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A regularized second order scheme for Cahn–Hilliard equation with Cahn–Hilliard type dynamic boundary conditions

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Abstract

In this paper, a numerical scheme is proposed and analyzed for Liu-Wu model: Cahn–Hilliard equation with Cahn-Hilliard type dynamic boundary conditions (Liu and Wu, Arch Ration Mech Anal 233(1):167–247, 2019). Inspired by the convex-concave decomposition of the Cahn–Hilliard free energy, prescribed with Neumann boundary condition, we propose a regularized second-order temporal discretization for the coupled PDE system. The unique solvability, unconditional dissipation of a modified free energy and second order convergence analysis (in the H^{-1} norm) are theoretically established. Finally, several numerical experiments are presented to illustrate the effectiveness of the proposed numerical scheme.

Keywords Cahn–Hilliard equation · Dynamic boundary conditions · Liu-Wu model · Convex splitting · Unique solvability · Energy stability

Mathematics Subject Classification 35K35 · 35K55 · 65M12 · 65M60

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1 Introduction

Gradient flow models have been widely used in many physical, chemical, material and other engineering fields such as image inpainting, fluid flows, see [3–5, 17, 21]. Given free energy functional $E(\phi)$, denote its variational derivative as $u = \dfrac{\delta E(\phi)}{\delta \phi}$, then a gradient flow process could be represented as

$$\partial_t \phi = \mathcal{G} u,$$

wherein $\mathcal{G}$ is a nonpositive symmetric operator, and determines the dissipation mechanism. Taking $\mathcal{G} = -I$ leads to an L^2 gradient flow, while $\mathcal{G} = \Delta$ implies an H^{-1} gradient flow. For example, with a free energy functional choice as $E_\Omega(\phi) = \int_\Omega \frac{\varepsilon^2}{2} |\nabla \phi|^2 + F(\phi) \ \mathrm{d}x$, and taking the H^{-1} gradient flow of $E_\Omega(\phi)$, then we get the standard Cahn–Hilliard equation:

$$\begin{aligned} &\partial_t \phi = \Delta u, && \text{in } \Omega \times (0, T], \\ &u = -\varepsilon^2 \Delta \phi + F'(\phi), && \text{in } \Omega \times (0, T]. \end{aligned}$$

Here $\Omega \subset \mathbb{R}^d (d = 2, 3)$ is an open domain with a smooth boundary $\Gamma = \partial \Omega$, ϕ represents the order parameter in the phase field, u is referred as chemical potential, and interface parameter ε prescribes the thickness of interfacial region. The bulk potential function $F(\phi)$, could be chosen as double well potential, logarithmic potential and obstacle potential [3, 7, 15]. Generally, homogeneous Neumann boundary conditions are widely used:

$$\partial_n u = 0, \qquad \text{on } \Gamma \times (0, T], \tag{1.1a}$$

$$\partial_n \phi = 0, \qquad \text{on } \Gamma \times (0, T]. \tag{1.1b}$$

The first boundary condition (1.1a) guarantees the mass conservation in Ω: $\int_\Omega \phi(t) \ \mathrm{d}x = \int_\Omega \phi(0) \ \mathrm{d}x = m_0$, for all $t \in (0, T)$, and the second boundary condition (1.1b) indicates that there is no interaction between the material and the container, see the related arguments [2]. Based on this boundary condition, the solution of the PDE system satisfies the following energy dissipation law:

$$\frac{\mathrm{d}}{\mathrm{d}t} E_\Omega(\phi(t)) + \int_\Omega |\nabla u|^2 \mathrm{d}x = 0, \quad \forall t \in (0, T).$$

However, this boundary condition ignores the influence of solid wall to the mixture. To take into consideration of short-range interaction near the boundary, some surface free energy functionals need to be introduced based on physical background, and boundary conditions for the system changed at the same time. For example, by using mean field theory, Sanjay et al. [31] proposed a dynamic boundary condition to describe the preference of container to mixture in one dimension:

$$\partial_t \phi = h + g\phi + \gamma \partial_x \phi, \qquad x = 0.$$

In fact, this boundary conditions latter became so called Allen-Cahn type dynamic boundary condition in $\mathbb{R}^d$ $(d = 2, 3)$:

$$\partial_t \phi = \kappa \Delta_\Gamma \phi - \varepsilon^2 \partial_n \phi - G'(\phi), \qquad \text{on } \Gamma \times (0, T], \tag{1.2}$$

wherein Δ_Γ is the Laplace-Beltrami operator on Γ, $\Delta_\Gamma \phi$ represents surface diffusion on the boundary, κ is surface diffuse interface thickness parameter and $G(\phi)$ is a selected surface potential (see [8, 20, 25, 30] for more details). By taking surface free energy functional as

$$E_{\Gamma,*}(\phi(t)) = \int_\Gamma \frac{\kappa}{2} |\nabla_\Gamma \phi|^2 + G(\phi) \ \mathrm{d}s,$$

where ∇_Γ is the tangential gradient operator on boundary Γ, equation (1.2) can be viewed as a L^2 gradient flow in terms of surface energy $E_{\Gamma,*}(\phi(t))$ on Γ. We also refer to [9, 10, 12, 34] for several examples of phase field model with dynamic boundary conditions.

In this paper, we focus on a new dynamic boundary condition proposed by Liu and Wu [26]. Based on three physical properties: mass conservation, energy dissipation, force balance, they came up with the Energetic Variational Approach, and obtained the following generalized Cahn–Hilliard system (abbreviated as Liu-Wu model in the following sections) with a Cahn–Hilliard-type dynamic boundary condition:

$$\begin{aligned}
&\partial_t \phi = \Delta u, && \text{in } \Omega \times (0, T], \\
&u = -\varepsilon^2 \Delta \phi + F'(\phi), && \text{in } \Omega \times (0, T], \\
&\partial_n u = 0, && \text{on } \Gamma \times (0, T], \\
&\partial_t \phi = \Delta_\Gamma u_\Gamma, && \text{on } \Gamma \times (0, T], \\
&u_\Gamma = -\kappa \varepsilon^2 \Delta_\Gamma \phi + \varepsilon^2 \partial_n \phi + G'(\phi), && \text{on } \Gamma \times (0, T].
\end{aligned} \tag{1.3}$$

In this system, mass in the bulk and boundary are individually conservative, due to the Neumann boundary condition of chemical potential u. Meanwhile, a boundary chemical potential u_Γ is introduced, which is not the trace of u. The total free energy of the system turns out to be

$$\begin{aligned}
E(\phi) &= E_\Omega(\phi) + E_\Gamma(\phi) \\
&= \int_\Omega \frac{\varepsilon^2}{2} |\nabla \phi|^2 + F(\phi) \ \mathrm{d}x + \int_\Gamma \frac{\kappa \varepsilon^2}{2} |\nabla_\Gamma \phi|^2 + G(\phi) \ \mathrm{d}s.
\end{aligned} \tag{1.4}$$

Following a standard calculation, we are able to verify that the system fulfills an energy dissipation law:

$$\frac{\mathrm{d}}{\mathrm{d}t}E(\phi(t)) + \int_\Omega |\nabla u|^2 \mathrm{d}x + \int_\Gamma |\nabla_\Gamma u|^2 \mathrm{d}s = 0, \quad \forall t \in (0,T). \tag{1.5}$$

Similar to Liu-Wu model, the GMS model proposed by Goldstein et al.[16] also introduces a Cahn–Hilliard type dynamic boundary condition, and satisfies energy dissipation property (1.5). The difference between the two models lies in the mass conservation law: while bulk mass and the surface mass are conserved separately for Liu-Wu model (see (1.6a)), only total mass is conserved for the GMS model (see (1.6b)). We also refer to [22, 23] for a new model that interpolates between the previous models.

$$\int_\Omega \phi(t)\mathrm{d}x = \int_\Omega \phi(0)\mathrm{d}x, \quad \int_\Gamma \phi(t)\mathrm{d}s = \int_\Gamma \phi(0)\mathrm{d}s. \tag{1.6a}$$

$$\int_\Omega \phi(t)\mathrm{d}x + \int_\Gamma \phi(t)\mathrm{d}s = \int_\Omega \phi(0)\mathrm{d}x + \int_\Gamma \phi(0)\mathrm{d}s. \tag{1.6b}$$

In the numerical simulation of phase field models, energy stability has always been a central issue in the theoretical analysis. Many different numerical approaches have been proposed to keep energy stability, such as stabilized linearly implicit algorithm [27], convex splitting method [18, 33, 35], invariant energy quadratization (IEQ) method [36, 37] and scalar auxiliary variable(SAV) method [32], etc.

In terms of the numerical approximation to Liu-Wu model (1.3), Garcke et al. [14] uses fully implicit discretization by solving a variation problem, and proves the convergence of the scheme to a weak solution. Metzger [28] applies the convex-concave decomposition and implicit temporal discretization to construct a first order in time scheme. Moreover, the author converts the ill-conditioned linear equation as the time step size $\tau \searrow 0$, to a time independent system, which greatly decreases the condition numbers at small time step size. Meng et al. [27] proposed a second-order in time, linear and energy stable scheme, and proves the convergence order of the semi-discrete scheme. To guarantee energy stability, Lipschitz property is assumed for the second derivative of double well potential functional F and G. Besides, as Liu-Wu model and the GMS model have similar constructions, several numerical schemes have been presented for these equations with Cahn–Hilliard-type dynamic boundary conditions [1, 19], and the temporal convergence rate could reach up to fifth order [19].

In this paper, we propose a second order in time, unconditionally energy stable scheme for the Liu-Wu model, inspired by the convex splitting approach for Cahn–Hilliard equation with Nuemann boundary condition [35]. In fact, this idea could be easily extended to a fully discrete scheme, with either finite difference or finite element spatial approximation. The primary difference between our approach and the existing work [27] is associated with the methodology to keep the total energy stability. In more details, a stabilized linearly implicit approach used in [27] requires four

ε-dependent parameters to ensure an unconditional energy stability, while the regularization coefficient in our proposed scheme is irrelevant to ε, and the implicit treatment of convex part provide an convenient way in the unique solvability analysis.

The rest of this paper is organized as follows. In Sect. 2 we introduce the semi-discrete scheme, prove the unique solvability and numerical energy dissipation. In Sect. 3 the H^{-1} convergence analysis is provided, and an extension to the fully discrete scheme is outlined, with Lagrange element. In Sect. 4 several numerical experiments are presented to demonstrate the system evolution, and verify the theoretical properties of the proposed numerical scheme.

2 The numerical scheme

2.1 Preliminary notations

For the convenience and conciseness of the paper, some notations are clarified here. (P1) As listed in the introduction, there are different choices for the potential functions F and G. Throughout the paper, we use double well potential functional with the following form:

$$F(\phi) = \frac{1}{4}\phi^4 - \frac{1}{2}\phi^2, \quad F'(\phi) = \phi^3 - \phi,$$

Surface potential G could be likewise defined. (P2) For Sobolev space $W^{0,p}(\Omega), W^{0,p}(\Gamma)$, we use $\|\cdot\|_{L^p,\Omega}, \|\cdot\|_{L^p,\Gamma}$ to denote the standard L^p norm, and abbreviated as $\|\cdot\|_{L^p}$ if the domain is Ω. Furthermore, when $p = 2$, we will use $\|\cdot\|, \|\cdot\|_\Gamma$ to denote the standard norm of $L^2(\Omega) = W^{0,2}(\Omega), L^2(\Gamma) = W^{0,2}(\Gamma)$, and use $(\cdot,\cdot), (\cdot,\cdot)_\Gamma$ to denote the corresponding inner product. (P3) Denote $L_0^2(\Omega) := \{u \in L^2(\Omega), (u, 1) = 0\}$ and $\mathring{H}^1(\Omega) := H^1(\Omega) \cap L_0^2(\Omega)$, then for every $f \in L_0^2(\Omega)$, the Poisson equation with Neumann boundary condition

$$\begin{aligned} -\Delta u &= f && \text{in } \Omega, \\ \partial_n u &= 0 && \text{on } \Gamma, \end{aligned} \tag{2.1}$$

has a unique weak solution in $\mathring{H}^1(\Omega)$. Similarly we could define space $\mathring{H}^1(\Gamma)$. Of course, for every $g \in L_0^2(\Gamma)$, equation

$$-\Delta_\Gamma v = g \qquad \text{on } \Gamma, \tag{2.2}$$

has a unique weak solution in $\mathring{H}^1(\Gamma)$.

In this paper, we denote the above weak solution and negative norm as:

$$\begin{aligned} u &= (-\Delta)^{-1} f, \quad \|f\|_{-1} = \|\nabla u\|, \\ v &= (-\Delta_\Gamma)^{-1} g, \quad \|g\|_{-1,\Gamma} = \|\nabla_\Gamma v\|_\Gamma. \end{aligned}$$

2.2 A semi-discrete numerical scheme

The following second order (in time) numerical scheme is proposed for the Liu-Wu model:

$$\frac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{2\tau} = \Delta u^{n+1}, \quad \text{in } \Omega, \tag{2.3a}$$

$$\begin{aligned} u^{n+1} = &-\varepsilon^2\Delta\phi^{n+1} + (\phi^{n+1})^3 - (2\phi^n - \phi^{n-1}) \\ &- A_1\tau(\Delta\phi^{n+1} - \Delta\phi^n), \qquad \text{in } \Omega, \end{aligned} \tag{2.3b}$$

$$\partial_n u^{n+1} = 0, \quad \text{on } \Gamma, \tag{2.3c}$$

$$\frac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{2\tau} = \Delta_\Gamma u_\Gamma^{n+1}, \quad \text{on } \Gamma, \tag{2.3d}$$

$$\begin{aligned} u_\Gamma^{n+1} = &-\kappa\varepsilon^2\Delta_\Gamma\phi^{n+1} + \varepsilon^2\partial_n\phi^{n+1} + (\phi^{n+1})^3 - (2\phi^n - \phi^{n-1}) \\ &+ A_1\tau\frac{\partial(\phi^{n+1}-\phi^n)}{\partial n} - A_2\tau(\Delta_\Gamma\phi^{n+1} - \Delta_\Gamma\phi^n), \quad \text{on } \Gamma. \end{aligned} \tag{2.3e}$$

Here τ is the time step size, tuple $(\phi^n, u^n, u_\Gamma^n)$ stands for the numerical solution of (ϕ, u, u_Γ) at time t^n respectively.

A second order backward differentiation formula (BDF) is applied in the temporal discretization, while the concave part of the chemical potential is treated by an explicit extrapolation $2\phi^n - \phi^{n-1}$. Two second order Douglas-Dupont-type regularization terms, namely $A_1\tau\Delta(\phi^{n+1}-\phi^n)$ and $A_2\tau\Delta_\Gamma(\Delta\phi^{n+1}-\Delta_\Gamma\phi^n)$, are added in the interior region and on the boundary section, respectively. These two additional stabilization terms ensure a total energy stability theoretically. Meanwhile, since the numerical scheme (2.3a)-(2.3e) is a three-level algorithm, an initialization process is needed in the first time step to obtain the numerical value of ϕ^1. In fact, any single-step scheme satisfying mass conservation and energy dissipation could be used in the first time step, such as the one from [28]:

$$\frac{\phi^1-\phi^0}{\tau} = \Delta u^1, \quad \text{in } \Omega, \tag{2.4a}$$

$$u^1 = -\varepsilon^2\Delta\phi^1 + (\phi^1)^3 - \phi^0, \quad \text{in } \Omega, \tag{2.4b}$$

$$\partial_n u^1 = 0, \quad \text{on } \Gamma, \tag{2.4c}$$

$$\frac{\phi^1-\phi^0}{\tau}=\Delta_\Gamma u_\Gamma^1, \quad \text{on} \quad \Gamma, \tag{2.4d}$$

$$u_\Gamma^1=-\kappa\varepsilon^2\Delta_\Gamma\phi^1+\varepsilon^2\partial_n\phi^1+(\phi^1)^3-\phi^0, \quad \text{on} \quad \Gamma. \tag{2.4e}$$

Moreover, a weak formulation of (2.3a)-(2.3e) is needed to facilitate the later analysis. Define space $\mathcal{V}:=\{u\in H^1(\Omega)|\,\gamma(u)\in H^1(\Gamma)\}$, where γ is the standard trace operator, which will be omitted when there is no ambiguity. Then the weak formulation is to find $(\phi^{n+1},u^{n+1},u_\Gamma^{n+1})\in\mathcal{V}\times H^1(\Omega)\times\in H^1(\Gamma)$ such that for all $(\xi,\zeta,\eta)\in H^1(\Omega)\times H^1(\Gamma)\times\mathcal{V}$, the following equalities hold:

$$\left(\frac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{2\tau},\xi\right)=-\left(\nabla u^{n+1},\nabla\xi\right), \tag{2.5a}$$

$$\left(\frac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{2\tau},\zeta\right)_\Gamma=-\left(\nabla_\Gamma u^{n+1},\nabla_\Gamma\zeta\right)_\Gamma, \tag{2.5b}$$

$$\begin{aligned}\left(u^{n+1},\eta\right)+\left(u_\Gamma^{n+1},\eta\right)_\Gamma=&\ \varepsilon^2\left(\nabla\phi^{n+1},\nabla\eta\right)+\kappa\varepsilon^2\left(\nabla_\Gamma\phi^{n+1},\nabla_\Gamma\eta\right)_\Gamma\\&+\left((\phi^{n+1})^3,\eta\right)-\left(2\phi^n-\phi^{n-1},\eta\right)\\&+\left((\phi^{n+1})^3,\eta\right)_\Gamma-\left(2\phi^n-\phi^{n-1},\eta\right)_\Gamma\\&+A_1\tau\left(\nabla\phi^{n+1}-\nabla\phi^n,\nabla\eta\right)+A_2\tau\left(\nabla_\Gamma\phi^{n+1}-\nabla_\Gamma\phi^n,\nabla_\Gamma\eta\right)_\Gamma.\end{aligned} \tag{2.5c}$$

With the help of this weak formulation, the mass conservation identity could be easily verified.

Lemma 2.1 *If $\int_\Omega\phi^1\,dx=\int_\Omega\phi^0\,dx$, $\int_\Gamma\phi^1\,ds=\int_\Gamma\phi^0\,ds$, then the numerical solution of (2.5a)-(2.5c) satisfies mass conservation in Ω and on Γ, respectively.*

Proof Assume that $\int_\Omega\phi^k\mathrm{d}x=\int_\Omega\phi^0\mathrm{d}x, k=1,2,...,n$ holds. Subsequently, taking a test function $\xi=1$ in (2.5a) gives

$$\frac{1}{2\tau}\left(3\int_\Omega\phi^{n+1}\mathrm{d}x-4\int_\Omega\phi^n\mathrm{d}x+\int_\Omega\phi^{n-1}\mathrm{d}x\right)=0. \tag{2.6}$$

Then it is straightforward to obtain $\int_\Omega\phi^{n+1}\mathrm{d}x=\int_\Omega\phi^0\mathrm{d}x$. In addition, the mass conservation identity on the boundary section could be proved analogously. □

By Lemma 2.1, it is clear that $(\phi^{n+1}-\phi^n)\in L_0^2(\Omega), \gamma(\phi^{n+1}-\phi^n)\in L_0^2(\Gamma)$, so that operators $(-\Delta)^{-1}$ and $(-\Delta_\Gamma)^{-1}$ could be applied on them respectively. In the following theorem we establish the unconditional energy dissipation property of the scheme, with respect to a numerically modified free energy.

Theorem 2.2 *The numerical solution of (2.5a)-(2.5c) preserves the following energy dissipation estimate, with the Douglas-Dupont regularization parameters satisfying* $A_1 \geqslant \frac{1}{16}, A_2 \geqslant \frac{1}{16}$:

$$\begin{aligned}&E(\phi^{n+1},\phi^n)+\frac{1}{\tau}\Big(1-\frac{1}{16A_1}\Big)\|\phi^{n+1}-\phi^n\|_{-1}^2+\frac{1}{\tau}\Big(1-\frac{1}{16A_2}\Big)\|\phi^{n+1}-\phi^n\|_{-1,\Gamma}^2\\&\leqslant E(\phi^n,\phi^{n-1}),\end{aligned}\tag{2.7}$$

where $E(\phi^{n+1},\phi^n), n\geqslant 1$ *is a modified total energy:*

$$\begin{aligned}E(\phi^{n+1},\phi^n)=E(\phi^{n+1})&+\frac{1}{4\tau}(\|\phi^{n+1}-\phi^n\|_{-1}^2+\|\phi^{n+1}-\phi^n\|_{-1,\Gamma}^2)\\&+\frac{1}{2}(\|\phi^{n+1}-\phi^n\|^2+\|\phi^{n+1}-\phi^n\|_\Gamma^2).\end{aligned}\tag{2.8}$$

Proof Let $\xi=(-\Delta)^{-1}(\phi^{n+1}-\phi^n)$, $\zeta=(-\Delta_\Gamma)^{-1}(\phi^{n+1}-\phi^n)$, and $\eta=-(\phi^{n+1}-\phi^n)$. Substituting ξ,ζ and η into (2.5a)-(2.5c) gives

$$\begin{aligned}&\big(\delta_\tau\phi^{n+1},(-\Delta)^{-1}(\phi^{n+1}-\phi^n)\big)+\big(\delta_\tau\phi^{n+1},(-\Delta_\Gamma)^{-1}(\phi^{n+1}-\phi^n)\big)_\Gamma\\&=-\varepsilon^2\left(\nabla\phi^{n+1},\nabla(\phi^{n+1}-\phi^n)\right)-\kappa\varepsilon^2\left(\nabla_\Gamma\phi^{n+1},\nabla_\Gamma(\phi^{n+1}-\phi^n)\right)_\Gamma\\&-\big((\phi^{n+1})^3,\phi^{n+1}-\phi^n\big)-\big((\phi^{n+1})^3,\phi^{n+1}-\phi^n\big)_\Gamma\\&+\big((2\phi^n-\phi^{n-1}),\phi^{n+1}-\phi^n\big)+\big((2\phi^n-\phi^{n-1}),\phi^{n+1}-\phi^n\big)_\Gamma\\&-A_1\tau\left(\nabla(\phi^{n+1}-\phi^n),\nabla(\phi^{n+1}-\phi^n)\right)-A_2\tau\left(\nabla_\Gamma(\phi^{n+1}-\phi^n),\nabla_\Gamma(\phi^{n+1}-\phi^n)\right)_\Gamma\\&:=Y_1+Y_2+Y_3+Y_4+Y_5+Y_6+Y_7+Y_8,\end{aligned}\tag{2.9}$$

with $\delta_\tau\phi^{n+1}=\dfrac{3\phi^{n+1}-4\phi^n+\phi^{n-1}}{2\tau}$. In terms of the above inner product involving time difference in the bulk, we see that

$$\begin{aligned}&\left(\delta_\tau\phi^{n+1},(-\Delta)^{-1}(\phi^{n+1}-\phi^n)\right)\\=&\frac{1}{\tau}\|\phi^{n+1}-\phi^n\|_{-1}^2+\frac{1}{4\tau}\left(\|\phi^{n+1}-\phi^n\|_{-1}^2-\|\phi^n-\phi^{n-1}\|_{-1}^2\right)\\+&\frac{1}{4\tau}\|\phi^{n+1}-2\phi^n+\phi^{n-1}\|_{-1}^2.\end{aligned} \tag{2.10}$$

Furthermore, on the right hand side of (2.9), the estimates of bulk part Y_1 could be derived as follows:

$$\begin{aligned}Y_1&=-\varepsilon^2\left(\nabla\phi^{n+1},\nabla(\phi^{n+1}-\phi^n)\right)\\&=-\frac{\varepsilon^2}{2}\left(\|\nabla\phi^{n+1}\|^2-\|\nabla\phi^n\|^2\right)-\frac{\varepsilon^2}{2}\|\nabla(\phi^{n+1}-\phi^n)\|^2.\end{aligned}$$

Regarding the nonlinear term Y_3, an application of identity $4(a^4-a^3b)=(a^4-b^4)+(a^2-b^2)^2+2(a(a-b))^2$ reveals that

$$\begin{aligned}Y_3=&-\left((\phi^{n+1})^3,\phi^{n+1}-\phi^n\right)\\=&-\frac{1}{4}(\|\phi^{n+1}\|_{L^4}^4-\|\phi^n\|_{L^4}^4)-\frac{1}{4}\|(\phi^{n+1})^2-(\phi^n)^2\|^2\\&-\frac{1}{2}\|\phi^{n+1}(\phi^{n+1}-\phi^n)\|^2.\end{aligned}$$

Similarly, based on the equality

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

the term Y_5 turns out to be

$$\begin{aligned}Y_5=&\left((2\phi^n-\phi^{n-1}),\phi^{n+1}-\phi^n\right)\\=&\frac{1}{2}(\|\phi^{n+1}\|^2-\|\phi^{n+1}-\phi^n\|^2)-\frac{1}{2}(\|\phi^n\|^2-\|\phi^n-\phi^{n-1}\|^2)\\&-\frac{1}{2}\|\phi^{n+1}-2\phi^n+\phi^{n-1}\|^2+\frac{1}{2}\|\phi^{n+1}-\phi^n\|^2.\end{aligned}$$

The Douglas-Dupont regularization part is introduced to bound the positive part $\frac{1}{2}\|\phi^{n+1}-\phi^n\|^2$ of Y_5, and it is straightforward to see that

$$Y_7=-A_1\tau\|\nabla(\phi^{n+1}-\phi^n)\|^2.$$

Meanwhile, inner products related to boundary Γ could be analyzed in the same way. A combination of all these estimates leads to

$$
\begin{aligned}
&\frac{\varepsilon^2}{2}\left(\|\nabla\phi^{n+1}\|^2-\|\nabla\phi^n\|^2\right)+\frac{\varepsilon^2\kappa}{2}\left(\|\nabla_\Gamma\phi^{n+1}\|_\Gamma^2-\|\nabla_\Gamma\phi^n\|_\Gamma^2\right)\\
&+\frac{1}{4}\left(\|\phi^{n+1}\|_{L^4}^4-\|\phi^n\|_{L^4}^4\right)+\frac{1}{4}\left(\|\phi^{n+1}\|_{L^4,\Gamma}^4-\|\phi^n\|_{L^4,\Gamma}^4\right)\\
&-\frac{1}{2}\left(\|\phi^{n+1}\|^2-\|\phi^n\|^2\right)-\frac{1}{2}\left(\|\phi^{n+1}\|_\Gamma^2-\|\phi^n\|_\Gamma^2\right)\\
&+\frac{1}{4\tau}\left(\|\phi^{n+1}-\phi^n\|_{-1}^2-\|\phi^n-\phi^{n-1}\|_{-1}^2\right)+\frac{1}{4\tau}\left(\|\phi^{n+1}-\phi^n\|_{-1,\Gamma}^2-\|\phi^n-\phi^{n-1}\|_{-1,\Gamma}^2\right)\\
&+\frac{1}{2}\left(\|\phi^{n+1}-\phi^n\|^2-\|\phi^n-\phi^{n-1}\|^2\right)+\frac{1}{2}\left(\|\phi^{n+1}-\phi^n\|_\Gamma^2-\|\phi^n-\phi^{n-1}\|_\Gamma^2\right)\\
&+\frac{1}{\tau}\|\phi^{n+1}-\phi^n\|_{-1}^2-\frac{1}{2}\|\phi^{n+1}-\phi^n\|^2+A_1\tau\|\nabla(\phi^{n+1}-\phi^n)\|^2\\
&+\frac{1}{\tau}\|\phi^{n+1}-\phi^n\|_{-1,\Gamma}^2-\frac{1}{2}\|\phi^{n+1}-\phi^n\|_\Gamma^2+A_2\tau\|\nabla_\Gamma(\phi^{n+1}-\phi^n)\|_\Gamma^2\\
&=-\frac{\varepsilon^2}{2}\|\nabla(\phi^{n+1}-\phi^n)\|^2-\frac{\varepsilon^2}{2}\|\nabla_\Gamma(\phi^{n+1}-\phi^n)\|_\Gamma^2\\
&-\frac{1}{4\tau}\|\phi^{n+1}-2\phi^n+\phi^{n-1}\|_{-1}^2-\frac{1}{4\tau}\|\phi^{n+1}-2\phi^n+\phi^{n-1}\|_{-1,\Gamma}^2\\
&-\frac{1}{4}\|(\phi^{n+1})^2-(\phi^n)^2\|^2-\frac{1}{4}\|(\phi^{n+1})^2-(\phi^n)^2\|_\Gamma^2\\
&-\frac{1}{2}\|\phi^{n+1}(\phi^{n+1}-\phi^n)\|^2-\frac{1}{2}\|\phi^{n+1}(\phi^{n+1}-\phi^n)\|_\Gamma^2\\
&\leqslant 0.
\end{aligned}
\tag{2.11}
$$

Subsequently, this inequality could be rewritten as

$$
\begin{aligned}
&E(\phi^{n+1},\phi^n)-E(\phi^n,\phi^{n-1})\\
&+\frac{1}{\tau}\|\phi^{n+1}-\phi^n\|_{-1}^2-\frac{1}{2}\|\phi^{n+1}-\phi^n\|^2+A_1\tau\|\nabla(\phi^{n+1}-\phi^n)\|^2\\
&+\frac{1}{\tau}\|\phi^{n+1}-\phi^n\|_{-1,\Gamma}^2-\frac{1}{2}\|\phi^{n+1}-\phi^n\|_\Gamma^2+A_2\tau\|\nabla_\Gamma(\phi^{n+1}-\phi^n)\|_\Gamma^2\\
&\leqslant 0.
\end{aligned}
\tag{2.12}
$$

On the other hand, an application of Cauchy-Schwarz inequality implies that

$$
\begin{aligned}
\frac{1}{2}\|\phi^{n+1}-\phi^n\|^2 &\leqslant \frac{1}{2}\|\nabla(\phi^{n+1}-\phi^n)\|\cdot\|\phi^{n+1}-\phi^n\|_{-1}\\
&\leqslant \frac{\tau}{4\alpha}\|\nabla(\phi^{n+1}-\phi^n)\|^2+\frac{\alpha}{4\tau}\|\phi^{n+1}-\phi^n\|_{-1}^2,\quad \forall\alpha>0.
\end{aligned}
$$

In turn, by taking $\alpha=\dfrac{1}{4A_1}$, and using the same trick on the boundary part, we finally arrive at

$$
\begin{aligned}
&E(\phi^{n+1},\phi^n)+\frac{1}{\tau}\Big(1-\frac{1}{16A_1}\Big)\|\phi^{n+1}-\phi^n\|_{-1}^2+\frac{1}{\tau}\Big(1-\frac{1}{16A_2}\Big)\|\phi^{n+1}-\phi^n\|_{-1,\Gamma}^2\\
&\leqslant E(\phi^n,\phi^{n-1}).
\end{aligned}
\tag{2.13}
$$

□

Following a similar procedure, it's analogical to verify the energy dissipation for the numerical solution at the initial time step, namely (2.4a)-(2.4e), and technical details are omitted for the sake of brevity.

Lemma 2.3 *The numerical solution at the initial time step, namely (2.4a)-(2.4e), preserves the following energy dissipation:*

$$E(\phi^1) + \frac{1}{\tau}\left(\|\phi^1 - \phi^0\|_{-1} + \|\phi^1 - \phi^0\|_{-1,\Gamma}\right) \leqslant E(\phi^0). \tag{2.14}$$

With the above energy estimates, we are able to verify that ϕ^n is uniformly bounded in $\mathcal{V}$, for any $n \geqslant 0$.

Lemma 2.4 *Assume an initial energy functional bound: $E(\phi^0) \leqslant C_0$. Then the numerical solution ϕ^n is uniformly bounded in $\mathcal{V}$.*

Proof Based on the equality $\frac{1}{4}\left(a^2-2\right)^2 = \frac{1}{4}a^4 + 1 - a^2$, the following quadratic inequality becomes available for any ϕ satisfying $\phi \in L^4(\Omega), \gamma\phi \in L^4(\Gamma)$:

$$\frac{1}{4}\left(\|\phi\|_{L^4}^4 + \|\phi\|_{L^4,\Gamma}^4\right) - \frac{1}{2}\left(\|\phi\|^2 + \|\phi\|_\Gamma^2\right) \geqslant \frac{1}{2}\left(\|\phi\|^2 + \|\phi\|_\Gamma^2\right) - |\Omega| - |\Gamma|, \tag{2.15}$$

where $|\cdot|$ stands for the measure of the domains. Then we get

$$\frac{1}{2}\|\phi^n\|^2 + \frac{\varepsilon^2}{2}\|\nabla\phi^n\|^2 + \frac{1}{2}\|\phi^n\|_\Gamma^2 + \frac{\kappa\varepsilon^2}{2}\|\nabla\phi^n\|_\Gamma^2 \leqslant E(\phi^n) + |\Omega| + |\Gamma|, \quad \forall n \geq 0. \tag{2.16}$$

With the help of definition (2.8), a combination of (2.14) and (2.16) implies that

$$\begin{aligned} E(\phi^1,\phi^0) &= E(\phi^1) + \frac{1}{4\tau}\left(\|\phi^1-\phi^0\|_{-1}^2 + \|\phi^1-\phi^0\|_{-1,\Gamma}^2\right) + \frac{1}{2}\left(\|\phi^1-\phi^0\|^2 + \|\phi^1-\phi^0\|_\Gamma^2\right) \\ &\leqslant E(\phi^0) + \frac{1}{2}\left(\|\phi^1-\phi^0\|^2 + \|\phi^1-\phi^0\|_\Gamma^2\right) \\ &\leqslant E(\phi^0) + \left(\|\phi^1\|^2 + \|\phi^1\|_\Gamma^2\right) + \left(\|\phi^0\|^2 + \|\phi^0\|_\Gamma^2\right) \\ &\leqslant 5E(\phi^0) + 4\left(|\Omega| + |\Gamma|\right). \end{aligned} \tag{2.17}$$

In turn, the following bound becomes valid:

$$E(\phi^{n+1}) \leqslant E(\phi^{n+1}, \phi^n) \leqslant E(\phi^1, \phi^0) \leqslant 5E(\phi^0) + 4\left(|\Omega| + |\Gamma|\right).$$

With an application of (2.16) again, we finally arrive at

$$\|\phi^{n+1}\|^2 + \varepsilon^2\|\nabla\phi^{n+1}\|^2 + \|\phi^{n+1}\|_\Gamma^2 + \kappa\varepsilon^2\|\nabla\phi^{n+1}\|_\Gamma^2 \leqslant 10\left(E(\phi^0) + |\Omega| + |\Gamma|\right).$$

□

When considering the fully discrete scheme, a uniform $H_h^1(\Omega)$ and $H_h^1(\Gamma)$ bound could be derived for the numerical solution ϕ_h^n, which is helpful to the convergence analysis. Here the symbol H_h^1 means a discretized version of H^1 norm, for example the same as H^1 norm when using conforming element like Lagrange element, or $\|\phi_h\|_{1,h}^2 := \|\phi\|^2 + \|\nabla_h\phi\|^2$, with ∇_h being piecewise gradient operator, for non-conforming element like CR element.

2.3 Unique solvability of the semi-discrete scheme

Unique solvability plays an important role to guarantee the well-posedness of proposed numerical scheme, and in this subsection we will construct a variational problem, since the variational problem is strictly convex, there exists a unique global minimizer for the variational problem, which exactly fulfills the weak formulation (2.5a)-(2.5c). This approach has been widely used in the existing numerical analysis, see [13, 15, 18], etc.

Lemma 2.5 *Define a strictly convex functional J_n over space K, where*

$$\begin{aligned} J_n(v) = {} & \frac{\varepsilon^2}{2}\|\nabla v\|^2 + \frac{1}{4}\|v\|_{L^4}^4 - \left(2\phi^n - \phi^{n-1}, v\right) \\ & + \frac{\kappa\varepsilon^2}{2}\|\nabla_\Gamma v\|_\Gamma^2 + \frac{1}{4}\|v\|_{L^4,\Gamma}^4 - \left(2\phi^n - \phi^{n-1}, v\right)_\Gamma \\ & + \frac{1}{3\tau}\left\|\frac{3v - 4\phi^n + \phi^{n-1}}{2}\right\|_{-1}^2 + \frac{A_1\tau}{2}\|\nabla v - \nabla\phi^n\|^2 \\ & + \frac{1}{3\tau}\left\|\frac{3v - 4\phi^n + \phi^{n-1}}{2}\right\|_{-1,\Gamma}^2 + \frac{A_2\tau}{2}\|\nabla_\Gamma v - \nabla_\Gamma\phi^n\|_\Gamma^2, \end{aligned} \tag{2.18}$$

and

$$K := \{v \in \mathcal{V}, (v, 1) = \left(\phi^0, 1\right), (v, 1)_\Gamma = \left(\phi^0, 1\right)_\Gamma\}. \tag{2.19}$$

Then there exists a unique global minimizer of J_n, and the minimizer is equivalent to the numerical solution of (2.5a)-(2.5c).

Proof It's obvious to see that J_n is coercive and strictly convex over K, thus the global minimizer exists and is unique [11], and we only need to verify the minimizer fulfills (2.5a)-(2.5c). For simplicity, the following space is defined:

$$K_0 := \{v \in \mathcal{V}, (v,1) = 0, (v,1)_\Gamma = 0\}.$$

Assume ϕ^{n+1} is a minimizer of the above problem. Then for all $\eta \in K_0$, we see that

$$\lim_{\alpha \to 0} \frac{J_n(\phi^{n+1} + \alpha\eta) - J_n(\phi^{n+1})}{\alpha} = 0. \tag{2.20}$$

An application of integration by parts leads to

$$\begin{aligned}
&-\Big((-\Delta)^{-1}\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\tau}, \eta\Big) - \Big((-\Delta_\Gamma)^{-1}\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\tau}, \eta\Big)_\Gamma \\
&= \varepsilon^2 \left(\nabla\phi^{n+1}, \nabla\eta\right) + \kappa\varepsilon^2 \left(\nabla_\Gamma\phi^{n+1}, \nabla_\Gamma\eta\right)_\Gamma \\
&+ \left((\phi^{n+1})^3, \eta\right) - \left(2\phi^n - \phi^{n-1}, \eta\right) \\
&+ \left((\phi^{n+1})^3, \eta\right)_\Gamma - \left(2\phi^n - \phi^{n-1}, \eta\right)_\Gamma \\
&+ A_1\tau \left(\nabla\phi^{n+1} - \nabla\phi^n, \nabla\eta\right) + A_2\tau \left(\nabla_\Gamma\phi^{n+1} - \nabla_\Gamma\phi^n, \nabla_\Gamma\eta\right)_\Gamma .
\end{aligned}$$

Meanwhile, we denote

$$\begin{aligned}
\mathring{u}^{n+1} &= -(-\Delta)^{-1}\Big(\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\tau}\Big), \\
\mathring{u}_\Gamma^{n+1} &= -(-\Delta_\Gamma)^{-1}\Big(\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\tau}\Big),
\end{aligned} \tag{2.21}$$

so that $\mathring{u}^{n+1} \in \mathring{H}^1(\Omega)$, $\mathring{u}_\Gamma^{n+1} \in \mathring{H}^1(\Gamma)$ is the unique solution to

$$\begin{aligned}
&\Delta u = \frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\tau} \quad \text{in } \Omega \quad \text{with} \quad \frac{\partial}{\partial n}u = 0 \quad \text{on } \Gamma, \\
&\Delta_\Gamma u_\Gamma = \frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\tau} \quad \text{on } \Gamma.
\end{aligned}$$

In turn, the following equalities are valid:

$$\begin{aligned}
\Big(\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\tau}, \xi\Big) &= -\left(\nabla\mathring{u}^{n+1}, \nabla\xi\right), \quad \forall\xi \in H^1(\Omega), \\
\Big(\frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\tau}, \zeta\Big)_\Gamma &= -\left(\nabla_\Gamma\mathring{u}^{n+1}, \nabla_\Gamma\zeta\right)_\Gamma, \quad \forall\zeta \in H^1(\Gamma), \\
\left(\mathring{u}^{n+1}, \eta\right) + \left(\mathring{u}_\Gamma^{n+1}, \eta\right)_\Gamma &= \varepsilon^2 \left(\nabla\phi^{n+1}, \nabla\eta\right) + \kappa\varepsilon^2 \left(\nabla_\Gamma\phi^{n+1}, \nabla_\Gamma\eta\right)_\Gamma \\
&+ \left((\phi^{n+1})^3, \eta\right) - \left(2\phi^n - \phi^{n-1}, \eta\right) \\
&+ \left((\phi^{n+1})^3, \eta\right)_\Gamma - \left(2\phi^n - \phi^{n-1}, \eta\right)_\Gamma \\
&+ A_1\tau \left(\nabla\phi^{n+1} - \nabla\phi^n, \nabla\eta\right) \\
&+ A_2\tau \left(\nabla_\Gamma\phi^{n+1} - \nabla_\Gamma\phi^n, \nabla_\Gamma\eta\right)_\Gamma, \quad \forall\eta \in K_0.
\end{aligned} \tag{2.22}$$

Next, as $\eta \in K_0$ has a zero-integral constraint, we want to construct $u^{n+1} = \mathring{u}^{n+1} + c^{n+1}, u_\Gamma^{n+1} = \mathring{u}_\Gamma^{n+1} + c_\Gamma^{n+1}, c^{n+1}, c_\Gamma^{n+1} \in \mathbb{R}$ such that (2.22) holds for all test function $\eta \in \mathcal{V}$ with $\left(\mathring{u}^{n+1}, \mathring{u}_\Gamma^{n+1}\right)$ substituted by $\left(u^{n+1}, u_\Gamma^{n+1}\right)$. In turn, given an arbitrary $\eta \in \mathcal{V}$, an alternate test function η_0 could be defined as

$$\eta_0 = \eta - c_1 - c_2\eta_1, \quad c_1, c_2 \in \mathbb{R},$$

in which $\eta_1 \in C_c^\infty(\Omega)$ is an arbitrary non-negative function that is not identically zero. Moreover, the values of c_1 and c_2 could be specified as

$$c_1 = \frac{1}{|\Gamma|}\int_\Gamma \eta \, \mathrm{d}s, \quad c_2 = \left(\int_\Omega \eta \, \mathrm{d}x - \frac{|\Omega|}{|\Gamma|}\int_\Gamma \eta \, \mathrm{d}s\right) \Big/ \int_\Omega \eta_1 \, \mathrm{d}x.$$

In fact, it is obvious to verify that $\eta_0 \in K_0$. Taking test function as η_0 with this definition in the third equation of (2.22), we get

$$\begin{aligned}
&\left(\mathring{u}^{n+1}, \eta\right) + \left(\mathring{u}_\Gamma^{n+1}, \eta\right)_\Gamma - c_2\left(\mathring{u}^{n+1}, \eta_1\right) + c_2\varepsilon^2\left(\nabla\phi^{n+1}, \nabla\eta_1\right) \\
&+ c_1\left((\phi^{n+1})^3, 1\right) + c_2\left((\phi^{n+1})^3, \eta_1\right) - c_1\left(2\phi^n - \phi^{n-1}, 1\right) - c_2\left(2\phi^n - \phi^{n-1}, \eta_1\right) \\
&+ c_1\left((\phi^{n+1})^3, 1\right)_\Gamma - c_1\left(2\phi^n - \phi^{n-1}, 1\right)_\Gamma + c_2A_1\tau\left(\nabla\phi^{n+1} - \nabla\phi^n, \nabla\eta_1\right) \\
=&\varepsilon^2\left(\nabla\phi^{n+1}, \nabla\eta\right) + \kappa\varepsilon^2\left(\nabla_\Gamma\phi^{n+1}, \nabla_\Gamma\eta\right)_\Gamma \\
&+ \left((\phi^{n+1})^3, \eta\right) - \left(2\phi^n - \phi^{n-1}, \eta\right) \\
&+ \left((\phi^{n+1})^3, \eta\right)_\Gamma - \left(2\phi^n - \phi^{n-1}, \eta\right)_\Gamma \\
&+ A_1\tau\left(\nabla\phi^{n+1} - \nabla\phi^n, \nabla\eta\right) + A_2\tau\left(\nabla_\Gamma\phi^{n+1} - \nabla_\Gamma\phi^n, \nabla_\Gamma\eta\right)_\Gamma.
\end{aligned} \tag{2.23}$$

Furthermore, the left hand side of (2.23) could be represented as $(u^{n+1}, \eta) + (u_\Gamma^{n+1}, \eta)_\Gamma$, with u^{n+1}, u_Γ^{n+1} defined as

$$\begin{aligned}
&u^{n+1} := \mathring{u}^{n+1} + c^{n+1}, \qquad u_\Gamma^{n+1} := \mathring{u}_\Gamma^{n+1} + c_\Gamma^{n+1}, \\
&c^{n+1} := \frac{1}{(1, \eta_1)}\left(-\left(\mathring{u}^{n+1}, \eta_1\right) + \varepsilon^2\left(\nabla\phi^{n+1}, \nabla\eta_1\right) + \left((\phi^{n+1})^3, \eta_1\right)\right) \\
&\qquad + \frac{1}{(1, \eta_1)}\left(-\left(2\phi^n - \phi^{n-1}, \eta_1\right) + A_1\tau\left(\nabla\phi^{n+1} - \nabla\phi^n, \nabla\eta_1\right)\right), \\
&c_\Gamma^{n+1} := -\frac{|\Omega|}{|\Gamma|}c^{n+1} \\
&\qquad + \frac{1}{|\Gamma|}\left(\left((\phi^{n+1})^3, 1\right) - \left(2\phi^n - \phi^{n-1}, 1\right) + \left((\phi^{n+1})^3, 1\right)_\Gamma - \left(2\phi^n - \phi^{n-1}, 1\right)_\Gamma\right).
\end{aligned} \tag{2.24}$$

As a result, identity (2.22) holds for all $\eta \in \mathcal{V}$ with $\left(\mathring{u}^{n+1}, \mathring{u}_\Gamma^{n+1}\right)$ substituted by $\left(u^{n+1}, u_\Gamma^{n+1}\right)$, and the variables $(\phi^{n+1}, u^{n+1}, u_\Gamma^{n+1})$ fulfill the weak formulation (2.5a)-(2.5c). □

In Lemma 2.5, the constructed variational problem is strictly convex, since the convex splitting method is used in the numerical scheme. Otherwise, the existence and uniqueness of the global minimizer could not be directly guaranteed. Besides, the uniqueness of the numerical solution could also be verified by the energy dissipation result in Theorem 2.2.

3 Convergence analysis

3.1 Convergence analysis for the semi-discrete scheme

In this subsection we provide a detailed convergence analysis for the semi-discrete scheme (2.5a)-(2.5c). First, the discrete Gronwall inequality [24] is recalled.

Lemma 3.1 *For fixed $T = N\tau$, here N is positive integer, $\tau > 0$. Assume that $\{a^n\}_{n=1}^{N}, \{b^n\}_{n=1}^{N}, \{c^n\}_{n=1}^{N-1}$ are non-negative sequences, and for all $\tau > 0$, the following inequalities hold:*

$$
\begin{aligned}
&\tau \sum_{n=1}^{N-1} c^n \leqslant C_1, \\
&a^N + \tau \sum_{n=1}^{N} b^n \leqslant C_2 + \tau \sum_{n=1}^{N-1} a^n c^n,
\end{aligned} \tag{3.1}
$$

where C_1, C_2 are positive numbers and C_1 are independent of τ but may depend on T, then we have

$$
a^N + \tau \sum_{n=1}^{N} b^n \leqslant (C_2 + \tau a^0 c^0) e^{C_1}. \tag{3.2}
$$

Some notations are introduced. Denote $e_\phi^n := \phi(t^n) - \phi^n, e_u^n := u(t^n) - u^n, e_\Gamma^n := u_\Gamma(t^n) - u_\Gamma^n$ the error functions at time t^n. Then we have

$$
\Big(\frac{3e_\phi^{n+1} - 4e_\phi^n + e_\phi^{n-1}}{2\tau}, \xi\Big) = \big(-\nabla e_u^{n+1}, \nabla \xi\big) + (R_\phi^{n+1}, \xi), \tag{3.3a}
$$

$$
\Big(\frac{3e_\phi^{n+1} - 4e_\phi^n + e_\phi^{n-1}}{2\tau}, \zeta\Big)_\Gamma = \big(-\nabla_\Gamma e_u^{n+1}, \nabla_\Gamma \zeta\big)_\Gamma + (R_\phi^{n+1}, \zeta)_\Gamma, \tag{3.3b}
$$

$$
\begin{aligned}
(e_u^{n+1},\eta)+(e_\Gamma^{n+1},\eta)_\Gamma =& \varepsilon^2(\nabla e_\phi^{n+1},\nabla\eta)+\kappa\varepsilon^2(\nabla_\Gamma e_\phi^{n+1},\nabla_\Gamma\eta)_\Gamma\\
&+\left(\phi^3(t^{n+1})-(\phi^{n+1})^3,\eta\right)-\Big((2e_\phi^n-e_\phi^{n-1}),\eta\Big)\\
&+\left(\phi^3(t^{n+1})-(\phi^{n+1})^3,\eta\right)_\Gamma-\Big((2e_\phi^n-e_\phi^{n-1}),\eta\Big)_\Gamma\\
&+\left(T^{n+1},\eta\right)+\left(T^{n+1},\eta\right)_\Gamma\\
&+A_1\tau\left(\nabla(e_\phi^{n+1}-e_\phi^n),\nabla\eta\right)-A_1\tau\left(\nabla(\phi(t^{n+1})-\phi(t^n)),\nabla\eta\right)\\
&+A_2\tau\left(\nabla_\Gamma(e_\phi^{n+1}-e_\phi^n),\nabla_\Gamma\eta\right)_\Gamma-A_2\tau\left(\nabla_\Gamma(\phi(t^{n+1})-\phi(t^n)),\nabla_\Gamma\eta\right)_\Gamma,
\end{aligned}
\tag{3.3c}
$$

in which

$$
\begin{aligned}
R_\phi^{n+1}&=\frac{3\phi(t^{n+1})-4\phi(t^n)+\phi(t^{n-1})}{2\tau}-\partial_t\phi(t^{n+1}),\\
T^{n+1}&=-\phi(t^{n+1})+2\phi(t^n)-\phi(t^{n-1}),
\end{aligned}
$$

are the truncation error functions arose from time difference and Adams extrapolation respectively.

The exact solution $\phi(t)$ is assumed to satisfy the following regularity:

$$
\begin{aligned}
&\int_0^T\|\partial_t\nabla\phi(t)\|^2\mathrm{d}t\leqslant C, && \int_0^T\|\partial_t\nabla_\Gamma\phi(t)\|_\Gamma^2\mathrm{d}t\leqslant C,\\
&\int_0^T\|\Delta^{-1}\partial_{ttt}\phi(t)\|_{-1}^2\mathrm{d}t\leqslant C, && \int_0^T\|\Delta_\Gamma^{-1}\partial_{ttt}\phi(t)\|_{-1,\Gamma}^2\mathrm{d}t\leqslant C,\\
&\int_0^T\|\partial_{tt}\phi(t)\|_{-1}^2\mathrm{d}t\leqslant C, && \int_0^T\|\partial_{tt}\phi(t)\|_{-1,\Gamma}^2\mathrm{d}t\leqslant C,
\end{aligned}
\tag{3.4}
$$

and the initial step numerical error is assumed to preserve the following bound:

$$
\begin{aligned}
&\|e_\phi^1\|^2+\tau^2\|\nabla e_\phi^1\|^2\leqslant C\tau^4,\\
&\|e_\phi^1\|_\Gamma^2+\tau^2\|\nabla_\Gamma e_\phi^1\|_\Gamma^2\leqslant C\tau^4.
\end{aligned}
\tag{3.5}
$$

Theorem 3.2 *Under the assumption (3.4), (3.5), for fixed $T=N\tau$, we have the following error estimate:*

$$
\|e_\phi^N\|_{-1}+\|e_\phi^N\|_{-1,\Gamma}\leqslant C\tau^2.
\tag{3.6}
$$

Proof A substitution of $\xi=(-\Delta)^{-1}e_\phi^{n+1}$, $\zeta=(-\Delta_\Gamma)^{-1}e_\phi^{n+1}$ and $\eta=-e_\phi^{n+1}$ into (3.3a)-(3.3c) gives

$$
\begin{aligned}
&\Big(\delta_\tau e_\phi^{n+1}, (-\Delta)^{-1} e_\phi^{n+1}\Big) + \Big(\delta_\tau e_\phi^{n+1}, (-\Delta_\Gamma)^{-1} e_\phi^{n+1}\Big)_\Gamma \\
&+ \varepsilon^2 (\nabla e_\phi^{n+1}, \nabla e_\phi^{n+1}) + \kappa\varepsilon^2 (\nabla_\Gamma e_\phi^{n+1}, \nabla_\Gamma e_\phi^{n+1})_\Gamma \\
&+ A_1\tau\Big(\nabla(e_\phi^{n+1} - e_\phi^n), \nabla e_\phi^{n+1}\Big) + A_2\tau\Big(\nabla_\Gamma(e_\phi^{n+1} - e_\phi^n), \nabla_\Gamma e_\phi^{n+1}\Big)_\Gamma \\
&= -\Big(\phi^3(t^{n+1}) - (\phi^{n+1})^3, e_\phi^{n+1}\Big) - \Big(\phi^3(t^{n+1}) - (\phi^{n+1})^3, e_\phi^{n+1}\Big)_\Gamma \\
&+ (2e_\phi^n - e_\phi^{n-1}, e_\phi^{n+1}) + (2e_\phi^n - e_\phi^{n-1}, e_\phi^{n+1})_\Gamma \\
&+ A_1\tau\Big(\nabla(\phi(t^{n+1}) - \phi(t^n)), \nabla e_\phi^{n+1}\Big) + A_2\tau\Big(\nabla_\Gamma(\phi(t^{n+1}) - \phi(t^n)), \nabla_\Gamma e_\phi^{n+1}\Big)_\Gamma \\
&+ (R_\phi^{n+1}, (-\Delta)^{-1} e_\phi^{n+1}) + (R_\phi^{n+1}, (-\Delta)^{-1} e_\phi^{n+1})_\Gamma - (T^{n+1}, e_\phi^{n+1}) - (T^{n+1}, e_\phi^{n+1})_\Gamma \\
&:= J_1 + J_2 + J_3 + J_4 + J_5 + J_6 + J_7 + J_8 + J_9 + J_{10}.
\end{aligned}
\tag{3.7}
$$

The estimates of inner product in the bulk are derived in details, and similar results hold for the inner product on the boundary. In terms of left hand side terms of (3.7), we see that

$$
\begin{aligned}
\Big(\frac{3e_\phi^{n+1} - 4e_\phi^n + e_\phi^{n-1}}{2\tau}, (-\Delta)^{-1} e_\phi\Big) &\geqslant \frac{1}{4\tau}(\|e_\phi^{n+1}\|_{-1}^2 - \|e_\phi^n\|_{-1}^2) \\
&\quad + \frac{1}{4\tau}(\|2e_\phi^{n+1} - e_\phi^n\|_{-1}^2 - \|2e_\phi^n - e_\phi^{n-1}\|_{-1}^2), \\
\varepsilon^2(\nabla e_\phi^{n+1}, \nabla e_\phi^{n+1}) &= \varepsilon^2 \|\nabla e_\phi^{n+1}\|^2, \\
A_1\tau\Big(\nabla(e_\phi^{n+1} - e_\phi^n), \nabla e_\phi^{n+1}\Big) &\geqslant \frac{A_1\tau}{2}(\|\nabla e_\phi^{n+1}\|^2 - \|\nabla e_\phi^n\|^2).
\end{aligned}
$$

The right hand side terms of (3.7) have to be separately analyzed. Because of the convexity of $y = x^4$, the following inequality is obvious:

$$
J_1 = -\Big(\phi^3(t^{n+1}) - (\phi^{n+1})^3, e_\phi^{n+1}\Big) = -\left(\phi^3(t^{n+1}) - (\phi^{n+1})^3, \phi(t^{n+1}) - \phi^{n+1}\right) \leqslant 0.
\tag{3.8}
$$

Based on the definition of inverse Laplacian and Cauchy-Schwarz inequality, the following bound becomes available for all $f \in L_0^2(\Omega)$ and $g \in L^2(\Omega)$ and $c \in \mathbb{R}^+$:

$$
(f, g) = (-\Delta(-\Delta)^{-1} f, g) = (\nabla(-\Delta)^{-1} f, \nabla g) \leqslant c\|f\|_{-1}^2 + \frac{1}{4c}\|\nabla g\|^2.
$$

As a result, it follows that

$$
\begin{aligned}
J_3 &= (2e_\phi^n - e_\phi^{n-1}, e_\phi^{n+1}) \leqslant \frac{\varepsilon^2}{8}\|\nabla e_\phi^{n+1}\|^2 + \frac{2}{\varepsilon^2}\|2e_\phi^n - e_\phi^{n-1}\|_{-1}^2, \\
J_5 &= A_1\tau\Big(\nabla(\phi(t^{n+1}) - \phi(t^n)), \nabla e_\phi^{n+1}\Big) \\
&\leqslant \frac{2A_1^2\tau^2}{\varepsilon^2}\|\nabla\phi(t^{n+1}) - \nabla\phi(t^n)\|^2 + \frac{\varepsilon^2}{8}\|\nabla e_\phi^{n+1}\|^2, \\
J_7 &= \Big(R_\phi^{n+1}, (-\Delta)^{-1}e_\phi^{n+1}\Big) \leqslant 2\varepsilon^{-2}\|\Delta^{-1}R_\phi^{n+1}\|_{-1}^2 + \frac{\varepsilon^2}{8}\|\nabla e_\phi^{n+1}\|^2, \\
J_9 &= -(T^{n+1}, e_\phi^{n+1}) \leqslant 2\varepsilon^{-2}\|T^{n+1}\|_{-1}^2 + \frac{\varepsilon^2}{8}\|\nabla e_\phi^{n+1}\|^2.
\end{aligned}
$$

A combination of the above estimates yields

$$
\begin{aligned}
&\frac{1}{4\tau}\Big(\|e_\phi^{n+1}\|_{-1}^2 - \|e_\phi^n\|_{-1}^2 + \|2e_\phi^{n+1} - e_\phi^n\|_{-1}^2 - \|2e_\phi^n - e_\phi^{n-1}\|_{-1}^2\Big) + \varepsilon^2\|\nabla e_\phi^{n+1}\|^2 \\
&+ \frac{1}{4\tau}\Big(\|e_\phi^{n+1}\|_{-1,\Gamma}^2 - \|e_\phi^n\|_{-1,\Gamma}^2 + \|2e_\phi^{n+1} - e_\phi^n\|_{-1,\Gamma}^2 - \|2e_\phi^n - e_\phi^{n-1}\|_{-1,\Gamma}^2\Big) \\
&+ \kappa\varepsilon^2\|\nabla e_\phi^{n+1}\|_\Gamma^2 + \frac{A_1\tau}{2}(\|\nabla e_\phi^{n+1}\|^2 - \|\nabla e_\phi^n\|^2) + \frac{A_2\tau}{2}(\|\nabla e_\phi^{n+1}\|_\Gamma^2 - \|\nabla e_\phi^n\|_\Gamma^2) \\
&\leqslant \frac{\varepsilon^2}{2}\|\nabla e_\phi^{n+1}\|^2 + \frac{\kappa\varepsilon^2}{2}\|\nabla_\Gamma e_\phi^{n+1}\|_\Gamma^2 + \frac{2}{\varepsilon^2}\|2e_\phi^n - e_\phi^{n-1}\|_{-1}^2 + \frac{2}{\kappa\varepsilon^2}\|2e_\phi^n - e_\phi^{n-1}\|_{-1,\Gamma}^2 \\
&+ \frac{2A_1^2\tau^2}{\varepsilon^2}\|\nabla\phi(t^{n+1}) - \nabla\phi(t^n)\|^2 + \frac{2A_2^2\tau^2}{\kappa\varepsilon^2}\|\nabla_\Gamma\phi(t^{n+1}) - \nabla_\Gamma\phi(t^n)\|_\Gamma^2 \\
&+ \frac{2}{\varepsilon^2}\|\Delta^{-1}R_\phi^{n+1}\|_{-1}^2 + \frac{2}{\kappa\varepsilon^2}\|\Delta_\Gamma^{-1}R_\phi^{n+1}\|_{-1,\Gamma}^2 + \frac{2}{\varepsilon^2}\|T^{n+1}\|_{-1}^2 + \frac{2}{\kappa\varepsilon^2}\|T^{n+1}\|_{-1,\Gamma}^2.
\end{aligned}
\tag{3.9}
$$

Furthermore, the truncation error terms are analyzed. For example, the term $\|\nabla\phi(t^{n+1}) - \nabla\phi(t^n)\|^2$ could be bounded as follows:

$$
\begin{aligned}
\|\nabla\phi(t^{n+1}) - \nabla\phi(t^n)\|^2 &= \int_\Omega \Big(\int_{t^n}^{t^{n+1}} \partial_t\nabla\phi(t)\mathrm{d}t\Big)^2 \mathrm{d}x \\
\leqslant \int_\Omega \tau \int_{t^n}^{t^{n+1}} (\partial_t\nabla\phi(t))^2\,\mathrm{d}t\mathrm{d}x &= \tau\int_{t^n}^{t^{n+1}} \|\partial_t\nabla\phi(t)\|^2\mathrm{d}t.
\end{aligned}
$$

Similarly, the following inequalities could be derived as well:

$$
\begin{aligned}
&\|\nabla_\Gamma\phi(t^{n+1})-\nabla_\Gamma\phi(t^n)\|_\Gamma^2 \leqslant C\tau\int_{t^n}^{t^{n+1}}\|\partial_t\nabla_\Gamma\phi(t)\|_\Gamma^2\mathrm{d}t,\\
&\|(-\Delta)^{-1}R_\phi^{n+1}\|_{-1}^2 \leqslant C\tau^3\int_{t^n}^{t^{n+1}}\|(-\Delta)^{-1}\partial_{ttt}\phi(t)\|_{-1}^2\mathrm{d}t,\\
&\|(-\Delta_\Gamma)^{-1}R_\phi^{n+1}\|_{-1,\Gamma}^2 \leqslant C\tau^3\int_{t^n}^{t^{n+1}}\|(-\Delta_\Gamma)^{-1}\partial_{ttt}\phi(t)\|_{-1,\Gamma}^2\mathrm{d}t,\\
&\|T^{n+1}\|_{-1}^2 \leqslant C\tau^3\int_{t^{n-1}}^{t^{n+1}}\|\partial_{tt}\phi(t)\|_{-1}^2\mathrm{d}t,\\
&\|T^{n+1}\|_{-1,\Gamma}^2 \leqslant C\tau^3\int_{t^{n-1}}^{t^{n+1}}\|\partial_{tt}\phi(t)\|_{-1,\Gamma}^2\mathrm{d}t.
\end{aligned}
\tag{3.10}
$$

For a fixed time $T=t^N$, a summation from $n=1$ to $n=N-1$ gives

$$
\begin{aligned}
&\frac{1}{4\tau}\Big(\|e_\phi^N\|_{-1}^2-\|e_\phi^1\|_{-1}^2+\|2e_\phi^N-e_\phi^{N-1}\|_{-1}^2-\|2e_\phi^1-e_\phi^0\|_{-1}^2\Big)+\sum_{n=2}^{N}\frac{\varepsilon^2}{2}\|\nabla e_\phi^n\|^2\\
&+\frac{1}{4\tau}\Big(\|e_\phi^N\|_{-1,\Gamma}^2-\|e_\phi^1\|_{-1,\Gamma}^2+\|2e_\phi^N-e_\phi^{N-1}\|_{-1,\Gamma}^2-\|2e_\phi^1-e_\phi^0\|_{-1,\Gamma}^2\Big)\\
&+\sum_{n=2}^{N}\frac{\kappa\varepsilon^2}{2}\|\nabla e_\phi^n\|_\Gamma^2+\frac{A_1\tau}{2}\left(\|\nabla e_\phi^N\|^2-\|\nabla e_\phi^1\|^2\right)+\frac{A_2\tau}{2}\left(\|\nabla_\Gamma e_\phi^N\|_\Gamma^2-\|\nabla_\Gamma e_\phi^1\|_\Gamma^2\right)\\
\leqslant&2\varepsilon^{-2}\sum_{n=1}^{N-1}\Big(\|2e_\phi^n-e_\phi^{n-1}\|_{-1}^2+\frac{1}{\kappa}\|2e_\phi^n-e_\phi^{n-1}\|_{-1,\Gamma}^2\Big)\\
&+2\tau^2\varepsilon^{-2}\Big(A_1^2\tau\int_{t^1}^{t^N}\|\partial_t\nabla\phi(t)\|^2\mathrm{d}t+\frac{A_2^2\tau}{\kappa}\int_{t^1}^{t^N}\|\partial_t\nabla_\Gamma\phi(t)\|_\Gamma^2\mathrm{d}t\Big)\\
&+2\varepsilon^{-2}\Big(C\tau^3\int_{t_1}^{t^N}\|\partial_{ttt}(-\Delta)^{-1}\phi(t)\|_{-1}^2\mathrm{d}t+C\kappa^{-1}\tau^3\int_{t_1}^{t^N}\|\partial_{ttt}(-\Delta_\Gamma)^{-1}\phi(t)\|_{-1,\Gamma}^2\mathrm{d}t\Big)\\
&+2\varepsilon^{-2}\Big(C\tau^3\int_{t_0}^{t^N}\|\partial_{tt}\phi(t)\|_{-1}^2\mathrm{d}t+C\kappa^{-1}\tau^3\int_{t_0}^{t^N}\|\partial_{tt}\phi(t)\|_{-1,\Gamma}^2\mathrm{d}t\Big).
\end{aligned}
\tag{3.11}
$$

Based on the regularity assumption of regularity for the exact solution and accuracy order for the initial numerical error, we see that

$$
\begin{aligned}
&\|e_\phi^N\|_{-1}^2 + \|e_\phi^N\|_{-1,\Gamma}^2 \\
\leqslant& C\tau^4 + 3\|e_\phi^1\|_{-1}^2 + 3\|e_\phi^1\|_{-1,\Gamma}^2 + 2A_1\tau^2\|\nabla e_\phi^1\|^2 + 2A_2\tau^2\|\nabla_\Gamma e_\phi^1\|_\Gamma^2 \\
&+ 8\varepsilon^{-2}\tau \sum_{n=1}^{N-1} \Big(\|2e_\phi^n - e_\phi^{n-1}\|_{-1}^2 + \frac{1}{\kappa}\|2e_\phi^n - e_\phi^{n-1}\|_{-1,\Gamma}^2 \Big) \\
\leqslant& C\tau^4 + 8\varepsilon^{-2}\tau \sum_{n=1}^{N-1} \Big(8\|e_\phi^n\|_{-1}^2 + 2\|e_\phi^{n-1}\|_{-1}^2 + \frac{1}{\kappa}(8\|e_\phi^n\|_{-1,\Gamma}^2 + 2\|e_\phi^{n-1}\|_{-1,\Gamma}^2) \Big) \\
\leqslant& C\tau^4 + 80\varepsilon^{-2}\tau \sum_{n=1}^{N-1} \Big(\|e_\phi^n\|_{-1}^2 + \frac{1}{\kappa}\|e_\phi^n\|_{-1,\Gamma}^2 \Big).
\end{aligned}
\tag{3.12}
$$

Finally, an application of discrete Gronwall inequality gives a second order error estimate for $\|e_\phi^N\|_{-1} + \|e_\phi^N\|_{-1,\Gamma}$. □

3.2 The spatial discretization

Let $\{\mathcal{T}_h\}$ be a quasi-uniform triangular or rectangular mesh over the physical domain Ω, $\{\mathcal{T}_h^\Gamma\}$ be the corresponding compatibility mesh on the boundary Γ. In other words,

$\{\mathcal{T}_h^\Gamma\}$ is consistent with the mesh $\{\mathcal{T}_h\}$ on the boundary. In turn, we are able to define the standard P_1 Lagrange element or Q_1 bilinear element over the physical domain. In this section we use P_1 Lagrange element as an example in the spatial discretization, and state the corresponding results. The technical details are skipped for the sake of brevity.

3.3 The fully-discrete numerical scheme

Let S_h denote the P_1 Lagrange element in the bulk, S_h^Γ the compatibility P_1 Lagrange element on the boundary:

$$
\begin{aligned}
S_h &:= \{u \in C^0(\Omega), u|_K \in P_1(K), \forall K \in \mathcal{T}_h\} \subset H^1(\Omega), \\
S_h^\Gamma &:= \{v \in C^0(\Gamma), v|_K^\Gamma \in P_1(K^\Gamma), \forall K^\Gamma \in \mathcal{T}_h^\Gamma\} \subset H^1(\Gamma).
\end{aligned}
$$

Subsequently, the weak formulation of the fully-discrete scheme becomes: Given $\phi_h^{n-1}, \phi_h^n \in S_h$, find $(\phi_h^{n+1}, u_h^{n+1}, u_{h,\Gamma}^{n+1}) \in S_h \times S_h \times S_h^\Gamma$ such that the following equalities hold for any $\xi_h \in S_h$, $\zeta_h \in S_h^\Gamma$, $\eta_h \in S_h$:

$$\Big(\frac{3\phi_h^{n+1}-4\phi_h^n+\phi_h^{n-1}}{2\tau},\xi_h\Big)=-\left(\nabla u_h^{n+1},\nabla\xi_h\right), \tag{3.13a}$$

$$\Big(\frac{3\phi_h^{n+1}-4\phi_h^n+\phi_h^{n-1}}{2\tau},\zeta_h\Big)_\Gamma=-\left(\nabla_\Gamma u_h^{n+1},\nabla_\Gamma\zeta_h\right)_\Gamma, \tag{3.13b}$$

$$\begin{aligned}(u_h^{n+1},\eta_h)+(u_{h,\Gamma}^{n+1},\eta)_\Gamma=&\ \varepsilon^2\left(\nabla\phi_h^{n+1},\nabla\eta_h\right)+\kappa\varepsilon^2\left(\nabla_\Gamma\phi_h^{n+1},\nabla_\Gamma\eta_h\right)_\Gamma\\&+\left((\phi_h^{n+1})^3,\eta_h\right)-\left(2\phi_h^n-\phi_h^{n-1},\eta_h\right)\\&+\left((\phi_h^{n+1})^3,\eta_h\right)_\Gamma-\left(2\phi_h^n-\phi_h^{n-1},\eta_h\right)_\Gamma\\&+A_1\tau\left(\nabla\phi_h^{n+1}-\nabla\phi_h^n,\nabla\eta_h\right)+A_2\tau\left(\nabla_\Gamma\phi_h^{n+1}-\nabla_\Gamma\phi_h^n,\nabla_\Gamma\eta_h\right)_\Gamma.\end{aligned} \tag{3.13c}$$

Moreover, the numerical values of ϕ_h^0 and ϕ_h^1 are needed in the initialization process. In terms of ϕ_h^0, we define the Ritz projection from $H^1(\Omega)$ to S_h such that $P_h\phi$ is the unique solution satisfying

$$\left(\nabla\left(P_h\phi-\phi\right),\nabla\chi_h\right)=0,\ \forall\chi_h\in S_h,\quad (P_h\phi-\phi,1)=0.$$

Of course, if the initial function ϕ^0 lies in $H^2(\Omega)$, then nodal interpolation is more convenient to define ϕ_h^0. In addition, we could extend (2.4a)-(2.4e) to the fully-discrete version to compute ϕ_h^1 (see [29] for a similar process). The following discrete mass conservation law is satisfied for (3.13a)-(3.13c)

Lemma 3.3 *If $\int_\Omega\phi_h^1\,dx=\int_\Omega\phi_h^0\,dx$, $\int_\Gamma\phi_h^1\,ds=\int_\Gamma\phi_h^0\,ds$, then the numerical solution of (3.13a)-(3.13c) the satisfies mass conservation in Ω and on Γ, respectively.*

3.4 Unique solvability and energy dissipation of the fully-discrete scheme

The following definitions will be used in the subsequent theorems.

Definition 3.4 For any Hilbert space V defined on D, and $V\subset L^2(D)$, define the zero mean space as $\mathring{V}=V\cup L_0^2(D)$.

Definition 3.5 For any $u_h\in S_h$, define discrete Laplacian $\Delta_h:S_h\to\mathring{S}_h$, and $\Delta_h u_h$ as the unique solution of

$$\left(\Delta_h u_h,\chi_h\right)=-\left(\nabla u_h,\nabla\chi_h\right),\quad\forall\chi_h\in S_h. \tag{3.14}$$

If we restrict the domain to $\mathring{S}_h$, then $\Delta_h : \mathring{S}_h \to \mathring{S}_h$ is invertible, and it satisfies

$$\left(\nabla(-\Delta_h)^{-1} u_h, \nabla \chi_h\right) = \left(u_h, \chi_h\right), \quad \forall \chi_h \in S_h. \tag{3.15}$$

Definition 3.6 For $u_h \in \mathring{S}_h$, define the discrete H^{-1} norm as $\|u_h\|_{-1,h} := \|\nabla \left(-\Delta_h\right)^{-1} u_h\|$.

Analogously, we could define the discrete Laplace–Beltrami operator $\Delta_{h,\Gamma} : S_h^\Gamma \to \mathring{S}_h^\Gamma$ and H^{-1} norm on the boundary: $\|v_h\|_{-1,h,\Gamma} := \|\nabla_\Gamma \left(-\Delta_{h,\Gamma}\right)^{-1} v_h\|_\Gamma$ for $v_h \in \mathring{S}_h^\Gamma$.

Theorem 3.7 *The numerical solution of scheme (3.13a)-(3.13c) preserves the following energy dissipation estimate with coefficients of Douglas–Dupont term satisfying* $A_1 \geqslant \frac{1}{16}, A_2 \geqslant \frac{1}{16}$.

$$E_h(\phi_h^{n+1}, \phi_h^n) + \frac{1}{\tau}\Big(1 - \frac{1}{16A_1}\Big)\|\phi_h^{n+1} - \phi_h^n\|_{-1,h}^2 + \frac{1}{\tau}\Big(1 - \frac{1}{16A_2}\Big)\|\phi_h^{n+1} - \phi_h^n\|_{-1,h,\Gamma}^2 \leqslant E_h(\phi_h^n, \phi_h^{n-1}),$$

where $E_h(\phi_h^{n+1}, \phi_h^n), n \geqslant 1$ *is given by*

$$\begin{aligned} E_h(\phi_h^{n+1}, \phi_h^n) = E(\phi_h^{n+1}) &+ \frac{1}{4\tau}(\|\phi_h^{n+1} - \phi_h^n\|_{-1,h}^2 + \|\phi_h^{n+1} - \phi_h^n\|_{-1,h,\Gamma}^2) \\ &+ \frac{1}{2}(\|\phi_h^{n+1} - \phi_h^n\|^2 + \|\phi_h^{n+1} - \phi_h^n\|_\Gamma^2). \end{aligned}$$

Lemma 3.8 *The solution to numerical scheme (3.13a)-(3.13c) is equivalent to the minimizer of functional* $J_{h,n}$ *in space* K_h*, where*

$$\begin{aligned} J_{h,n}(v_h) = &\frac{\varepsilon^2}{2}\|\nabla v_h\|^2 + \frac{1}{4}\|v_h\|_{L^4}^4 - \left(2\phi_h^n - \phi_h^{n-1}, v_h\right) \\ &+ \frac{\kappa\varepsilon^2}{2}\|\nabla_\Gamma v_h\|_\Gamma^2 + \frac{1}{4}\|v_h\|_{L^4,\Gamma}^4 - \left(2\phi_h^n - \phi_h^{n-1}, v_h\right)_\Gamma \\ &+ \frac{1}{3\tau}\|\frac{3v_h - 4\phi_h^n + \phi_h^{n-1}}{2}\|_{-1,h}^2 + \frac{A_1\tau}{2}\|\nabla v_h - \nabla\phi_h^n\|^2 \\ &+ \frac{1}{3\tau}\|\frac{3v_h - 4\phi_h^n + \phi_h^{n-1}}{2}\|_{-1,h,\Gamma}^2 + \frac{A_2\tau}{2}\|\nabla_\Gamma v_h - \nabla_\Gamma\phi_h^n\|_\Gamma^2, \end{aligned}$$

and

$$K_h := \{v_h \in S^h, (v_h, 1) = \left(\phi_h^0, 1\right), (v_h, 1)_\Gamma = \left(\phi_h^0, 1\right)_\Gamma\}.$$

The proof of Lemma 3.3, Theorem 3.7 and Lemma 3.8 are similar to Lemma 2.1, Theorem 2.2 and Lemma 2.5. We omit the proof and use numerical experiments to illustrate these properties in next section.

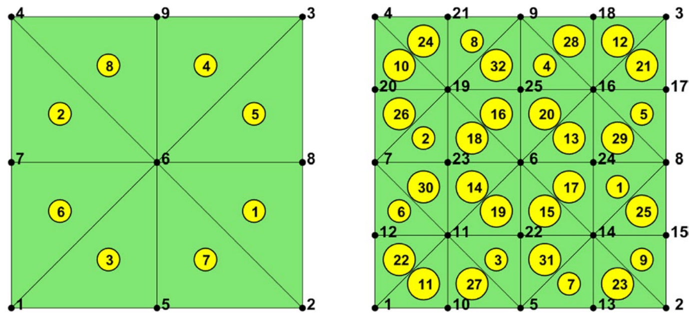

Fig. 1 Different meshes and interpolation from coarse mesh(left) to fine mesh(right)

Table 1 Numerical errors in different norms for the second order scheme

1/*h*	16	32	64	128	256
$L^2(\Omega)$	$1.3890 \cdot 10^{-3}$	$3.5076 \cdot 10^{-4}$	$8.4145 \cdot 10^{-5}$	$1.7098 \cdot 10^{-5}$	Reference
rate		1.9855	2.0595	2.2990	
$L^2(\Gamma)$	$6.7963 \cdot 10^{-5}$	$1.7095 \cdot 10^{-5}$	$4.1759 \cdot 10^{-6}$	$9.0751 \cdot 10^{-7}$	Reference
rate		1.9911	2.0334	2.2021	
$L^\infty(\Omega)$	$2.1778 \cdot 10^{-3}$	$5.6007 \cdot 10^{-4}$	$1.3749 \cdot 10^{-5}$	$3.0148 \cdot 10^{-6}$	Reference
rate		1.9592	2.0263	2.1892	

4 Numerical experiments

In this section, we present several numerical experiments, based on Matlab codes. The finite element spatial discretization is taken, as illustrated in previous Sect. 3.2, and iFEM [6] is used as a powerful tool to generate mesh, record boundary node, interpolate from coarse mesh to fine mesh, etc.

4.1 The convergence test

Here we verify the accuracy order of the proposed numerical scheme (2.3a)-(2.3e). The physical parameters are set as: $\varepsilon = 0.05, \kappa = 1$, and the final time is taken to be $T = 0.01$. The initial datum is chosen as

$$\phi_0(x, y) = 0.1 \sin(2\pi x) \sin(2\pi y).$$

The spatial and time step sizes are denoted as and τ, respectively. A sequence of

spatial mesh size is taken as $h = 2^{-k}, k = 4, 5, 6, 7, 8$, and we set the time step size as $\tau = hT$. Since an exact solution could be not represented as an explicit formula, numerical solution of the finest mesh (when $h = 2^{-8}$) will be used as a reference solution. In terms of numerical error calculation, the interpolation and projection between different meshes need to be introduced. For interpolation from coarse mesh to fine mesh, we use the mean value at the two sides of the edge to get the value at new node. For example, in Fig. 1, for a nodal function defined in coarse mesh (a),

Table 2 Numerical errors in different norms for the first order scheme, $\tau = O(h^2)$

$1/h$	16	32	64	128
$L^2(\Omega)$	$1.3619 \cdot 10^{-3}$	$3.3263 \cdot 10^{-4}$	$6.7921 \cdot 10^{-5}$	Reference
rate		2.0336	2.2920	
$L^2(\Gamma)$	$7.8377 \cdot 10^{-5}$	$1.9049 \cdot 10^{-5}$	$4.0789 \cdot 10^{-6}$	Reference
rate		2.0406	2.2235	
$L^\infty(\Omega)$	$2.1364 \cdot 10^{-3}$	$5.3855 \cdot 10^{-4}$	$1.1947 \cdot 10^{-4}$	Reference
rate		1.9880	2.1725	

Table 3 Numerical errors in different norms for the first order scheme, $\tau = O(h)$

$1/h$	16	32	64	128
$L^2(\Omega)$	$7.7097 \cdot 10^{-4}$	$1.1086 \cdot 10^{-4}$	$4.269 \cdot 10^{-5}$	Reference
rate		2.7979	1.3768	
$L^\infty(\Omega)$	$9.2066 \cdot 10^{-4}$	$2.3322 \cdot 10^{-4}$	$1.2536 \cdot 10^{-4}$	Reference
rate		1.9810	0.9856	

the mean value of node 1 and 6 is taken to get the value at node 11 in fine mesh (b). On the other hand, we delete the additional nodes and nodal functions to get the projection from fine mesh to coarse mesh, which is the inverse process of interpolation defined above.

The numerical error and convergence order of the proposed numerical scheme are displayed in Table 1. Here $L^2(\Omega)$, $L^2(\Gamma)$ and $L^\infty(\Omega)$ stand for the L^2 error in the bulk, L^2 error on the boundary and L^∞ error in the bulk at the final time *T*, respectively. In the calculation of the L^2 norms, the numerical solution is interpolated to the finest mesh; while in the calculation of L^∞ norms, the reference solution is projected to coarse mesh. In the convergence analysis section we have only proved an H^{-1} error estimate, while in most numerical experiments all the above norms have exhibited the second order convergence rate.

As a comparison, the numerical errors of the first order scheme (2.4a) - (2.4e), are listed in Tables 2 and 3, with $h = 2^{-k}, k = 4, 5, 6, 7$. Moreover, the time step size is taken to be $\tau = h^2 T$ in Table 2, and $\tau = hT$ in Table 3. A second order spatial convergence rate and the first order temporal convergence rate have been clearly observed.

Remark 4.1 Convergence rate in the case where takes values of $64 - 128$ in Table 1 behaves slightly worse than the others, because the inexact reference solution has a greater “relative" influence with $1/h = 128$, in comparison with other coarser mesh sizes.

4.2 Spinodal decomposition

The same configuration is used, as in the example of section 5.2 in [28]. The computational domain is taken to be $\Omega = (0,1)^2$, the mesh and time step sizes are set to be $h = 0.01$, $\tau = 1 \times 10^{-5}$, respectively. The initial profile ϕ is given by: $(x_1, x_2) \mapsto \max\{0.1\sin\pi x_1, 0.1\sin\pi x_2\}$, and the PDE system turns out to be

$$\begin{aligned}
&\partial_t \phi = m\Delta u, && \text{in } \Omega \times (0,T],\\
&u = -\delta\sigma\Delta\phi + \delta^{-1}\sigma F'(\phi), && \text{in } \Omega \times (0,T],\\
&\partial_n u = 0, && \text{on } \Gamma \times (0,T],\\
&\partial_t \phi = m_\Gamma \Delta_\Gamma u_\Gamma, && \text{on } \Gamma \times (0,T],\\
&u_\Gamma = -\kappa\delta_\Gamma\Delta_\Gamma\phi + \delta\sigma\partial_n\phi + \delta_\Gamma^{-1}G'(\phi), && \text{on } \Gamma \times (0,T].
\end{aligned} \tag{4.1}$$

Here $m = 0.01, \delta = 0.02, \sigma = 2; m_\Gamma = 0.02, \delta_\Gamma = 0.02, \kappa = 1$. Fig. 2 displays the evolution of ϕ at a sequence of time instants. A phase transition is observed, both in the bulk and the boundary, which is consistent with the result listed in [28].

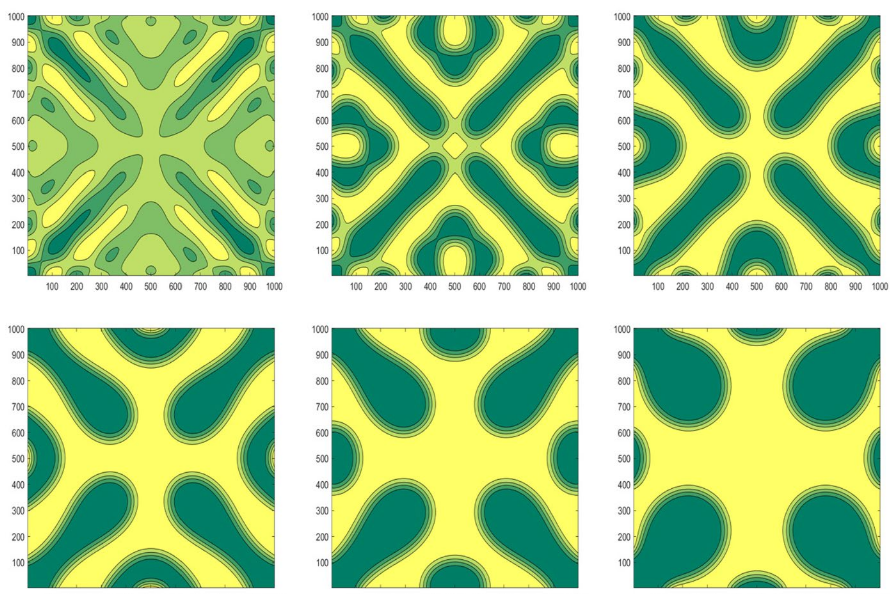

Fig. 2 Level set of ϕ at time 0.01, 0.02, 0.04, 0.1, 0.2 and 0.5

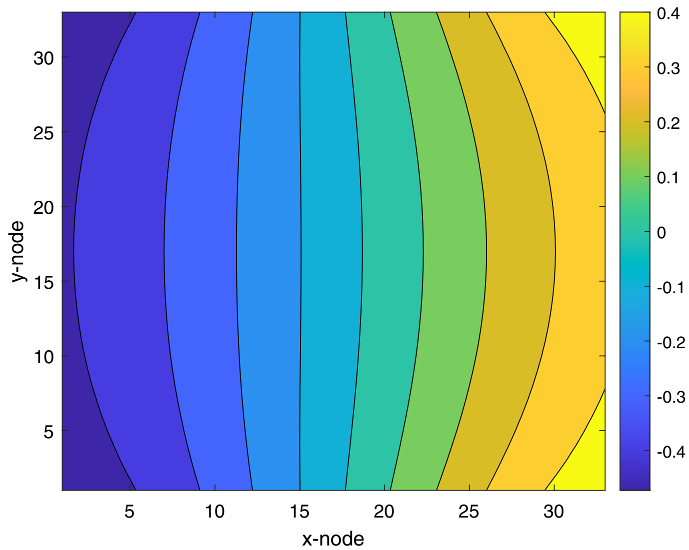

Fig. 3 Level set of the numerical solution at $T = 0.5$

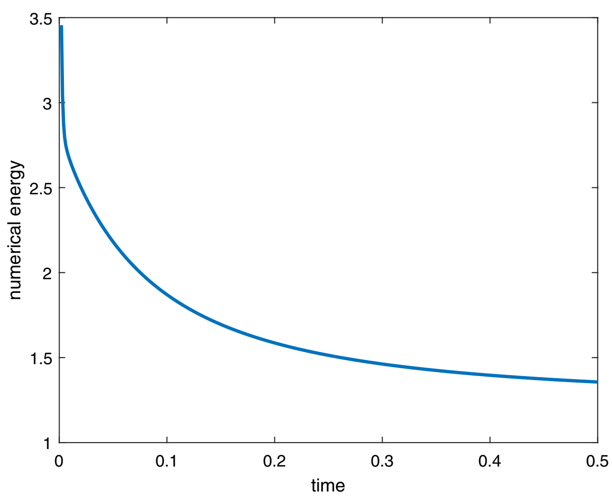

Fig. 4 The free energy evolution

4.3 Mass conservation and energy dissipation test

In this example, we provide the mass conservation and energy dissipation test for the proposed numerical scheme. Set $\Omega = (0, 1)^2, h = 1/32, \tau = 1 \times 10^{-3}$, and the initial profile ϕ_0 is chosen as

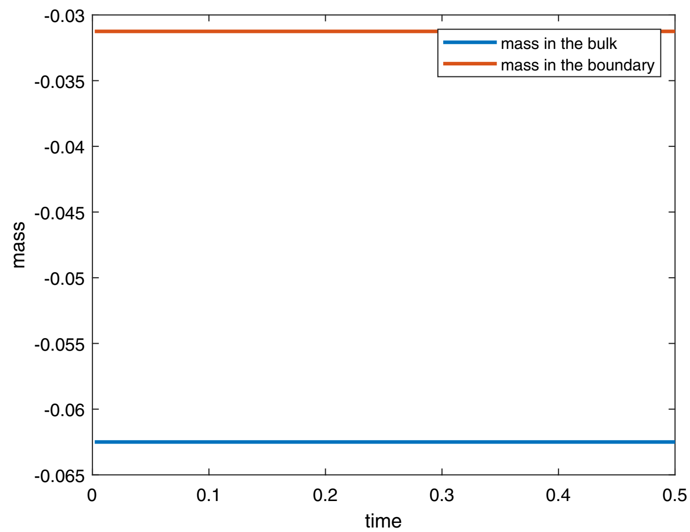

Fig. 5 The mass evolution in the bulk and on the boundary

$$\phi_0(x,y) = \begin{cases} 1 & x > 1/2, \\ -1 & x \leqslant 1/2. \end{cases} \tag{4.2}$$

Interface parameter is given by $\varepsilon = 1$ in the bulk, $\kappa = 0.01$ on the boundary. The artificial regularization parameters are chosen as $A_1 = A_2 = 5$.

Figure 3 presents the level set of the numerical solution at $T = 0.5$. Given the boundary-bulk diffuse ratio $\kappa = 0.01$, it is observed that numerical solution is smoother in the bulk, while there is a rapid shift on the boundary. Figure 4 plots the numerical energy evolution over time, and Fig. 5 gives the mass evolution in the bulk and on the boundary. These results are consistent with the theoretical analysis.

Remark 4.2 As mentioned in the introduction section, the numerical method in [28] reduces the condition number of the numerical system if time step size τ becomes small. This technique takes the advantage of Schur complement, and such an approach could be applied to our proposed scheme; see Sect. 2 in [28] for more details.

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Declarations

Conflict of interest The authors declare that they have no Conflict of interest.

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