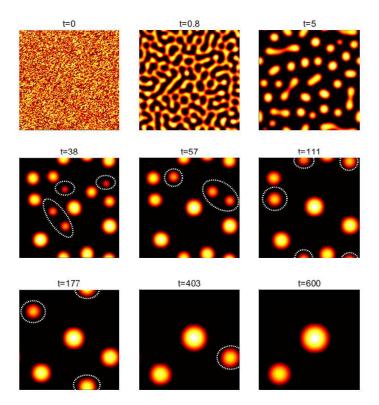


Figure 4: Snapshots of the computed height function ϕ at the indicated times for the parameters $L=12.8, \varepsilon=0.08.$

where $r_{i,j}$ are uniformly distributed random numbers in [0,1]. We employ a grid resolution of 128×128 with a time step $\tau = 0.002$, and the parameters are set to $A = A_0 = 1, \varepsilon = 0.08$. As shown in Fig. 3, the energy decays rapidly initially, followed by a slower decay process. The inclusion of phase diagrams is benefit to observe the phase state changes corresponding to energy variations.

The time snapshots of the evolution are presented in Fig. 4, allowing for clear observation of significant coarsening in the system. In the early stages, numerous small hills (yellow) with flat bases (black) are present. As the coarsening process advances, it is noteworthy that the regions marked by dashed ellipses in Fig. 4 gradually disappear. Undoubtedly, after t=600, a single hill structure will emerge, and further coarsening will not occur, consistent with the findings reported in [38]. Furthermore, Fig. 5 is composed of two sections. The upper panel illustrates the evolution of the maximum and minimum values of the phase variable. The red solid line indicates that the height function ϕ is numerically greater than zero. The lower panel presents the temporal evolution of mass. These numerical results are in agreement with both theoretical predictions and empirical observations, thereby validating the accuracy of the numerical scheme and the reliability of the theoretical analysis.

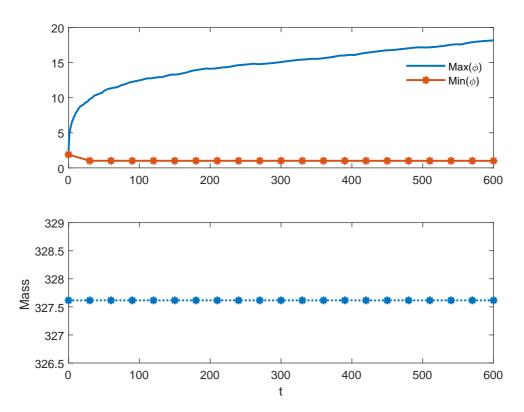


Figure 5: Evolution of the maximum and minimum values of the computed height function ϕ (top) and mass evolution (bottom) for the parameters $L=12.8, \varepsilon=0.08$.

7. Conclusions

A mass lumped mixed finite element numerical scheme is proposed and analyzed for the droplet liquid film model by using the convex splitting idea, in which a singular Leonard-Jones energy potential is involved. The BDF temporal discrete and second-order Adams-Bashforth extrapolation formula has been used to construct the full discrete scheme. Combined Douglas-Dupont regularization term, the modified energy stability property is estimated. In order to facilitate error analysis, we designed a convex-concave decomposition, so that the concave part corresponds to a quadratic energy. Further, an optimal rate convergence analysis for the proposed scheme is established as well. Finally, mass conservation, energy stability, bound of the numerical solution and the second order accurate are demonstrated in the numerical experiments.

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