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Finite element approximation of the Cahn–Hilliard equation on surfaces ☆

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ABSTRACT

In this paper, we consider the phase separation on general surfaces by solving the nonlinear Cahn–Hilliard equation using a finite element method. A fully discrete approximation scheme is introduced, and we establish a priori estimates for the discrete solution that does not rely on any knowledge of the exact solution beyond the initial time. This in turn leads to convergence and optimal error estimates of the discretization scheme. Numerical examples are also provided to substantiate the theoretical results.

1. Introduction

The Cahn–Hilliard equation introduced in [7] is a very general mathematical model that describes phase separations. It has found many applications in various fields, such as foams modeling, solidification processes, dendritic flow, image processing, planet formation and so on [5,8,13,28,32,35,38,43,47]. The phase separation processes have been successfully investigated with the Cahn–Hilliard equation in a wide variety of non-equilibrium systems. There have been many algorithms and simulations performed using a variety of discretization methods including finite difference, finite volume, finite element and spectral methods, see, e.g., [1,2,8,10, 24–27,33,35,36,40,44–46] and the references cited therein.

Various experimental studies have shown that interesting phase separations could occur on static or dynamic surfaces, such as phase separation on lipid bilayer membranes, crystal growth on curved surfaces, and phase separations within thin films, see [3,4,21,41]. Thus, theoretical analysis and numerical implementation of the phase transition models on general surfaces are attracting more and more attentions. For instance, a finite volume method for Cahn–Hilliard equations on the sphere was studied in [42], the numerical approximations of the Ginzburg–Landau model for a superconducting hollow sphere were studied using a gauge invariant finite volume discretization on a spherical centroidal Voronoi tesselation [16]. The finite element method has been used for the discretization of partial differential equations (PDEs) defined on surfaces including the Cahn–Hilliard equation [12,11,21].

Development of fully discrete approximation schemes for nonlinear PDEs is important because these schemes not only directly reduce differential equations to systems of algebraic equations, but also suggest what kinds of ordinary differential equation solvers are needed for the semi-discrete approximation schemes. For fully discrete approximations of the Cahn–Hilliard equation that are most relevant to the work presented here, let us mention that in [18], Du and Nicolaides proposed and analyzed a fully discrete approximation scheme for one dimensional Cahn–Hilliard equations. One of its features is the existence of a Lyapunov functional associated with the approximation scheme. This leads to some estimates for the discrete solution in a certain Sobolev space. Combining these with a Sobolev imbedding theorem in one space dimension, they are able to prove the point-wise boundedness of the discrete solution, and consequently, they obtain the Lipschitz property of the nonlinear term, which guarantees the existence and uniqueness of a discrete solution and make the error analysis possible. This idea was studied further in [29]. We note that a point-wise estimate for solutions of fully discrete schemes is important for the mathematical analysis, since, as pointed out in [37], the linear part of the equation does not always control the

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nonlinear term automatically. Nevertheless, in higher dimensional spaces, the imbedding theorem used in [18] is no longer valid and point-wise boundedness does not follow directly from the existence of the Lyapunov functional. Thus, new a priori estimates for the discrete solution are needed.

In this paper, we demonstrate wellposedness and convergence of a fully discrete finite element approximation scheme of the Cahn–Hilliard equation defined on a general surface. Our approach requires a combination of both standard and nonstandard techniques due to the lack of maximum principle for fourth-order equations. On one hand, the approach is similar to the usual arguments for establishing a priori estimates of discrete solutions of PDEs. For example, some estimates for the discrete potential function are provided first, then we apply the idea of elliptic regularity to get high order estimates. On the other hand, we present a more delicate analysis of the initial approximation in our derivation. This type of analysis is an important part of the estimation, but it appears rarely in the literature on the approximation of non-linear or semi-linear parabolic type equations. It is done here through some technical discussions on the approximation space.

We now give an outline of this paper. In Sections 2 and 3, we present the model problem on general surfaces, and the fully discrete finite element approximation scheme. In Section 4, we discuss some properties of the initial approximation, some estimates on the discrete chemical potential p, and then the desired point-wise boundedness of the discrete solution. Then we show the existence and uniqueness of the solution to the fully discrete scheme, and give the error analysis in Section 6. Finally, some numerical experiments are presented to validate our theoretical results in Section 7.

2. The model problem

Before setting up the model, we introduce some basic notations first, where we closely follow the framework introduced in [20,21], see also the discussion in [17]. Given an open connected and bounded $C^{\nu,\alpha}$ surface $\mathbf{S}$ in $\mathbb{R}^3$ with $\nu \in \mathbb{N} \cup \{0\}$ and $0 < \alpha \leqslant 1$, we assume that it can be represented globally by some oriented distance function (level set function) $d = d(\mathbf{x})$ defined in an open subset Ω in $\mathbb{R}^3$, such that $\mathbf{S} = \{\mathbf{x} \in \Omega | d(\mathbf{x}) = 0\}$ with $d \in C^{\nu,\alpha}$ and $\nabla d \neq 0$ in Ω with ∇ being the standard gradient operator in $\mathbb{R}^3$. Moreover, we assume that on a strip (band)

$$\mathbf{U} = \{\mathbf{x} \in \mathbb{R}^3 \| d(\mathbf{x})| < \delta\}, \quad \text{for some } \delta > 0,$$

around $\mathbf{S}$, there is a unique decomposition for any $\mathbf{x} \in \mathbf{U}$,

$$\mathbf{x} = \mathbf{p}(\mathbf{x}) + d(\mathbf{x})\vec{\mathbf{n}}(\mathbf{p}(\mathbf{x})) \tag{2.1}$$

with $\mathbf{p}(\mathbf{x}) \in \mathbf{S}$ and $\vec{\mathbf{n}}(\mathbf{p}(\mathbf{x}))$ being the unit outward normal to the surface $\mathbf{S}$ at $\mathbf{p}(\mathbf{x})$. The parameter δ is usually determined by the surface curvature if $\mathbf{S}$ is sufficiently smooth. One can prove that given $\partial\Omega$ is smooth enough, there always exists $\delta > 0$ such that $d(\mathbf{x})$ is smooth in $\mathbf{U}$, see Lemma 14.16 in [30] for details. Without loss of generality, we assume that $|\nabla d| \equiv 1$ in $\mathbf{U}$. Let $\nabla_s = (\nabla_{s,1}, \nabla_{s,2}, \nabla_{s,3}) = \nabla - (\vec{\mathbf{n}} \cdot \nabla)\vec{\mathbf{n}}$ denote the tangential (surface) gradient operator, and $\Delta_s = \nabla_s \cdot \nabla_s$ be the so-called Laplace–Beltrami operator on $\mathbf{S}$. We use the standard notation for $L^q(\mathbf{S})$ on $\mathbf{S}$, and we define the Sobolev spaces as follows:

$$W^{m,q}(\mathbf{S}) = \{u \in L^q(\mathbf{S}) | u \text{ possesses weak tangential derivatives up to order } m \text{ which are in } L^q(\mathbf{S})\}.$$

We denote, in addition, that $H^m(\mathbf{S}) = W^{m,2}(\mathbf{S})$ on $\mathbf{S}$. To make the space $H^m(\mathbf{S})$ well defined, it is customary to assume $\nu + \alpha \geqslant \max\{1, m\}$ [34]. To avoid technical complications, we further assume that $\mathbf{S}$ and $\partial\mathbf{S}$ are sufficiently smooth (say with $\nu = 4$) and $\partial\mathbf{S} \neq \emptyset$ for the rest of the paper unless stated otherwise.

To introduce the Cahn–Hilliard equation, we begin with the free energy functional

$$I(u) = \int_{\mathbf{S}} \left\{\mathcal{H}(u(\mathbf{x})) + \frac{\sigma}{2}|\nabla_s u(\mathbf{x})|^2\right\} ds \tag{2.2}$$

for any $u = u(x) \in H^1(\mathbf{S})$ with $\mathcal{H}$ being the bulk free energy density, and a positive constant $\sigma > 0$ which symbolizes the so-called diffuse interfacial width. Let $u = u(\mathbf{x}, t)$ be a function for $\mathbf{x}$ on $\mathbf{S}$ at time t which, in the original works of [6,7], denotes the concentration of one species of the binary mixture. The chemical potential of the system is then of the form

$$p = \frac{\partial I}{\partial u} = \mathcal{H}'(u) - \sigma\Delta_s u = \phi(u) - \sigma\Delta_s u. \tag{2.3}$$

By assuming a constant unit mobility, we get the dynamic equation

$$u_t = \Delta_s p, \tag{2.4}$$

which leads to a simple form of the Cahn–Hilliard equation:

$$u_t = \Delta_s(\phi(u) - \sigma\Delta_s u). \tag{2.5}$$

As a model case, the function ϕ is assumed to be of the form:

$$\phi(u) = \mathcal{H}'(u) = \gamma_2 u^3 + \gamma_1 u^2 + \gamma_0 u, \tag{2.6}$$

where γ_0, γ_1 and γ_2 are given constants and $\gamma_2 > 0$ is assumed which implies that $H(u)$ reaches its minima at finite values of u. Then we state a property of function $\mathcal{H}$ in the following lemma,

Lemma 1. *There exists a constant $k > 0$ such that*

$$\mathcal{H}(x) - \mathcal{H}(y) - \phi(y)(x - y) \geqslant -k(x - y)^2, \quad \forall x, y \in \mathbb{R}.$$

Proof. For any $x \in \mathbb{R}$, we have

$$\mathcal{H}''(x) = \phi'(x) = 3\gamma_2 x^2 + 2\gamma_1 x + \gamma_0 \geqslant \gamma_0 - \frac{1}{3\gamma_2}\gamma_1^2.$$

By the mean value theorem, we can always find a constant $k > 0$ such that

$$\mathcal{H}(x) - \mathcal{H}(y) - \phi(y)(x - y) \geqslant -k(x - y)^2 \tag{2.7}$$

for any $x, y \in \mathbb{R}$. ☐

It is worth noting that Lemma 1 is typical for gradient flows and similar result was proven in [25,40]. The initial condition for u is given by

$$u(\mathbf{x}, 0) = u_0(\mathbf{x}), \quad \text{for } \mathbf{x} \in \mathbf{S}. \tag{2.8}$$

For technical analysis, we assume that $u_0 \in H_0^1(\mathbf{S}) \cap H^2(\mathbf{S})$ and $\Delta_s u_0 \in H_0^1(\mathbf{S}) \cap W^{1,2+\epsilon}(\mathbf{S})$ for $\epsilon \in (0, 1)$.

As for boundary conditions, the Cahn–Hilliard equation is usually supplemented by either conditions on u and p (the Dirichlet case) or their normal derivatives (the Neumann case), with the former corresponding to specifying a given concentration at the boundary while the latter corresponding to the more popular case of conserved dynamics. For simpler presentation, here we study the homogenous Dirichlet type boundary value problem for both the concentration and the chemical potential, that is,

$$u(\mathbf{x}) = 0, \quad \text{for } \mathbf{x} \in \partial\mathbf{S} \tag{2.9}$$

and

$$p(\mathbf{x}) = 0, \quad \text{for } \mathbf{x} \in \partial\mathbf{S}. \tag{2.10}$$

Our method and analysis are directly applicable to the case of Neumann boundary condition as well.

In order to introduce numerical discretization to the above equations, we first uniquely extend the functions defined on $\mathbf{S}$ to

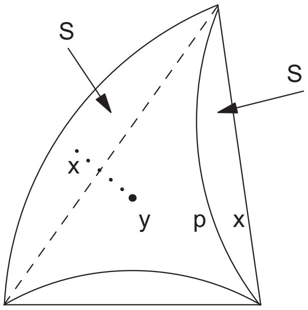

Fig. 1. Surface **S** and its discretization $\mathbf{S}^h$.

U. That is, given a function u defined on **S**, its extension in **U** is given by

$$u^l(\mathbf{x}) = u(\mathbf{p}(\mathbf{x})), \quad \forall \mathbf{x} \in \mathbf{U}. \tag{2.11}$$

The same extension can be done for the unit normal. For simplicity, we still use the same notation for the extension, that is, for $\mathbf{x} \in \mathbf{U}$, we simply let $\vec{\mathbf{n}}(\mathbf{x}) = \vec{\mathbf{n}}(\mathbf{p}(\mathbf{x}))$.

Let $\mathbf{S}^h$ be a polyhedral approximation to **S** having triangular faces. We assume that for each point $\mathbf{y} \in \mathbf{S}$ there is at most one point $\mathbf{x} \in \mathbf{S}^h$ such that $\mathbf{p}(\mathbf{x}) = \mathbf{y}$ as suggested in [21], and vertices of each triangular face of $\mathbf{S}^h$ are on **S**, as shown in Fig. 1. The mesh size of $\mathbf{S}^h$ is often defined to be

$$h = \max_{Q \in \mathbf{S}^h} h_Q,$$

where h_Q denotes the diameter of the circumscribed circle of the triangular face Q.

We then do the similar extension from $\mathbf{S}^h$ to **U**. Given a function u^h defined on $\mathbf{S}^h$, first project it onto **S** by $\tilde{u}^h(\mathbf{p}(\mathbf{y})) = u^h(\mathbf{y})$ for $\mathbf{y} \in \mathbf{S}^h$, then we apply (2.11) again to extend $\tilde{u}^h$ to **U**, i.e.,

$$u^{h,l}(\mathbf{x}) = \tilde{u}^h(\mathbf{p}(\mathbf{x})), \quad \forall \mathbf{x} \in \mathbf{U}. \tag{2.12}$$

We may equivalently write $u^{h,l}(\mathbf{x}) = u^h(\mathbf{y})$ for any pair of $\mathbf{x} \in \mathbf{U}$ and $\mathbf{y} \in \mathbf{S}^h$ such that $\mathbf{p}(\mathbf{x}) = \mathbf{p}(\mathbf{y}) \in \mathbf{S}$. Note that all extensions of functions to **U** are constant along normals to **S**, thus, extensions of functions defined on **S** and those on $\mathbf{S}^h$ share much the same properties.

We use $ds(\mathbf{x})$ and $ds_h(\mathbf{y})$ to denote the surface measures of **S** and $\mathbf{S}^h$ respectively at the points $\mathbf{x} \in \mathbf{S}$ and $\mathbf{y} \in \mathbf{S}^h$. Let

$$\mu_h(\mathbf{p}(\mathbf{x})) = \frac{ds(\mathbf{p}(\mathbf{x}))}{ds_h(\mathbf{x})} \tag{2.13}$$

for any $\mathbf{x} \in \mathbf{S}^h$. We then assume, since **S** and $\partial\mathbf{S}$ are sufficiently smooth, that

$$|1 - \mu_h(\mathbf{x})| \leqslant ch^2, \tag{2.14}$$

where h is the mesh size parameter. Moreover, here and in the sequel, c is used to denote a generic postive constant which is independent of h as $h \to 0$, that is, it may take different values but remain uniformly bounded as the discretization gets refined. We note that the assumption (2.14) is generally true for regular and quasi-uniform triangulations of a smooth surface **S** [20].

3. The fully discrete approximation scheme

Let $\mathcal{U}$ denote a finite dimensional subspace of $H^1(\mathbf{S}^h)$. In the context of finite element approximations, we take $\mathcal{U}$ to be a continuous finite element space with respect to a certain triangulation of the general surface **S** with mesh size parameter h. In this paper, we take $\mathcal{U}$ to be continuous piecewise linear function space, equipped with the corresponding boundary condition, for simplicity. Let $(0, T)$ be the time interval of interest, which is discretized into N subintervals, each with a step size $\Delta t = T/N$. The choice of a uniform time step size is not essential to our following discussion.

For notational convenience, for any $v, w \in H_0^1(\mathbf{S})$, and any $V^h, W^h \in \mathcal{U}$, we let

$$(v, w)_s = \int_{\mathbf{S}} v(\mathbf{x}) \cdot w(\mathbf{x}) ds, \quad (V^h, W^h)_{s_h} = \int_{\mathbf{S}^h} V^h(\mathbf{x}) W^h(\mathbf{x}) ds_h.$$

To approximate the nonlinear term in the equation, we define the function $\tilde{\phi} : \mathbb{R}^2 \to \mathbb{R}$ by (see [18] for the original formulation which was reviewed in [23])

$$\tilde{\phi}(x, y) = \begin{cases} (\mathcal{H}(x) - \mathcal{H}(y))/(x - y), & \text{if } x \neq y, \\ \phi(x), & \text{if } x = y, \end{cases} \tag{3.1}$$

where $\mathcal{H}$ is as in Eq. (2.2). We note that for such an $\mathcal{H}, \tilde{\phi}(x, y)$ is in fact a single globally defined cubic polynomial of x and y. With this notation, we obtain the following fully discrete scheme: find $\left(U_{n+1}^h, P_n^h\right) \in \mathcal{U} \times \mathcal{U}, n = 0, 1, \ldots, N-1$, such that for any $V^h, W^h \in \mathcal{U}$:

$$U_0^h = u_0^{h,l}, \tag{3.2}$$

$$\left(\delta_t U_n^h, V^h\right)_{s_h} + \left(\nabla_{s_h} P_n^h, \nabla_{s_h} V^h\right)_{s_h} = 0, \tag{3.3}$$

$$-\left(P_n^h, W^h\right)_{s_h} + \sigma\left(\nabla_{s_h} U_{n+1/2}^h, \nabla_{s_h} W^h\right)_{s_h} + \left(\tilde{\phi}\left(U_n^h, U_{n+1}^h\right), W^h\right)_{s_h} = 0, \tag{3.4}$$

where $u_0^{h,l}$ is an approximation to the initial condition u_0 onto $\mathbf{S}^h$ given by the H^1 projection,

$$U_{n+1/2}^h = \frac{U_n^h + U_{n+1}^h}{2} \quad \text{and} \quad \delta_t U_n^h = \frac{U_{n+1}^h - U_n^h}{\Delta t}.$$

Similar notations are used for P_n^h.

Notice that (3.2)–(3.4) is an extension to surfaces of the one-dimensional Cahn–Hillard formulation with Dirichlet boundary conditions presented and analysed in [18,23].

Define the Lyapunov functional: $\forall U^h \in \mathcal{U}$, let

$$I^h(U^h) = \int_{\mathbf{S}^h} \left\{\mathcal{H}(U^h) + \frac{\sigma}{2}|\nabla_{s_h} U^h|^2\right\} ds_h,$$

thus we have the following lemma (see also Lemma 3.1 in [18]), assume that there exists a solution of (3.2) and (3.3):

Lemma 2. *For n = 0, 1, …, N − 1, we have*

$$\frac{I^h\left(U_{n+1}^h\right) - I^h\left(U_n^h\right)}{\Delta t} + \|\nabla_{s_h} P_n^h\|_0^2 = 0. \tag{3.5}$$

Proof. From Eqs. (2.2), (3.3) and (3.4), we have

$$\begin{aligned} I^h\left(U_{n+1}^h\right) - I^h\left(U_n^h\right) &= \sigma\Delta t\left(\nabla_{s_h} U_{n+1/2}^h, \nabla_{s_h} \delta_t U_n^h\right)_{s_h} \\ &\quad + \Delta t\left(\tilde{\phi}\left(U_n^h, U_{n+1}^h\right), \delta_t U_n^h\right)_{s_h} \\ &= \Delta t\left(P_n^h, \delta_t U_n^h\right)_{s_h} = -\Delta t\left(\nabla_{s_h} P_n^h, \nabla_{s_h} P_n^h\right)_{s_h} \\ &= -\Delta t\left\|\nabla_{s_h} P_n^h\right\|_{L^2(\mathbf{S}^h)}^2. \end{aligned}$$

Hence, we obtain (3.5) which proves the lemma. □

One can easily verify that Lemma 2 implies the following theorem (see also Corollary 3.1 in [18]):

Theorem 1. *Let* $u_0(\mathbf{x}) \in H_0^1(\mathbf{S})$. *Assuming that there is a constant c > 0, independent of h, such that* $\left\|u_0^{h,l}\right\|_{H^1(\mathbf{S})} \leqslant c\|u_0\|_{H^1(\mathbf{S})}$. *Then, the solution* $\left(U_n^h, P_{n-1}^h\right)$ *of* (3.3) and (3.4) *satisfies for n = 1, 2, …, N,*

$$\left\|U_n^h\right\|_{H^1(\mathbf{S}^h)} \leqslant c \tag{3.6}$$

and

$$\sum_{j=0}^{n} \Delta t \left\| \nabla_{s_h} P_j^h \right\|^2_{L^2(\mathbf{S}^h)} \leqslant c, \tag{3.7}$$

where the generic constant c in the above two equations is independent of h, n, Δt and N.

Proof. By summing up (3.5) over n, we get (3.7) and also that $I^h\left(U_n^h\right) \leqslant c$ for some generic constant c. It is easy to establish the coercivity of the functional I^h in $H^1(\mathbf{S}^h)$ which then gives (3.6). □

4. Pointwise boundedness of discrete solutions

As stated in [18], one needs to prove the point-wise boundedness of U_n^h for any n, such that $\tilde{\phi}\left(U_n^h, U_{n+1}^h\right)$ becomes Lipschitz continuous with some Lipschitz constant independent of h, n and Δt, then the error estimates of the proposed fully discrete finite element scheme can be analyzed in a standard manner. Since the imbedding theorem used in [18] is no longer valid in the manifold case, we see that the point-wise boundedness does not follow directly from the existence of the Lyapunov functional. Thus, some further estimates are needed.

4.1. Some technical lemmas

We first present some technical results that are of later use.

For any $u \in H_0^1(\mathbf{S}) \cap H^2(\mathbf{S})$, we define the projection of u, say $\Pi^h u$, onto the finite element space $\mathcal{U}$ as follows: let $f = -\Delta_s u \in L^2(\mathbf{S})$, then $\Pi^h u$ is defined by

$$(\nabla_{s_h} \Pi^h u, \nabla_{s_h} W^h)_{s_h} = (f^l, W^h)_{s_h}, \quad \forall W^h \in \mathcal{U}.$$

As discussed in [20], one can easily deduce that if $u \in H^2(\mathbf{S})$, $\Pi^h u$ actually is the discrete solution of $-\Delta_s u = f$ over the triangulation $\mathbf{S}^h$ and one has the following energy norm error estimate: for $u \in H_0^1(\mathbf{S}) \cap H^2(\mathbf{S})$, there exists a generic constant $c > 0$, such that

$$\|u - (\Pi^h u)^l\|_{H^1(\mathbf{S})} \leqslant ch\|u\|_{H^2(\mathbf{S})}. \tag{4.1}$$

Furthermore, concerning the extension defined earlier, we have the following two lemmas (see [20])

Lemma 3. *For any u, $v \in H^1(\mathbf{S})$, there exist generic constants c_1, $c_2 > 0$ such that*

$$c_1\|u - v\|_{H^1(\mathbf{S})} \leqslant \|u^l - v^l\|_{H^1(\mathbf{S}^h)} \leqslant c_2\|u - v\|_{H^1(\mathbf{S})}. \tag{4.2}$$

Proof. From the definition of $\|\cdot\|_{H^1(S^h)}$, we have

$$\begin{aligned} \|u^l - v^l\|_{H^1(\mathbf{S}^h)} &= \left(\int_{\mathbf{S}^h} |u^l - v^l|^2 ds_h\right)^{1/2} + \left(\int_{\mathbf{S}^h} |\nabla_{s_h}(u^l - v^l)|^2 ds_h\right)^{1/2} \\ &= \left(\int_{\mathbf{S}} \frac{1}{\mu_h}|u - v|^2 ds\right)^{1/2} + \left(\int_{\mathbf{S}} \frac{1}{\mu_h}|\mathbf{P}_h(\mathbf{I} - d\mathbf{H})\nabla_s(u - v)|^2 ds\right)^{1/2}, \end{aligned} \tag{4.3}$$

where $\mathbf{P}_h(\mathbf{x}) = \mathbf{I} - \vec{\mathbf{n}}_h(\mathbf{x}) \otimes \vec{\mathbf{n}}_h(\mathbf{x}), \mathbf{H} = D^2 d(\mathbf{x}) : \mathbb{R}^3 \to \mathbb{R}^3$ denotes the Weingarten map [12], $d = d(\mathbf{x})$ is the oriented distance function we defined before, and $\mathbf{H}$ is well-defined by Lemma 14.17 in [30].

From the discussions in [20], we know that when h is sufficiently small, there always exists a generic constant $c_0 > 0$ such that

$$\frac{1}{c_0} \leqslant \mu_h \leqslant c_0, \quad \frac{1}{c_0} \leqslant \mathbf{P}_h(\mathbf{I} - d\mathbf{H}) \leqslant c_0,$$

which implies the existence of generic constants c_1, $c_2 > 0$ satisfying (4.2). □

Lemma 4. *For $\epsilon \in (0,1)$, there exist some generic constants c_1, $c_2 > 0$ such that for any $U \in H^1(\mathbf{S}^h)$,*

$$c_1\|U^l\|_{W^{1,2+\epsilon}(\mathbf{S})} \leqslant \|U\|_{W^{1,2+\epsilon}(\mathbf{S}^h)} \leqslant c_2\|U^l\|_{W^{1,2+\epsilon}(\mathbf{S})}. \tag{4.4}$$

Proof. Since the surface is sufficiently smooth, we have $U^l \in H^1(\mathbf{S})$, therefore $U^l \in W^{1,2+\epsilon}(\mathbf{S})$. By using the fact (see [20]) that when h is sufficiently small, there always exists a generic constant $c > 0$ such that

$$\frac{1}{c}\left|\nabla_s U^l\right| \leqslant |\nabla_{s_h} U| \leqslant c\left|\nabla_s U^l\right|,$$

we can easily obtain the conclusion. □

Lemma 5. *For $\epsilon \in (0,1)$, there exists a generic constant $c > 0$, such that for any $u \in H_0^1(\mathbf{S}) \cap H^2(\mathbf{S})$,*

$$\|\Pi^h u\|_{W^{1,2+\epsilon}(\mathbf{S}^h)} \leqslant c\|u\|_{H^2(\mathbf{S})}. \tag{4.5}$$

Proof. For $u \in H_0^1(\mathbf{S}) \cap H^2(\mathbf{S})$, by the inverse inequality for finite element functions, the Lemmas 4, 3 and the inequality (4.1), we can find a generic constant $c > 0$ satisfying

$$\begin{aligned} \|\Pi^h u\|_{W^{1,2+\epsilon}(\mathbf{S}^h)} &\leqslant \|u^l\|_{W^{1,2+\epsilon}(\mathbf{S}^h)} + \|u^l - \Pi^h u\|_{W^{1,2+\epsilon}(\mathbf{S}^h)} \\ &\leqslant \|u^l\|_{W^{1,2+\epsilon}(\mathbf{S}^h)} + ch^{\frac{2}{2+\epsilon} - \frac{2}{2}}\|u^l - \Pi^h u\|_{H^1(\mathbf{S}^h)} \\ &\leqslant \|u^l\|_{W^{1,2+\epsilon}(\mathbf{S}^h)} + ch^{\frac{2}{2+\epsilon} - 1}\|u - (\Pi^h u)^l\|_{H^1(\mathbf{S})} \\ &\leqslant c\|u\|_{W^{1,2+\epsilon}(\mathbf{S})} + ch^{\frac{2}{2+\epsilon}}\|u\|_{H^2(\mathbf{S})}. \end{aligned} \tag{4.6}$$

Now, using the Sobolev imbedding theorem $H^2(\mathbf{S}) \hookrightarrow W^{1,2+\epsilon}(\mathbf{S})$, we have

$$\|\Pi^h u\|_{W^{1,2+\epsilon}(\mathbf{S}^h)} \leqslant c\|u\|_{H^2(\mathbf{S})}$$

for some constant $c > 0$. □

We would like to note that some results equivalent to Lemmas 3–5 can be found in [20]. Similarly, we define another projection Λ^h, onto $\mathbf{S}^h$, as follows: for any $u \in H_0^1(\mathbf{S})$,

$$(\Lambda^h u, V^h)_{s_h} = (u, V^{h,l})_s, \quad \forall V^h \in \mathcal{U}, \tag{4.7}$$

i.e., equivalently,

$$(\Lambda^h u, V^h)_{s_h} = (\mu_h u^l, V^h)_{s_h}, \quad \forall V^h \in \mathcal{U}, \tag{4.8}$$

then for any $V^h \in \mathcal{U}$, we have

$$\|\Lambda^h u - V^h\|_{L^2(\mathbf{S}^h)} \leqslant \|\mu_h u^l - V^h\|_{L^2(\mathbf{S}^h)}.$$

Then we can prove the following lemma:

Lemma 6. *For $\epsilon \in (0,1)$, there exists a generic constant $c > 0$ such that for any $u \in H_0^1(\mathbf{S}) \cap W^{1,2+\epsilon}(\mathbf{S})$,*

$$\|\Lambda^h u\|_{H^1(\mathbf{S}^h)} \leqslant c\|u\|_{W^{1,2+\epsilon}(\mathbf{S})}. \tag{4.9}$$

Proof. By the best approximation property, the inverse theorem in finite element space [9] and (2.14), we can always find $U^h \in \mathcal{U}$ satisfying the following inequality:

$$\begin{aligned} \|\Lambda^h u\|_{H^1(\mathbf{S}^h)} &\leqslant \|u^l\|_{H^1(\mathbf{S}^h)} + \|u^l - U^h\|_{H^1(\mathbf{S}^h)} + \|\Lambda^h u - U^h\|_{H^1(\mathbf{S}^h)} \\ &\leqslant c\|u^l\|_{W^{1,2+\epsilon}(\mathbf{S}^h)} + c\|u^l - U^h\|_{W^{1,2+\epsilon}(\mathbf{S}^h)} + ch^{-1}\|\Lambda^h u - U^h\|_{L^2(\mathbf{S}^h)} \\ &\leqslant c\|u^l\|_{W^{1,2+\epsilon}(\mathbf{S}^h)} + ch^{-1}\|\mu_h u^l - U^h\|_{L^2(\mathbf{S}^h)} \leqslant c\|u^l\|_{W^{1,2+\epsilon}(\mathbf{S}^h)} \\ &\quad + ch^{-1}\|u^l - U^h\|_{L^2(\mathbf{S}^h)} + ch^{-1}\|(1 - \mu_h)u^l\|_{L^2(\mathbf{S}^h)} \leqslant c\|u^l\|_{W^{1,2+\epsilon}(\mathbf{S}^h)} \\ &\quad + c\|u^l\|_{H^1(\mathbf{S}^h)} \leqslant c\|u^l\|_{W^{1,2+\epsilon}(\mathbf{S}^h)} \leqslant c\|u\|_{W^{1,2+\epsilon}(\mathbf{S})} \end{aligned}$$

for some constant $c > 0$. □

4.2. Estimates on the initial approximation

In order to get energy type estimates for the discretization scheme, first we consider the approximation of the initial condition, especially the initial chemical potential.

Let $U_0^h = \Pi^h u_0 = u_0^{h,l}, p_0^h = \Lambda^h p_0$ where $p_0 = \phi(U_0^{h,l}) - \sigma\Delta_s u_0$. Then we have.

Lemma 7. *There exists a constant $c > 0$ such that*

$$\|p_0^h\|_{H^1(\mathbf{S}^h)} \leqslant c.$$

Proof. Under the assumptions on u_0, we have from Lemmas 4–6

$$\|U_0^h\|_{W^{1,2+\epsilon}(\mathbf{S}^h)} \leqslant c, \quad \|\Lambda^h \Delta_s u_0\|_{H^1(\mathbf{S}^h)} \leqslant c,$$

where the constant c is independent of h. Since

$$W^{1,2+\epsilon}(\mathbf{S}^h) \hookrightarrow L^\infty(\mathbf{S}^h),$$

we then get

$$\|U_0^h\|_{W^{0,\infty}(\mathbf{S}^h)} \leqslant c.$$

This implies that $\left\|\phi'\left(U_0^h\right)\right\|_{W^{0,\infty}(\mathbf{S}^h)}$ is bounded, and so is $\left\|\phi'\left(U_0^h\right)\nabla_{s_h} U_0^h\right\|_{W^{0,2+\epsilon}(\mathbf{S}^h)}$ for arbitrary $\epsilon \in (0,1)$. Thus,

$$\|\phi(U_0^h)\|_{W^{1,2+\epsilon}(\mathbf{S}^h)} \leqslant c,$$

where the generic constant c does not depend on h.

Using Lemma 6 again, we also have

$$\left\|\Lambda^h \phi\left(U_0^h\right)\right\|_{H^1(\mathbf{S}^h)} \leqslant c,$$

and by the definition of p_0^h, we get that

$$\|p_0^h\|_{H^1(\mathbf{S}^h)} \leqslant c,$$

for a generic constant c independent of h. □

By the definition of p_0, for any $v \in H^1(\mathbf{S})$, we have

$$-(p_0, v)_s + \sigma(\nabla_s u_0, \nabla_s v)_s + \left(\phi\left(U_0^{h,l}\right), v\right)_s = 0. \tag{4.10}$$

Using the definition of Π^h and under the assumption that $u_0 \in H^2(\mathbf{S})$, we have that for any $V^h \in \mathcal{U}$,

$$\begin{aligned}\sigma\left(\nabla_{s_h} U_0^h, \nabla_{s_h} V^h\right)_{s_h} &= \left(\left(p_0 - \phi\left(U_0^{h,l}\right)\right)^l, V^h\right)_{s_h} \\ &= \left(p_0^l, V^h\right)_{s_h} - \left(\phi\left(U_0^h\right), V^h\right)_{s_h}.\end{aligned} \tag{4.11}$$

Using the definition of Λ_h, the following equation also holds

$$\begin{aligned}&-\left(p_0^h, V^h\right)_{s_h} + \sigma\left(\nabla_{s_h} U_0^h, \nabla_{s_h} V^h\right)_{s_h} + \left(\phi\left(U_0^h\right), V^h\right)_{s_h} \\ &\quad = \left(\left(\frac{1}{\mu_h} - 1\right)p_0, V^{h,l}\right)_s.\end{aligned} \tag{4.12}$$

Next we want to show the boundedness of P_0^h, which is an important component of the discrete solution to the fully discrete scheme (3.2)–(3.4) when $n = 0$.

Theorem 2. *Let Δt be sufficiently small, i.e. $\Delta t < \sigma/(4k^2)$, where k is as stated in Lemma 1, then there exists a generic constant $c > 0$, such that*

$$\|\nabla_{s_h} P_0^h\|^2_{L^2(\mathbf{S}^h)} \leqslant c\left(\left(1 - \frac{4k^2\Delta t}{\sigma}\right)^{-1/2} \|\nabla_{s_h} p_0^h\|_{L^2(\mathbf{S}^h)} + h\|p_0^l\|_{L^2(\mathbf{S}^h)}\right).$$

Proof. Let $\eta = \left(U_1^h - U_0^h\right)/\Delta t$. By (3.4), it holds that for any $V^h \in \mathcal{U}$,

$$-\left(P_0^h, V^h\right)_{s_h} + \frac{\sigma}{2}\left(\nabla_{s_h}\left(U_1^h + U_0^h\right), \nabla_{s_h} V^h\right)_{s_h} + \left(\tilde{\phi}\left(U_0^h, U_1^h\right), V^h\right)_{s_h} = 0.$$

Subtracting the above equation from (4.12) and setting $V^h = \eta$, we then obtain

$$\begin{aligned}\left(P_0^h - p_0^h, \eta\right)_{s_h} &= \frac{\sigma}{2}\left(\nabla_{s_h}\left(U_1^h - U_0^h\right), \nabla_{s_h}\eta\right)_{s_h} + \left(\tilde{\phi}\left(U_0^h, U_1^h\right) - \phi\left(U_0^h\right), \eta\right)_{s_h} \\ &\quad + \left(\left(\frac{1}{\mu_h} - 1\right)p_0, V^{h,l}\right)_s = \frac{\Delta t}{2}\sigma(\nabla_{s_h}\eta, \nabla_{s_h}\eta)_{s_h} \\ &\quad + ((1-\mu_h)p_0^l, \eta)_{s_h} + \frac{1}{\Delta t}\int_{\mathbf{S}^h}[\mathcal{H}\left(U_1^h\right) - \mathcal{H}\left(U_0^h\right) \\ &\quad - \phi\left(U_0^h\right)\left(U_1^h - U_0^h\right)]ds_h \geqslant \frac{\Delta t\sigma}{2}\|\nabla_{s_h}\eta\|^2_{L^2(\mathbf{S}^h)} \\ &\quad - 2k\Delta t\|\eta\|^2_{L^2(\mathbf{S}^h)} - ch^2\|p_0^l\|^2_{L^2(\mathbf{S}^h)},\end{aligned}$$

where the last step is a result of Lemma 1, and $c > 0$ is a generic constant derived from (2.14) and Cauchy's inequality.

Now, from Eq. (3.3), it follows that for any $V^h \in \mathcal{U}$,

$$(\eta, V^h)_{s_h} = -\left(\nabla_{s_h} P_0^h, \nabla_{s_h} V^h\right)_{s_h}.$$

Letting $V^h = \eta$ and using Cauchy's inequality, we have

$$\|\eta\|^2_{L^2(\mathbf{S}^h)} \leqslant \frac{\sigma}{4k}\|\nabla_{s_h}\eta\|^2_{L^2(\mathbf{S}^h)} + \frac{k}{\sigma}\|\nabla_{s_h} P_0^h\|^2_{L^2(\mathbf{S}^h)}.$$

So we obtain

$$\begin{aligned}\left(P_0^h - p_0^h, \eta\right)_{s_h} &\geqslant \frac{\Delta t\sigma}{2}\|\nabla_{s_h}\eta\|^2_{L^2(\mathbf{S}^h)} - \frac{\Delta t\sigma}{2}\|\nabla_{s_h}\eta\|^2_{L^2(\mathbf{S}^h)} - ch^2\|p_0^l\|^2_{L^2(\mathbf{S}^h)} \\ &\quad - \frac{2k^2\Delta t}{\sigma}\|\nabla_{s_h} P_0^h\|^2_{L^2(\mathbf{S}^h)} \\ &= -\frac{2k^2\Delta t}{\sigma}\left\|\nabla_{s_h} P_0^h\right\|^2_{L^2(\mathbf{S}^h)} - ch^2\|p_0^l\|^2_{L^2(\mathbf{S}^h)}.\end{aligned}$$

With (3.3), we get

$$\left(\eta, P_0^h - p_0^h\right)_{s_h} = -\left(\nabla_{s_h} P_0^h, \nabla_{s_h}\left(P_0^h - p_0^h\right)\right)_{s_h}$$

and so

$$\begin{aligned}\left\|\nabla_{s_h} P_0^h\right\|^2_{L^2(\mathbf{S}^h)} &= \left(\nabla_{s_h} P_0^h, \nabla_{s_h} p_0^h\right)_{s_h} + \left(\nabla_{s_h} P_0^h, \nabla_{s_h}\left(P_0^h - p_0^h\right)\right)_{s_h} \\ &\leqslant \left\|\nabla_{s_h} P_0^h\right\|_{L^2(\mathbf{S}^h)}\|\nabla_{s_h} p_0^h\|_{L^2(\mathbf{S}^h)} - \left(\eta, P_0^h - p_0^h\right)_{s_h} \\ &\leqslant \left\|\nabla_{s_h} P_0^h\right\|_{L^2(\mathbf{S}^h)}\|\nabla_{s_h} p_0^h\|_{L^2(\mathbf{S}^h)} + \frac{2k^2\Delta t}{\sigma}\left\|\nabla_{s_h} P_0^h\right\|^2_{L^2(\mathbf{S}^h)} \\ &\quad + ch^2\|p_0^l\|^2_{L^2(\mathbf{S}^h)}.\end{aligned}$$

Since $\Delta t < \sigma/(4\ k^2)$, we then get for $a = 1/4 - k^2\Delta t/\sigma > 0$,

$$\left\|\nabla_{s_h} P_0^h\right\|_{L^2(\mathbf{S}^h)}\|\nabla_{s_h} p_0^h\|_{L^2(\mathbf{S}^h)} \leqslant 2a\|\nabla_{s_h} P_0^h\|^2_{L^2(\mathbf{S}^h)} + \frac{1}{8a}\|\nabla_{s_h} p_0^h\|^2_{L^2(\mathbf{S}^h)},$$

which leads to

$$\begin{aligned}\left\|\nabla_{s_h} P_0^h\right\|^2_{L^2(\mathbf{S}^h)} &\leqslant 2a\left\|\nabla_{s_h} P_0^h\right\|^2_{L^2(\mathbf{S}^h)} + \frac{1}{8a}\|\nabla_{s_h} p_0^h\|^2_{L^2(\mathbf{S}^h)} \\ &\quad + \frac{2k^2\Delta t}{\sigma}\left\|\nabla_{s_h} P_0^h\right\|^2_{L^2(\mathbf{S}^h)} + ch^2\|p_0^l\|^2_{L^2(\mathbf{S}^h)}.\end{aligned}$$

We then obtain

$$\left\|\nabla_{s_h} P_0^h\right\|^2_{L^2(\mathbf{S}^h)} \leqslant \frac{1}{4a}\|\nabla_{s_h} p_0^h\|^2_{L^2(\mathbf{S}^h)} + ch^2\|p_0^l\|^2_{L^2(\mathbf{S}^h)},$$

or equivalently,

$$\|\nabla_{s_h} P_0^h\|_{L^2(\mathbf{S}^h)} \leqslant c\left(\left(1-\frac{4k^2\Delta t}{\sigma}\right)^{-1/2}\|\nabla_{s_h} p_0^h\|_{L^2(\mathbf{S}^h)} + h\|p_0^l\|_{L^2(\mathbf{S}^h)}\right). \tag{4.13}$$

Notice that the above c's are not essentially the same.

This completes the proof of the theorem. □

Finally, utilizing the boundary condition, we may apply the Poincaré inequality, Lemma 7 and Theorem 2 to obtain:

Corollary 1. *There exists a generic constant $c > 0$, independent of h, Δt and N, such that for sufficiently small Δt,*

$$\|P_0^h\|_{H^1(\mathbf{S}^h)} \leqslant c. \tag{4.14}$$

4.3. Estimates on the discrete chemical potential

In this section, we derive estimates for the discrete chemical potential function P_n^h when $n \geqslant 1$.

Let us use the notation

$$\delta_{2t} U_n^h = \frac{U_{n+2}^h - U_n^h}{2\Delta t} = \frac{\delta_t U_{n+1}^h + \delta_t U_n^h}{2}, \quad \forall n \geqslant 0.$$

From the discrete approximation scheme (3.3) and (3.4), it holds that for $n = 0, 1, 2, \ldots, N-2$,

$$\left(\delta_{2t} U_n^h, V^h\right)_{s_h} + \left(\nabla_{s_h} P_{n+1/2}^h, \nabla_{s_h} V^h\right)_{s_h} = 0, \quad \forall V^h \in \mathcal{U}, \tag{4.15}$$

$$-\left(\delta_t P_n^h, W^h\right)_{s_h} + \sigma\left(\nabla_{s_h}\delta_{2t} U_n^h, \nabla_{s_h} W^h\right)_{s_h} + (\delta_t \tilde{\phi}_{n+1}, W^h)_{s_h} = 0, \quad \forall W^h \in \mathcal{U}, \tag{4.16}$$

where $\tilde{\phi}_{n+1} = \tilde{\phi}\left(U_{n+2}^h, U_{n+1}^h\right)$ and

$$\delta_t \tilde{\phi}_{n+1} = \frac{\tilde{\phi}\left(U_{n+2}^h, U_{n+1}^h\right) - \tilde{\phi}\left(U_{n+1}^h, U_n^h\right)}{\Delta t}.$$

Theorem 3. *There exists a constant $c > 0$, independent of h, Δt, n and N, such that when Δt is sufficiently small, it holds*

$$\left\|\nabla_{s_h} P_n^h\right\|_{L^2(\mathbf{S}^h)} \leqslant c, \quad \forall n = 0, 1, 2, \ldots, N. \tag{4.17}$$

Proof. Take $V^h = \delta_t P_n^h, W^h = \delta_{2t} U_n^h$ in (4.15) and (4.16), then it holds

$$\begin{aligned}\frac{\left\|\nabla_{s_h} P_{n+1}^h\right\|_{L^2(\mathbf{S}^h)}^2 - \left\|\nabla_{s_h} P_n^h\right\|_{L^2(\mathbf{S}^h)}^2}{2\Delta t} &= -\left(\delta_{2t} U_n^h, \delta_t P_n^h\right)_{s_h} \\ &= -\sigma\left(\nabla_{s_h}\delta_{2t} U_n^h, \nabla_{s_h}\delta_{2t} U_n^h\right)_{s_h} - \left(\delta_t \tilde{\phi}_{n+1}, \delta_{2t} U_n^h\right)_{s_h}.\end{aligned}$$

For the last term of the above equation,

$$\begin{aligned}\delta_t \tilde{\phi}_{n+1} = \delta_{2t} U_n^h \cdot \Bigg[&\frac{\gamma_2}{4}\left(U_{n+2}^h + U_{n+1}^h + U_n^h\right)^2 + \frac{\gamma_2}{4}\left(\left(U_{n+2}^h\right)^2 + \left(U_{n+1}^h\right)^2 \right.\\ &\left. + \left(U_n^h\right)^2\right) + \frac{2\gamma_1}{3}\left(U_{n+2}^h + U_{n+1}^h + U_n^h\right) + \gamma_0\Bigg],\end{aligned} \tag{4.18}$$

so we get

$$\delta_t \tilde{\phi}_{n+1} \cdot \delta_{2t} U_n^h \geqslant \left(\gamma_0 - \frac{64\gamma_1^2}{3\gamma_2}\right) \cdot \left(\delta_{2t} U_n^h\right)^2,$$

which leads us to

$$\begin{aligned}&\frac{\left\|\nabla_{s_h} P_{n+1}^h\right\|_{L^2(\mathbf{S}^h)}^2 - \left\|\nabla_{s_h} P_n^h\right\|_{L^2(\mathbf{S}^h)}^2}{2\Delta t} \\ &\quad \leqslant -\sigma\left\|\nabla_{s_h}\delta_{2t} U_n^h\right\|_{L^2(\mathbf{S}^h)}^2 + c\left\|\delta_{2t} U_n^h\right\|_{L^2(\mathbf{S}^h)}^2\end{aligned} \tag{4.19}$$

for some constant $c > 0$.

Let $V^h = \delta_{2t} U_n^h$ in (4.15), and make use of the Young's inequality, we get that for some $\lambda > 0$,

$$\left\|\delta_{2t} U_n^h\right\|_{L^2(\mathbf{S}^h)}^2 \leqslant \lambda\left\|\nabla_{s_h}\delta_{2t} U_n^h\right\|_{L^2(\mathbf{S}^h)}^2 + \frac{1}{4\lambda}\left\|\nabla_{s_h} P_{n+1/2}^h\right\|_{L^2(\mathbf{S}^h)}^2.$$

Combining the above two inequalities, we easily obtain

$$\begin{aligned}&\frac{\left\|\nabla_{s_h} P_{n+1}^h\right\|_{L^2(\mathbf{S}^h)}^2 - \left\|\nabla_{s_h} P_n^h\right\|_{L^2(\mathbf{S}^h)}^2}{2\Delta t} \\ &\quad \leqslant (c\lambda - \sigma)\left\|\nabla_{s_h}\delta_{2t} U_n^h\right\|_{L^2(\mathbf{S}^h)}^2 + \frac{c}{4\lambda}\left\|\nabla_{s_h} P_{n+1/2}^h\right\|_{L^2(\mathbf{S}^h)}^2.\end{aligned} \tag{4.20}$$

Taking $\lambda = \sigma/2c$, the above inequality then becomes

$$\begin{aligned}&\frac{1}{\Delta t}\left(\left\|\nabla_{s_h} P_{n+1}^h\right\|_{L^2(\mathbf{S}^h)}^2 - \left\|\nabla_{s_h} P_n^h\right\|_{L^2(\mathbf{S}^h)}^2\right) + \sigma\left\|\nabla_{s_h}\delta_{2t} U_n^h\right\|_{L^2(\mathbf{S}^h)}^2 \\ &\quad \leqslant \frac{c^2}{2\sigma}\left(\left\|\nabla_{s_h} P_{n+1}^h\right\|_{L^2(\mathbf{S}^h)}^2 + \left\|\nabla_{s_h} P_n^h\right\|_{L^2(\mathbf{S}^h)}^2\right).\end{aligned}$$

Thus,

$$\begin{aligned}&\frac{1}{\Delta t}\left(\left\|\nabla_{s_h} P_{n+1}^h\right\|_{L^2(\mathbf{S}^h)}^2 - \left\|\nabla_{s_h} P_n^h\right\|_{L^2(\mathbf{S}^h)}^2\right) \\ &\quad \leqslant \frac{c^2}{2\sigma}\left(\left\|\nabla_{s_h} P_{n+1}^h\right\|_{L^2(\mathbf{S}^h)}^2 + \left\|\nabla_{s_h} P_n^h\right\|_{L^2(\mathbf{S}^h)}^2\right).\end{aligned}$$

Multiplying Δt to both sides of the above inequality, and summing the results over n from 0 to $m-1$ for any integer $m > 1$, we get

$$\left\|\nabla_{s_h} P_m^h\right\|_{L^2(\mathbf{S}^h)}^2 \leqslant \left\|\nabla_{s_h} P_0^h\right\|_{L^2(\mathbf{S}^h)}^2 + \frac{c^2}{\sigma}\left(\Delta t\sum_{n=0}^{m}\left\|\nabla_{s_h} P_n^h\right\|_{L^2(\mathbf{S}^h)}^2\right).$$

Using Theorem 1, it holds that there is a constant $c > 0$, independent of h, n, Δt and N, such that

$$\left\|\nabla_{s_h} P_m^h\right\|_{L^2(\mathbf{S}^h)}^2 \leqslant \left\|\nabla_{s_h} P_0^h\right\|_{L^2(\mathbf{S}^h)}^2 + c.$$

Combining this with Corollary 1, the proof of theorem is then complete. □

4.4. Pointwise boundedness of the discrete solution

In this section, we aim to prove the point-wise boundedness for the discrete solution $\{U_n^h, n = 1, 2, \ldots, N\}$ for (3.2)–(3.4). Assume the solution exists.

Theorem 4. *For $\epsilon \in (0,1)$, there exists a generic constant $c > 0$, independent of h, n, Δt and N, such that*

$$\left\|U_{n+1/2}^h\right\|_{W^{1,2+\epsilon}(\mathbf{S}^h)} \leqslant c, \quad \forall n = 0, 1, \ldots, N-1 \tag{4.21}$$

and

$$\left\|U_{n+1/2}^h\right\|_{L^\infty(\mathbf{S}^h)} \leqslant c, \quad \forall n = 0, 1, \ldots, N-1. \tag{4.22}$$

Proof. With (3.4), we have that for $n = 0, 1, \ldots, N-1$ and any $W^h \in \mathcal{U}$,

$$\sigma\left(\nabla_{s_h} U_{n+1/2}^h, \nabla_{s_h} W^h\right)_{s_h} = \left(P_n^h - \tilde{\phi}\left(U_n^h, U_{n+1}^h\right), W^h\right)_{s_h} = (F_n, W^h)_{s_h},$$

where $F_n = P_n^h - \tilde{\phi}\left(U_n^h, U_{n+1}^h\right)$.

Using Theorem 3 and the Poincaré inequality, we get

$$\left\|P_n^h\right\|_{L^2(\mathbf{S}^h)} \leqslant c.$$

Moreover, by the Sobolev embedding theorem, (3.6) indicates that

$$\left\|U_n^h\right\|_{L^6(\mathbf{S}^h)} \leqslant c,$$

which leads to

$$\left\|\tilde{\phi}\left(U_n^h, U_{n+1}^h\right)\right\|_{L^2(\mathbf{S}^h)} \leqslant c, \quad \forall n = 0, 1, \ldots, N-1,$$

since $\tilde{\phi}$ is actually a globally defined smooth cubic polynomial of its two arguments for the free energy density function used in this paper. Then we have for $n = 0,1,\ldots,N-1$,

$$\|F_n\|_{L^2(\mathbf{S}^h)} \leqslant c,$$

which is equivalent to

$$\left\|F_n^l\right\|_{L^2(\mathbf{S})} \leqslant c.$$

For a fixed n, let $\tilde{u}$ be the solution of the equation

$$-\Delta_s \tilde{u} = F_n^l/\sigma$$

over **S** with the homogeneous Dirichlet boundary condition, we can show that such $\tilde{u}$ exists and satisfies the following property

$$\|\tilde{u}\|_{H^2(\mathbf{S})} \leqslant c\left\|F_n^l\right\|_{L^2(\mathbf{S})}.$$

Using the weak form of the above equation

$$\sigma(\nabla_s \tilde{u}, \nabla_s w)_s = (F_n^l, w)_s, \quad \forall w \in H^1(\mathbf{S}),$$

as well as the definition of $\Pi^h(\cdot)$, we can find that

$$U_{n+1/2}^h = \Pi^h \tilde{u}.$$

Therefore, by Lemma 5, we get for $n = 0,1,\ldots,N-1$,

$$\left\|U_{n+1/2}^h\right\|_{W^{1,2+\epsilon}(\mathbf{S}^h)} = \|\Pi^h \tilde{u}\|_{W^{1,2+\epsilon}(\mathbf{S}^h)} \leqslant c\|\tilde{u}\|_{H^2(\mathbf{S})} \leqslant c\left\|F_n^l\right\|_{L^2(\mathbf{S})} \leqslant c,$$

where c is independent of h, n, Δt and N.

Thus, (4.22) follows directly from (4.21) and from the Sobolev imbedding Theorem, $W^{1,2+\epsilon}(\mathbf{S}^h) \hookrightarrow L^\infty(\mathbf{S}^h)$, for $\epsilon > 0$. □

Now, let us prove the the point-wise boundedness for the discrete solution under some stability conditions.

Theorem 5. *Let Δt be sufficiently small, i.e.*

$$\Delta t < \sigma/(4k^2) \tag{4.23}$$

and

$$\Delta t/h^2 \leqslant c_0, \tag{4.24}$$

where c_0 is a constant. Then, there exists a constant $c > 0$ which depends on the initial condition u_0 but is independent of h, n, Δt and N, such that

$$\left\|U_n^h\right\|_{W^{0,\infty}(\mathbf{S}^h)} \leqslant c, \quad \forall n = 1, 2, \ldots, N. \tag{4.25}$$

Proof. In (3.3), set $V^h = \partial_t U_n^h$, we have

$$\left\|\delta_t U_n^h\right\|_{L^2(\mathbf{S}^h)}^2 \leqslant \left\|\nabla_{s_h} \delta_t U_n^h\right\|_{L^2(\mathbf{S}^h)} \left\|\nabla_{s_h} P_n^h\right\|_{L^2(\mathbf{S}^h)}. \tag{4.26}$$

By Theorem 3, we get the following inequality

$$\left\|\delta_t U_n^h\right\|_{L^2(\mathbf{S}^h)}^2 \leqslant c\left\|\nabla_{s_h} \delta_t U_n^h\right\|_{L^2(\mathbf{S}^h)}. \tag{4.27}$$

Using the inverse inequality

$$\left\|\nabla_{s_h} \delta_t U_n^h\right\|_{L^2(\mathbf{S}^h)} \leqslant ch^{-1}\left\|\delta_t U_n^h\right\|_{L^2(\mathbf{S}^h)}$$

on the last term, we have

$$\left\|\delta_t U_n^h\right\|_{L^2(\mathbf{S}^h)} \leqslant ch^{-1}.$$

Applying the inverse estimate in [9] (theorem 3.2.6), we further obtain

$$\|\delta_t U_n^h\|_{W^{0,\infty}(\mathbf{S}^h)} \leqslant ch^{-2},$$

which leads to

$$\left\|U_{n+1}^h - U_n^h\right\|_{W^{0,\infty}(\mathbf{S}^h)} \leqslant c\Delta t h^{-2} \leqslant cc_0, \quad \forall n = 0, 1, \ldots, N-1. \tag{4.28}$$

Combining (4.28) and Theorem 4, we have for any $n = 0,1,\ldots,N-1$,

$$\left\|U_{n+1}^h\right\|_{W^{0,\infty}(\mathbf{S}^h)} \leqslant \left\|U_{n+1/2}^h\right\|_{W^{0,\infty}(\mathbf{S}^h)} + \left\|\frac{U_{n+1}^h - U_n^h}{2}\right\|_{W^{0,\infty}(\mathbf{S}^h)} \leqslant c,$$

which proves the theorem. □

The stability condition (4.24) needed for proving the above theorem requires the time step increment be refined at a faster rate than the spatial discretization parameter h, when refinement of the discretization is used. Since the scheme is implicit, this may not be essential to the stability of the approximation scheme. In fact, the stability condition is not necessary for the one dimensional problem. On the other hand, the stability condition for a typical fully explicit finite difference scheme for fourth-order problems requires $\Delta t \leqslant ch^4$, which is considerably more restrictive than the one specified here.

5. Iterative Solution of the Nonlinear System

We have derived some nice properties of the discrete solution in previous sections. However, to compute the discrete solution that satisfies Eqs. (3.3) and (3.4), systems of nonlinear algebaic equations have to be solved. It is thus interesting to know what types of iterative solution techniques are applicable. In this section, we present an iterative scheme that can be used to solve the resulting nonlinear systems at each time step. The iteration is based on a contraction mapping theorem which can also be used to show the existence and uniqueness of the discrete solution for the scheme (3.3), (3.4). Our approach is very similar to that of [18].

For a given element $V \in \mathcal{U}$, we first consider the nonlinear mapping $\mathcal{T}_V : \mathcal{U} \to \mathcal{U}$ defined as follows: for any $\overline{U} \in \mathcal{U}, U = \mathcal{T}_V(\overline{U})$ satisfies

$$(U, V^h)_{s_h} + \Delta t(\nabla_{s_h} P, \nabla_{s_h} V^h)_{s_h} = (V, V^h)_{s_h}, \quad \forall V^h \in \mathcal{U} \tag{5.1}$$

and

$$-(P, W^h)_{s_h} + \sigma\left(\nabla_{s_h} \frac{U+V}{2}, \nabla_{s_h} W^h\right)_{s_h} + (\tilde{\phi}(\overline{U}, V), W^h)_{s_h} = 0, \quad \forall W^h \in \mathcal{U} \tag{5.2}$$

for some $P \in S^h$.

In [18], $\mathcal{T}_V$ was shown to be well-defined and the solution (U_{n+1},P_n) for $n = 0,1,2,\ldots,N-1$, of (3.2)–(3.4) is the fixed point of the mapping $\mathcal{T}_V$ for $V = U_{n-1}$. The proof remains valid in higher space dimensions. Now, we show that under the proper assumptions, $\mathcal{T}_V$ is in fact a local contraction mapping for all V in a bounded subset $\mathcal{U}_M$ of $\mathcal{U}$ where

$$\mathcal{U}_M = \{V \in \mathcal{U} \| max\left\{\|V\|_{W^{0,\infty}(\mathbf{S}^h)}, \|V\|_{H^1(\mathbf{S}^h)}\right\} \leqslant M.\}.$$

We define another subset of $\mathcal{U}$ by

$$\mathcal{U}_{1,K} = \{V \in \mathcal{U} \,|\, \|V\|_{H^1(\mathbf{S}^h)} \leqslant K\}.$$

Now, let us show that first of all, if $\psi = \mathcal{T}_V(\overline{U})$ where $\overline{U} = 0 \in \mathcal{U}_{1,K}$, then ψ is bounded in some $\mathcal{U}_{1,K}$.

Lemma 8. *Let $V \in \mathcal{U}_M$, then*

$$\|\psi\|_{H^1(\mathbf{S}^h)} \leqslant c_1\ (M^3 + 1)$$

for some constant $c_1 > 0$, independent of h, Δt and M.

Proof. In (5.1) and (5.2), let us take $W^h = \psi - V$ and $V^h = P$ respectively, then add them together to get

$$\frac{\sigma}{2}(\nabla_{s_h}(\psi + V), \nabla_{s_h}(\psi - V))_{s_h} + \Delta t(\nabla_{s_h}P, \nabla_{s_h}P)_{s_h} + (\tilde{\phi}(0, V), \psi - V)_{s_h} = 0.$$

Noticing that $\psi \in H_0^1(\Omega)$ and the definition of $\tilde{\phi}$, we have

$$\begin{aligned}\|\nabla_{s_h}\psi\|^2_{L^2(\mathbf{S}^h)} &\leqslant \|\nabla_{s_h}V\|^2_{L^2(\mathbf{S}^h)} + \frac{2}{\sigma}\cdot(\tilde{\phi}(0, V), V - \psi)_{s_h} \\ &\leqslant M^2 + \frac{2}{\sigma}\cdot\|\tilde{\phi}(0, V)\|_{L^2(\mathbf{S}^h)}\|\psi\|_{L^2(\mathbf{S}^h)} + c \\ &\leqslant c + cM^6 + \frac{1}{2}\|\nabla_{s_h}\psi\|^2_{L^2(\mathbf{S}^h)}.\end{aligned}$$

Therefore, we get

$$\|\nabla_{s_h}\psi\|^2_{L^2(\mathbf{S}^h)} \leqslant c(1 + M^6),$$

which implies the inequality in Lemma 8 for some constant c_1. □

Next, let us define $|||\mathcal{T}_V|||_K$ as follows:

$$|||\mathcal{T}_V|||_K = \mathbf{Sup}\left\{\frac{\|\mathcal{T}_V(\chi_1) - \mathcal{T}_V(\chi_2)\|_{H^1(\mathbf{S}^h)}}{\|\chi_1 - \chi_2\|_{H^1(\mathbf{S}^h)}} \,|\, \forall \chi_1, \chi_2 \in \mathcal{U}_{1,K}, \chi_1 \neq \chi_2\right\}.$$

Using this notation, we have:

Lemma 9. *Let $V \in \mathcal{U}_M$, then, there exists a constant $c_2 > 0$, independent of h, Δt, K and M, such that*

$$|||\mathcal{T}_V|||_K \leqslant c_2\frac{\Delta t^{1/4}}{\sigma^{3/4}}(K^2 + M^2 + 1). \tag{5.3}$$

Proof. Let us take $\chi_i \in \mathcal{U}_{1,K}, i = 1, 2,$ and $\psi_i = \mathcal{T}_V(\chi_i)$, then from (5.1) and (5.2), we have

$$(\psi_1 - \psi_2, V^h)_{s_h} + \Delta t(\nabla_{s_h}(\rho_1 - \rho_2), \nabla_{s_h}V^h)_{s_h} = 0, \quad \forall\ V^h \in \mathcal{U} \tag{5.4}$$

for $\rho_i \in \mathcal{U}, i = 1, 2$ and for all $W^h \in \mathcal{U}$

$$\begin{aligned}&-(\rho_1 - \rho_2, W^h)_{s_h} + \sigma\left(\nabla_{s_h}\frac{\psi_1 - \psi_2}{2}, \nabla_{s_h}W^h\right)_{s_h} \\ &\quad = -(\tilde{\phi}(\chi_1, V) - \tilde{\phi}(\chi_2, V), W^h)_{s_h}.\end{aligned} \tag{5.5}$$

Taking $V^h = \psi_1 - \psi_2$ and $W^h = -2\Delta t(\rho_1 - \rho_2)/\sigma$, and adding the above two equations together, we get

$$\begin{aligned}&\|\psi_1 - \psi_2\|^2_{L^2(\mathbf{S}^h)} + \frac{2\Delta t}{\sigma}\|\rho_1 - \rho_2\|^2_{L^2(\mathbf{S}^h)} \\ &\quad = \frac{2\Delta t}{\sigma}(\tilde{\phi}(\chi_1, V) - \tilde{\phi}(\chi_2, V), \rho_1 - \rho_2)_{s_h} \\ &\quad \leqslant \frac{\Delta t}{\sigma}\|\tilde{\phi}(\chi_1, V) - \tilde{\phi}(\chi_2, V)\|^2_{L^2(\mathbf{S}^h)} + \frac{\Delta t}{\sigma}\|\rho_1 - \rho_2\|^2_{L^2(\mathbf{S}^h)},\end{aligned}$$

so

$$\|\psi_1 - \psi_2\|_{L^2(\mathbf{S}^h)} \leqslant \sqrt{\frac{\Delta t}{\sigma}}\|\tilde{\phi}(\chi_1, V) - \tilde{\phi}(\chi_2, V)\|_{L^2(\mathbf{S}^h)}.$$

Now, taking $W^h = \psi_1 - \psi_2$ and $V^h = \rho_1 - \rho_2$ in (5.4) and (5.5), and adding the two equations together, we get

$$\begin{aligned}\frac{\sigma}{2}\|\nabla(\psi_1 - \psi_2)\|^2_{L^2(\mathbf{S}^h)} &= (\tilde{\phi}(\chi_1, V) - \tilde{\phi}(\chi_2, V), \psi_1 - \psi_2)_{s_h} - \Delta t\|\rho_1 - \rho_2\|^2_{L^2(\mathbf{S}^h)} \\ &\leqslant \|\tilde{\phi}(\chi_1, V) - \tilde{\phi}(\chi_2, V)\|_{L^2(\mathbf{S}^h)}\|\psi_1 - \psi_2\|_{L^2(\mathbf{S}^h)},\end{aligned}$$

therefore,

$$\frac{\sigma}{2}\|\nabla(\psi_1 - \psi_2)\|^2_{L^2(\mathbf{S}^h)} \leqslant \sqrt{\frac{\Delta t}{\sigma}}\|\tilde{\phi}(\chi_1, V) - \tilde{\phi}(\chi_2, V)\|^2_{L^2(\mathbf{S}^h)}. \tag{5.6}$$

This implies that

$$\|\psi_1 - \psi_2\|_{H^1(\mathbf{S}^h)} \leqslant c\frac{\Delta t^{1/4}}{\sigma^{3/4}}\|\tilde{\phi}(\chi_1, V) - \tilde{\phi}(\chi_2, V)\|_{L^2(\mathbf{S}^h)}. \tag{5.7}$$

Since

$$\begin{aligned}&|\tilde{\phi}(\chi_1, V) - \tilde{\phi}(\chi_2, V)| \\ &\quad = |\chi_1 - \chi_2|\cdot\left|\frac{\gamma_2}{8}(\chi_1 + \chi_2 + V)^2 + \frac{\gamma_0}{2} + \frac{\gamma_1}{3}(\chi_1 + \chi_2 + V)\right. \\ &\quad\quad \left.+ \frac{\gamma_2}{8}\left(\chi_1^2 + \chi_2^2 + V^2\right)\right| \leqslant c|\chi_1 - \chi_2|\cdot\left(1 + \chi_1^2 + \chi_2^2 + V^2\right)\end{aligned}$$

for some constant c, we have

$$\begin{aligned}\|\tilde{\phi}(\chi_1, V) - \tilde{\phi}(\chi_2, V)\|^2_{L^2(\mathbf{S}^h)} &\leqslant c\|\chi_1 - \chi_2\|^2_{L^6(\mathbf{S}^h)}\cdot(\|\chi_1\|_{L^6(\mathbf{S}^h)} + \|\chi_2\|_{L^6(\mathbf{S}^h)} \\ &\quad + \|V\|_{L^6(\mathbf{S}^h)} + 1)^4 \\ &\leqslant c\|\chi_1 - \chi_2\|^2_{H^1(\mathbf{S}^h)}\cdot(\|\chi_1\|_{H^1(\mathbf{S}^h)} \\ &\quad + \|\chi_2\|_{H^1(\mathbf{S}^h)} + \|V\|_{H^1(\mathbf{S}^h)} + 1)^4 \\ &\leqslant c\|\chi_1 - \chi_2\|^2_{H^1(\mathbf{S}^h)}\cdot(M^2 + K^2 + 1)^2.\end{aligned}$$

In above derivation, we have used the imbedding theorem: $H^1(\mathbf{S}) \hookrightarrow L^6(\mathbf{S})$.

Hence, we have

$$\|\psi_1 - \psi_2\|_{H^1(\mathbf{S}^h)} \leqslant c\frac{\Delta t^{1/4}}{\sigma^{3/4}}(M^2 + K^2 + 1)\|\chi_1 - \chi_2\|_{H^1(\mathbf{S}^h)}.$$

The theorem follows from the definition of $|||\mathcal{T}_V|||_K$. □

We now prove a fixed point theorem. For simplicity, we define a constant ϱ such that

$$\varrho = c_2\frac{\Delta t^{1/4}}{\sigma^{3/4}}(M^2 + (2K)^2 + 1),$$

where $K = c_1(M^3 + 1)$ and the constants c_i, $i = 1, 2$, are defined according to Lemmas 8 and 9. Then, by Lemma 9, we have

$$|||\mathcal{T}_V|||_{2K} \leqslant \varrho. \tag{5.8}$$

Theorem 6. *Let $V \in \mathcal{U}_M$, and Δt be small such that*

$$\varrho = c_2\frac{\Delta t^{1/4}}{\sigma^{3/4}}(M^2 + [2c_1(M^3 + 1)]^2 + 1) < \frac{1}{2}. \tag{5.9}$$

Then, there exists a constant $c > 0$, independent of h, Δt and M, such that $\mathcal{T}_V$ has a unique fixed point in $\mathcal{U}_{1,2K}$ where $K = c_1(M^3 + 1)$.

Proof. Let $\psi = \mathcal{T}_V(\overline{U})$ where $\overline{U} = 0 \in \mathcal{U}$ and consider the sequence $\left\{\mathcal{T}_v^i(\psi), i = 0, 1, \ldots\right\}$. Clearly, $\psi \in \mathcal{U}_{1,K}$ by Lemma 8 and thus $\psi \in \mathcal{U}_{1,2K}$. So, by (5.8),

$$\|\mathcal{T}_V(\psi) - \psi\|_{H^1(\mathbf{S}^h)} \leqslant \varrho\|\psi\|_{H^1(\mathbf{S}^h)}.$$

By triangle inequality,

$$\|\mathcal{T}_V(\psi)\|_{H^1(\mathbf{S}^h)} \leqslant (1 + \varrho)\|\psi\|_{H^1(\mathbf{S}^h)} \leqslant (1 + \varrho)K \leqslant 2K.$$

So, we can apply Lemma 9 again to get

$$\|\mathcal{T}_V^2(\psi) - \mathcal{T}_V(\psi)\|_{H^1(\mathbf{S}^h)} \leqslant \varrho \|\mathcal{T}_V(\psi) - \psi\|_{H^1(\mathbf{S}^h)} \leqslant \varrho^2 \|\psi\|_{H^1(\mathbf{S}^h)}.$$

Again, triangle inequality gives us:

$$\|\mathcal{T}_V^2(\psi)\|_{H^1(\mathbf{S}^h)} \leqslant (1 + \varrho + \varrho^2)\|\psi\|_{H^1(\mathbf{S}^h)}.$$

If we continue this process, we get that for $i = 0,1,\ldots$,

$$\left\|\mathcal{T}_V^{i+1}(\psi) - \mathcal{T}_V^i(\psi)\right\|_{H^1(\mathbf{S}^h)} \leqslant \varrho^{i+1}\|\psi\|_{H^1(\mathbf{S}^h)}$$

and

$$\left\|\mathcal{T}_V^{i+1}(\psi)\right\|_{H^1(\mathbf{S}^h)} \leqslant \left(\sum_{j=0}^{i+1} \varrho^j\right)\|\psi\|_{H^1(\mathbf{S}^h)} \leqslant 2\|\psi\|_{H^1(\mathbf{S}^h)} \leqslant 2K.$$

This shows that the sequence $\left\{\mathcal{T}_V^i(\psi), i = 0,1,\ldots\right\}$ is a Cauchy sequence in the finite dimensional space $\mathcal{U}$, thus it converges to some limit which is, naturally, a fixed point of the nonlinear mapping $\mathcal{T}_V$ in $\mathcal{U}_{1,2K}$. The uniqueness follows directly from (5.8). □

Remark 1. Comparing the above theorem with Lemma 3.3 of [18], we see that by a more careful argument, we have proved the fixed point theorem without assuming the dependence of Δt on h.

Based on the above theorem, a fixed-point iteration using the mapping $\mathcal{T}_{U_n^h}$ gives a globally convergent scheme for solving the nonlinear system (3.3) and (3.4). Thus, we propose the following algorithm: At time step t_n, $(n = 0,1,2,\ldots,N-1)$, define

$$\psi_0 = U_n^h. \tag{5.10}$$

then, for $j = 0,1,2,\ldots$, let

$$\psi_{j+1} = \mathcal{T}_{U_n^h}(\psi_j). \tag{5.11}$$

Then, as a consequence of the above theorem, we have

Corollary 2. *Under the assumptions in Theorem 6, the sequence defined by (5.10) and (5.11) satisfies*

$$\psi_j \to U_{n+1}^h, \quad \text{as } j \to \infty. \tag{5.12}$$

In practice, one may choose to use the fixed-point iteration for a few times, then switch to a Newton-like iteration to accelerate the convergence.

Finally, by applying the above theorems and the uniform pointwise bound we have obtained in previous sections, the existence and uniqueness of the fully discrete scheme can be easily established in the same way as previously demonstrated in [18].

6. Error estimates for the approximation scheme

Given the analysis already presented, deriving the error estimate becomes rather standard, except for the additional complication due to the projections between the surface and its planar triangulation.

To simplify the notation, we use the abbreviation $u(t)$ and $p(t)$ to denote the exact solution $u(\cdot,t)$ and the corresponding chemical potential at time t, both of which are assumed to be sufficiently smooth. We let u_t, u_{tt} be the time derivatives of u, p_t be that of p. The next lemma follows Lemma 4.3 and Corollary 4.2 in [18].

Lemma 10. *Let $u \in L^\infty(\mathbf{S} \times (0,T))$ and there exists a constant $c > 0$ such that*

$$\left\|U_n^h\right\|_{W^{0,\infty}(\mathbf{S}^h)} \leqslant c, \quad \forall n = 0,1,\ldots,N. \tag{6.1}$$

Then there exists a generic constant $c > 0$ such that

$$\left\|\tilde{\phi}\left(U_n^h, U_{n+1}^h\right) - \phi(u^l(t_n))\right\|_{L^2(\mathbf{S}^h)} \leqslant c\left(\left\|U_{n+1}^h - u^l(t_{n+1})\right\|_{L^2(\mathbf{S}^h)} + \left\|U_n^h - u^l(t_n)\right\|_{L^2(\mathbf{S}^h)} + \|u^l(t_n) - u^l(t_{n+1})\|_{L^4(\mathbf{S}^h)}^2\right)$$

Proof. By the triangle inequality,

$$\begin{aligned}\left\|\tilde{\phi}\left(U_n^h, U_{n+1}^h\right) - \phi(u^l(t_n))\right\|_{L^2(\mathbf{S}^h)} &\leqslant \Big\|\tilde{\phi}\left(U_n^h, U_{n+1}^h\right) - \tilde{\phi}\left(U_n^h, u^l(t_{n+1})\right)\Big\|_{L^2(\mathbf{S}^h)} + \left\|\tilde{\phi}\left(U_n^h, u^l(t_{n+1})\right) - \tilde{\phi}(u^l(t_n), u^l(t_{n+1}))\right\|_{L^2(\mathbf{S}^h)} \\ &\quad + \|\tilde{\phi}(u^l(t_n), u^l(t_{n+1})) - \phi(u^l(t_n))\|_{L^2(\mathbf{S}^h)} = I_1 + I_2 + I_3,\end{aligned}$$

where $\{I_i\}(i = 1,2,3)$ denote the terms in the previous summation in their corresponding orders.

Due to the uniform boundedness of U_n^h and $u(t)$, it easily follows that

$$I_1 \leqslant c\left\|U_{n+1}^h - u^l(t_{n+1})\right\|_{L^2(\mathbf{S}^h)},$$

$$I_2 \leqslant c\left\|U_n^h - u^l(t_n)\right\|_{L^2(\mathbf{S}^h)}$$

for some constant $c > 0$.

For the term I_3, recall the algebraic identities

$$\frac{u^2 + uv + v^2}{3} - \left(\frac{u+v}{2}\right)^2 = \frac{1}{12}(u-v)^2,$$

$$\frac{u^3 + u^2v + uv^2 + v^3}{4} - \left(\frac{u+v}{2}\right)^3 = \frac{1}{8}(u+v)(u-v)^2,$$

then we have

$$\tilde{\phi}(u^l(t_n), u^l(t_{n+1})) - \phi(u^l(t_n)) = \left(\frac{\gamma_2}{4}u^l(t_n) + \frac{\gamma_1}{12}\right)[u^l(t_n) - u^l(t_{n+1})]^2,$$

thus

$$I_3 \leqslant c\|u^l(t_n) - u^l(t_{n+1})\|_{L^4(\mathbf{S}^h)}^2,$$

which finishes the proof. □

We remark that in Lemma 10, if we change $\phi(u^l(t_n))$ to $\phi(u^l(t_{n+1}))$, a similar result follows. By Theorem 5, the conditions on the pointwise bounds assumed in the above lemma can be established under suitable conditions as stated earlier. Then we have the following error estimate for our fully discrete finite element scheme.

Theorem 7. *For $n = 1,2,\ldots,N$, under the assumptions on u and U_n^h in Lemma 10, and the additional assumptions that*

$$u \in C^1\left([0,T], H_0^1(\mathbf{S}) \cap H^2(\mathbf{S})\right) \cap C^3([0,T], L^2(\mathbf{S})), \tag{6.2}$$

$$p \in L^\infty\left([0,T], H_0^1(\mathbf{S}) \cap H^2(\mathbf{S})\right) \cap C^2([0,T], L^2(\mathbf{S})), \tag{6.3}$$

then there exists a generic constant $c > 0$ independent of h, Δt and n, such that

$$\begin{aligned}\left\|U_n^h - u^l(t_n)\right\|_{L^2(\mathbf{S}^h)}^2 &\leqslant \|u^l(t_n) - \Pi^h u(t_n)\|_{L^2(\mathbf{S}^h)}^2 + c\Delta t\sum_{i=0}^{n-1}\Big[\|\delta_t(u^l(t_i) - \Pi^h u(t_i))\|_{L^2(\mathbf{S}^h)}^2 + \|u^l(t_i) - \Pi^h u(t_i)\|_{L^2(\mathbf{S}^h)}^2 + \|p^l(t_{i+1/2}) \\ &\quad - \Pi^h p(t_{i+1/2})\|_{L^2(\mathbf{S}^h)}^2 + \Delta t^4\Big(\left\|u_{ttt}^l(t_{i+\theta_i})\right\|_{L^2(\mathbf{S}^h)}^2 + \left\|u_{ttt}^l(t_{i+\kappa_i})\right\|_{L^2(\mathbf{S}^h)}^2 \\ &\quad + \left\|p_{tt}^l(t_{n+\tau_i})\right\|_{L^2(\mathbf{S}^h)}^2 + \left\|p_{tt}^l(t_{n+v_i})\right\|_{L^2(\mathbf{S}^h)}^2 + \left\|u_t^l(t_{i+\gamma_i})\right\|_{L^4(\mathbf{S}^h)}^4\Big)\Big],\end{aligned} \tag{6.4}$$

where $t_j = j\Delta t, t_{j+\theta_j} = (j+\theta_j)\Delta t$ for $0 < \theta_j < 1, j = 1,2,\ldots,n-1$, adopt the same definition for κ_j, τ_j, v_j and γ_j.

Proof. For $n = 0, 1, 2, \ldots, N$, let us define

$$E_n = U_n^h - \Pi^h u(t_n), \quad F_n = P_n^h - \Pi^h p(t_n), \quad F_{n+1/2} = P_n^h - \Pi^h p(t_{n+1/2})$$

and

$$\xi(t) = u^l(t) - \Pi^h u(t), \quad \eta(t) = p^l(t) - \Pi^h p(t).$$

By the definition of the fully discrete scheme we see that the above quantities satisfy the following equations:

$$\begin{aligned}
&\left(\frac{E_{n+1} - E_n}{\Delta t}, V^h\right)_{s_h} + (\nabla_{s_h} F_{n+1/2}, \nabla_{s_h} V^h)_{s_h} \\
&\quad = \left(\frac{\xi(t_{n+1}) - \xi(t_n)}{\Delta t}, V^h\right)_{s_h} - (\delta_t u^l(t_n), V^h)_{s_h} \\
&\qquad - (\nabla_{s_h} \Pi^h p(t_{n+1/2}), \nabla_{s_h} V^h)_{s_h},
\end{aligned} \tag{6.5}$$

$$\begin{aligned}
&-(F_{n+1/2}, W^h)_{s_h} + \sigma\left(\nabla_{s_h} \frac{E_{n+1} + E_n}{2}, \nabla_{s_h} W^h\right)_{s_h} \\
&\quad = -(\eta(t_{n+1/2}), W^h)_{s_h} + (p^l(t_{n+1/2}), W^h)_{s_h} \\
&\qquad - \sigma\left(\nabla_{s_h} \frac{\Pi^h u(t_{n+1}) + \Pi^h u(t_n)}{2}, \nabla_{s_h} W^h\right)_{s_h} \\
&\qquad - \left(\tilde{\phi}\left(U_n^h, U_{n+1}^h\right), W^h\right)_{s_h}.
\end{aligned} \tag{6.6}$$

Set $V^h = \frac{E_{n+1}+E_n}{2}$ in (6.5), $W^h = F_{n+1/2}$ in (6.6), multiply the first result by σ and subtract by the second result, we then obtain

$$\begin{aligned}
&\sigma\left(\frac{E_{n+1} - E_n}{\Delta t}, \frac{E_{n+1} + E_n}{2}\right)_{s_h} + (F_{n+1/2}, F_{n+1/2})_{s_h} \\
&\quad = \sigma\left(\frac{\xi(t_{n+1}) - \xi(t_n)}{\Delta t}, V^h\right)_{s_h} - \sigma(\delta_t u^l(t_n), V^h)_{s_h} \\
&\qquad - \sigma(\nabla_{s_h} \Pi^h p(t_{n+1/2}), \nabla_{s_h} V^h)_{s_h} + (\eta(t_{n+1/2}), W^h)_{s_h} \\
&\qquad - (p^l(t_{n+1/2}), W^h)_{s_h} \\
&\qquad + \sigma\left(\nabla_{s_h} \frac{\Pi^h u(t_{n+1}) + \Pi^h u(t_n)}{2}, \nabla_{s_h} W^h\right)_{s_h} \\
&\qquad + \left(\tilde{\phi}\left(U_n^h, U_{n+1}^h\right), W^h\right)_{s_h} \\
&\quad = T_1 + T_2 + T_3 + T_4,
\end{aligned} \tag{6.7}$$

where

$$\begin{aligned}
T_1 &= \sigma\left(\frac{\xi(t_{n+1}) - \xi(t_n)}{\Delta t}, V^h\right)_{s_h}, \\
T_2 &= -\sigma(\delta_t u^l(t_n), V^h)_{s_h} - \sigma(\nabla_{s_h} \Pi^h p(t_{n+1/2}), \nabla_{s_h} V^h)_{s_h}, \\
T_3 &= (\eta(t_{n+1/2}), W^h)_{s_h}, \\
T_4 &= -(p^l(t_{n+1/2}), W^h)_{s_h} + \sigma\left(\nabla_{s_h} \frac{\Pi^h u(t_{n+1}) + \Pi^h u(t_n)}{2}, \nabla_{s_h} W^h\right)_{s_h} \\
&\quad + \left(\tilde{\phi}\left(U_n^h, U_{n+1}^h\right), W^h\right)_{s_h}.
\end{aligned}$$

As for the estimates of T_2 and T_4, to avoid tedious derivations, we omit most details of our analysis and only give the following main results:

$$\begin{aligned}
T_2 &= -\sigma\left(\frac{1}{\mu_h}\left(\frac{u(t_{n+1}) - u(t_n)}{\Delta t} - u_t(t_{n+1/2})\right), V^{h,l}\right)_s \\
&= -\frac{\sigma\Delta t^2}{48}\left(u_{ttt}(t_{n+\theta_n}) + u_{ttt}(t_{n+\kappa_n}), V^h\right)_{s_h}
\end{aligned}$$

$$\begin{aligned}
T_4 &= -(p^l(t_{n+1/2}), W^h)_{s_h} + \left(\tilde{\phi}\left(U_n^h, U_{n+1}^h\right), W^h\right)_{s_h} \\
&\quad + \left(\frac{p^l(t_{n+1}) + p^l(t_n)}{2} - \frac{\phi(u^l(t_{n+1})) + \phi(u^l(t_n))}{2}, W^h\right)_{s_h} \\
&= \left(\frac{p^l(t_{n+1}) + p^l(t_n)}{2} - p^l(t_{n+1/2}), W^h\right)_{s_h} + \left(\frac{\tilde{\phi}\left(U_n^h, U_{n+1}^h\right) - \phi(u^l(t_{n+1}))}{2}, W^h\right)_{s_h} \\
&\quad + \left(\frac{\tilde{\phi}\left(U_n^h, U_{n+1}^h\right) - \phi(u^l(t_n))}{2}, W^h\right)_{s_h} \\
&= \frac{\Delta t^2}{16}\left(p_{tt}^l(t_{n+\tau_n}) + p_{tt}^l(t_{n+\nu_n}), W^h\right)_{s_h} + \left(\frac{\tilde{\phi}\left(U_n^h, U_{n+1}^h\right) - \phi(u^l(t_{n+1}))}{2}, W^h\right)_{s_h} \\
&\quad + \left(\frac{\tilde{\phi}\left(U_n^h, U_{n+1}^h\right) - \phi(u^l(t_n))}{2}, W^h\right)_{s_h}.
\end{aligned}$$

With all the above approximations and Lemma 10, we sum both sides of (6.7) with n ranging from 0 to $n - 1$. It follows that

$$\begin{aligned}
&\frac{\sigma}{2\Delta t}\|E_n\|_{L^2(\mathbf{S}^h)}^2 + \sum_{i=0}^{n-1}\|F_{i+1/2}\|_{L^2(\mathbf{S}^h)}^2 - \frac{\sigma}{2\Delta t}\|E_0\|_{L^2(\mathbf{S}^h)}^2 \\
&\quad \leqslant \frac{\sigma}{2}\sum_{i=0}^{n-1}\|\delta_t\xi(t_i)\|_{L^2(\mathbf{S}^h)}^2 + \frac{\sigma\Delta t^4}{1304} \\
&\qquad \times \sum_{i=0}^{n-1}\left(\left\|u_{ttt}^l(t_{i+\theta_i})\right\|_{L^2(\mathbf{S}^h)}^2 + \left\|u_{ttt}^l(t_{i+\kappa_i})\right\|_{L^2(\mathbf{S}^h)}^2\right) + \frac{1}{2} \\
&\qquad \times \sum_{i=0}^{n-1}\|\eta(t_{i+1/2})\|_{L^2(\mathbf{S}^h)}^2 + \frac{\sigma}{4}\sum_{i=0}^{n-1}\|E_{i+1} + E_i\|_{L^2(\mathbf{S}^h)}^2 + \frac{\Delta t^4}{512} \\
&\qquad \times \sum_{i=0}^{n-1}\left(\left\|p_{tt}^l(t_{i+\tau_i})\right\|_{L^2(\mathbf{S}^h)}^2 + \left\|p_{tt}^l(t_{i+\nu_i})\right\|_{L^2(\mathbf{S}^h)}^2\right) + c \\
&\qquad \times \sum_{i=0}^{n-1}\left(\|E_i\|_{L^2(\mathbf{S}^h)}^2 + \|\xi(t_i)\|_{L^2(\mathbf{S}^h)}^2 + \|u^l(t_i) - u^l(t_{i+1})\|_{L^4(\mathbf{S}^h)}^4\right) + \frac{1}{2} \\
&\qquad \times \sum_{i=0}^{n-1}\|F_{i+1/2}\|_{L^2(\mathbf{S}^h)}^2,
\end{aligned}$$

which leads to

$$\begin{aligned}
\|E_n\|_{L^2(\mathbf{S}^h)}^2 &\leqslant \|E_0\|_{L^2(\mathbf{S}^h)}^2 + \Delta t\sum_{i=0}^{n-1}\|\delta_t\xi(t_i)\|_{L^2(\mathbf{S}^h)}^2 + \frac{\Delta t^5}{652} \\
&\quad \times \sum_{i=0}^{n-1}\left(\left\|u_{ttt}^l(t_{i+\theta_i})\right\|_{L^2(\mathbf{S}^h)}^2 + \left\|u_{ttt}^l(t_{i+\kappa_i})\right\|_{L^2(\mathbf{S}^h)}^2\right) + \Delta t \\
&\quad \times \sum_{i=0}^{n-1}\|E_i\|_{L^2(\mathbf{S}^h)}^2 + \frac{\Delta t}{2}\|E_n\|_{L^2(\mathbf{S}^h)}^2 + \frac{\Delta t}{\sigma}\sum_{i=0}^{n-1}\|\eta(t_{i+1/2})\|_{L^2(\mathbf{S}^h)}^2 \\
&\quad + \frac{\Delta t^5}{256\sigma}\sum_{i=0}^{n-1}\left(\left\|p_{tt}^l(t_{i+\tau_i})\right\|_{L^2(\mathbf{S}^h)}^2 + \left\|p_{tt}^l(t_{i+\nu_i})\right\|_{L^2(\mathbf{S}^h)}^2\right) + c\Delta t \\
&\quad \times \sum_{i=0}^{n-1}\|E_i\|_{L^2(\mathbf{S}^h)}^2 + c\Delta t\sum_{i=0}^{n-1}\|\xi(t_i)\|_{L^2(\mathbf{S}^h)}^2 + c\Delta t^5 \\
&\quad \times \sum_{i=0}^{n-1}\|u_t^l(t_{i+\gamma_i})\|_{L^4(\mathbf{S}^h)}^4.
\end{aligned}$$

Apply the discrete Gronwall inequality and consider the definition of E_0 and U_0^h, we see that there exists a constant $c > 0$ such that

$$\begin{aligned}
\|E_n\|_{L^2(\mathbf{S}^h)}^2 &\leqslant c\Delta t\sum_{i=0}^{n-1}\Big[\|\delta_t\xi(t_i)\|_{L^2(\mathbf{S}^h)}^2 + \|\xi(t_i)\|_{L^2(\mathbf{S}^h)}^2 + \|\eta(t_{i+1/2})\|_{L^2(\mathbf{S}^h)}^2 \\
&\quad + \Delta t^4\Big(\left\|u_{ttt}^l(t_{i+\theta_i})\right\|_{L^2(\mathbf{S}^h)}^2 + \left\|u_{ttt}^l(t_{i+\kappa_i})\right\|_{L^2(\mathbf{S}^h)}^2 + \left\|p_{tt}^l(t_{i+\tau_i})\right\|_{L^2(\mathbf{S}^h)}^2 \\
&\quad + \left\|p_{tt}^l(t_{i+\nu_i})\right\|_{L^2(\mathbf{S}^h)}^2 + \left\|u_t^l(t_{i+\gamma_i})\right\|_{L^4(\mathbf{S}^h)}^4\Big)\Big].
\end{aligned}$$

Thus the conclusion (6.4) follows. □

By the definition of $\mathcal{U}$ and the conclusions in [20], it can be seen that if $u \in C^1((0,T), H_0^1(\mathbf{S}) \cap H^2(\mathbf{S}))$ and $p \in L^\infty\left((0,T), H_0^1(\mathbf{S}) \cap H^2(\mathbf{S})\right)$, then there exists some constant $c > 0$ which satisfies

$$\|u^l(t_i) - \Pi^h u(t_i)\|_{L^2(\mathbf{S}^h)} \leqslant ch^2,$$
$$\|p^l(t_i) - \Pi^h p(t_i)\|_{L^2(\mathbf{S}^h)} \leqslant ch^2,$$
$$\|\delta_t(u^l(t_i) - \Pi^h u(t_i))\|_{L^2(\mathbf{S}^h)} \leqslant ch^2$$

and under some regularity assumptions for time derivatives of u and p, we can deduce the following corollary from Theorem 7,

Corollary 3. *Under the assumptions in Theorem 7, it holds that for $n = 1, 2, \ldots, N$, there exists a constant $c > 0$ independent of h, Δt and n, such that*

$$\left\|U_n^h - u^l(t_n)\right\|_{L^2(\mathbf{S}^h)} \leqslant c(h^2 + \Delta t^2).$$

From discussions in previous sections, we know that the condition (6.1) is automatically satisfied under the conditions specified in Theorem 5. The error estimate is of optimal order, with respect to the approximation space.

7. Numerical experiments

We now present some numerical simulations using the proposed method to solve the Cahn–Hilliard equation. In the experiments, we first show the numerical approximate solutions for one surface (*half-sphere*, *saddle-like surface* or *unit sphere*) at some specific time steps on two meshes with different degrees of freedom to demonstrate the convergence. Similar experiments can be found in [22,31,39]. Then we also study the numerical spatial and temporal convergence rates of our scheme in details. To ensure the accurate finite element solution, the meshes of the surface $\mathbf{S}$ to be used in our numerical experiments for discretization are generated by the so-called *constrained centroidal Voronoi Delaunay triangulation* (CCVDT) algorithm [15]. We now give a brief description below.

Given a density function $\rho(\mathbf{x})$ defined on $\mathbf{S}$, for any region $V \subset \mathbf{S}$, we call $\mathbf{x}^c$ the constrained mass centroid of V on $\mathbf{S}$ if

$$\mathbf{x}^c = \arg\min_{\mathbf{x} \in V} F(\mathbf{x}), \quad \text{where } F(\mathbf{x}) = \int_V \rho(\mathbf{y}) \|\mathbf{y} - \mathbf{x}\|^2 \, ds(\mathbf{y}). \tag{7.1}$$

The existence of solutions of (7.1) can be easily obtained by using the continuity and compactness of F; however, solutions may not be unique. In general, given a Voronoi tessellation $\mathcal{W} = \{\mathbf{x}_i, V_i\}_{i=1}^n$ of $\mathbf{S}$, the generators $\{\mathbf{x}_i\}_{i=1}^n$ do not coincide with $\{\mathbf{x}_i^c\}_{i=1}^n$, where $\mathbf{x}_i^c$ denotes the constrained mass centroid of V_i for $i = 1, \ldots, n$. We refer to a Voronoi tessellation of $\mathbf{S}$ as a *constrained centroidal Voronoi tessellation*(CCVT) if and only if the points $\{\mathbf{x}_i\}_{i=1}^n$ which serve as the generators of the associated Voronoi tessellation $\{V_i\}_{i=1}^n$ are also the constrained mass centroids of those regions [15], i.e., if and only if we have that

$$\mathbf{x}_i = \mathbf{x}_i^c \quad \text{for } i = 1, \ldots, n.$$

The CCVT is a generalization of the standard centroidal Voronoi tessellation [14] which is a concept with many applications including mesh generation and optimization. The dual tessellation of CCVT of $\mathbf{S}$ is then called a CCVDT. Constrained centroidal Voronoi meshes on surfaces in $\mathbb{R}^3$ have many good geometric properties, see [15,19] for detailed studies as well as efficient algorithms for constructing CCVT/CCVDT meshes.

For all the experiments shown here, the meshes are all generated by CCVDT algorithm with a constant density function, and we always set $\phi(u) = u^3 - u$. As in Lemma 1, a simple computation gives $k = 0.5$, so that

$$\Delta t < \frac{\sigma}{4k^2} \leqslant \sigma, \tag{7.2}$$

according to the theoretical analysis.

Numerical tests are performed on different surfaces, with different σ. And we use Newton's method to solve nonlinear system (3.2)–(3.4). Notice that our analysis can be applied to natural boundary condition problems without any major modification, so we do not restrict ourselves with Dirichlet boundary conditions in the numerical experiments.

Firstly, we present the approximate solutions on the half unit sphere with $\sigma = 0.008$, $\Delta t = 0.004$ in Fig. 2 which shows the results on meshes with 1219 and 4777 nodes, respectively. The initial condition for the coarse mesh is a small zero mean perturbation across the surface, then is projected onto the finer mesh, such that the two experiments have the same initial condition. We can see the excellent agreement between these two cases.

Our second experiment is performed on a saddle-like surface defined by

$$\mathbf{S} = \left\{\mathbf{x} \in \mathbb{R}^3 | (x_3 - x_2^2)^2 + x_1^2 + x_2^2 = 1, \; x_3 \geqslant x_2^2, \; x_1 \geqslant 0\right\}.$$

We set $\sigma = 0.006$, $\Delta t = 0.005$ and Fig. 3 shows the numerical results at different time with 3420 and 13493 nodes. The initial conditions

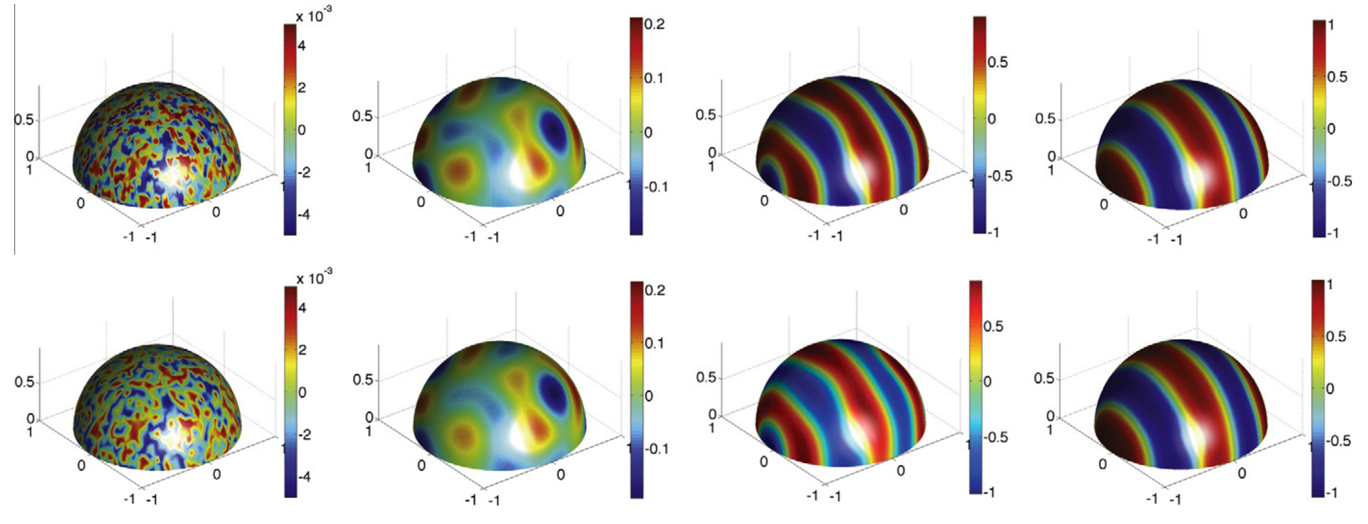

Fig. 2. Numerical solutions of the concentration u at t = 0, 0.2, 0.4, 0.6 (from left to right), on meshes with 1219 (top row) and 4777 (bottom row) nodes in the first example.

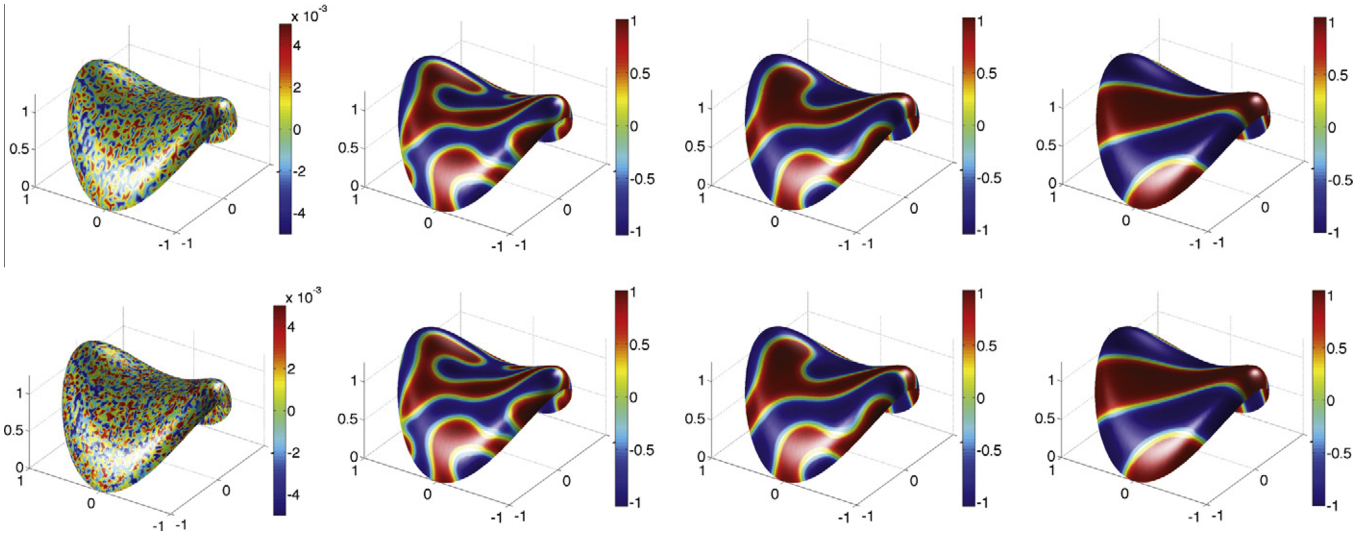

Fig. 3. Numerical solutions of the concentration u at $t = 0, 1, 2, 10$ (left to right), on meshes with 3420 (top row) and 13493 (bottom row) nodes in the second example.

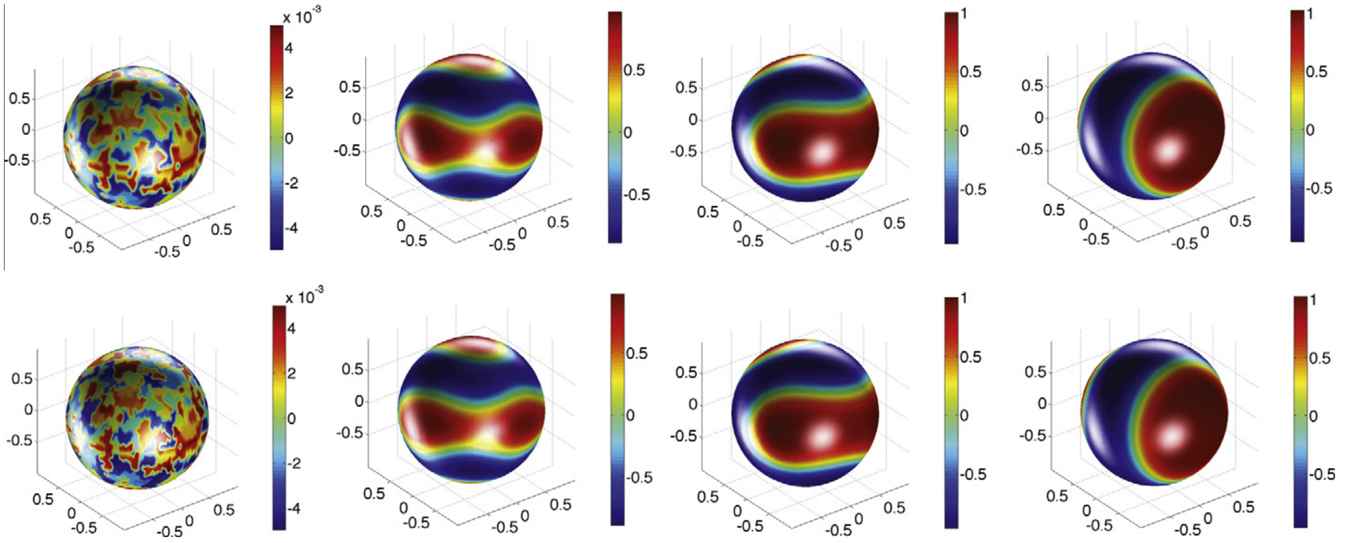

Fig. 4. Numerical solutions of the concentration u at $t = 0, 1, 2, 5$ (from left to right), on meshes with 2018 (top row) and 8066 (bottom row) nodes in the third example.

for different meshes are determined in the same way as in the first example. We can observe the solution finally converges to a steady state and the solutions agree well on two different meshes.

Thirdly, we test our scheme on a closed surface. The surface **S** is chosen to be the unit sphere, defined by $\mathbf{S} = \{\mathbf{x} \in \mathbb{R}^3 | x_1^2 + x_2^2 + x_3^2 = 1\}$. We set $\sigma = 0.01$ and $\Delta t = 0.005$ and solve the equation on meshes with 2018 and 8066 nodes. The initial conditions on two meshes are again chosen, as in the previous two examples, to guarantee the consistency. Results at different time steps are presented in Fig. 4. It can be seen that our method also works well for closed surface, though the theoretical analysis is only done for an open surface.

In the following we investigate the numerical spatial and temporal convergence rates of our scheme. We first test the spatial convergence rate by solving the Cahn–Hilliard equations with $\sigma = 0.01$ over the half unit sphere, and the initial conditions are set using the same way as in the first example. Since there is no analytic solution available in general for this nonlinear problem, we use the numerical solution on a sufficiently fine mesh (64897 nodes) as the *exact solution*. To obtain accurate spatial convergence rates, we need keep Δt much smaller than h. Thus we take a small time step $\Delta t = 0.001$ and compare numerical solutions on coarser meshes (277, 1057, 4129 and 16321 nodes, respectively) with the *exact solution* at $t = 1$. These four meshes have mesh size $h = 0.2695$, 0.1354, 0.0678 and 0.0339 respectively. We note that although the continuously refined CCVDT meshes are not exactly nested, they are very close to uniform refinement. As shown in Table 1, the observed spatial convergence rates are consistent with our theoretical results.

To check the temporal convergence rate, we solve the Cahn–Hilliard equation with $\sigma = 0.3$ over the half sphere on the fine spatial

Table 1
Results on the numerical spatial convergence rates.

# of nodes	# of triangles	h	L^2 error	CR
277	504	0.2695	0.12643	–
1057	2016	0.1354	0.02331	2.45
4129	8064	0.0678	0.00613	1.93
16321	32256	0.0339	0.00144	2.08

Table 2
Results on the numerical temporal convergence rates.

Δt	L^2 error	CR
0.2	0.02714	–
0.1	0.00774	1.87
0.05	0.00263	1.71

mesh with 64897 nodes ($h = 0.0169$). We first take a sufficient small time step $\Delta t = 0.005$, solve for the numerical solution on this mesh until $t = 2$, and use it as the *exact solution*. Then we solve the same problem until $t = 2$ with $\Delta t = 0.2$, 0.1 and 0.05 respectively. We compare the three numerical solutions with the *exact solution* and list the results in Table 2. The observed temporal convergence rates are also close to the theoretical results.

8. Conclusions

In this paper, we rigorously analyzed the well-posedness and convergence of a fully discrete finite element approximation scheme for solving the Cahn–Hilliard equation defined on a general surface which is often used to model the phase separation process. In particular, we derived some uniform a priori estimates for the discrete solution that does not rely on any knowledge of the exact solution beyond the initial time. Given the nonlinear nature of the underlying PDE, such estimates are very useful to control (and compare) the nonlinear terms. They lead to the global Lipshitz property of the nonlinear term in the proper function space which in turn gives the optimal error estimates of the scheme. Various numerical examples are presented to validate our theoretical results. We note that while a uniform time discretization is used in the analysis given here for the purpose of simplifying notations, much of the conclusions remain valid for nonuniform and adaptive time steps. The approximation scheme as well as the analysis presented here can be easily modified to deal with the Neumann type boundary value problems for the Cahn–Hilliard equation where the reductions to coupled systems and the mixed forms are again allowed. In the future, it will be interesting to study the extensions to more complex situation where the surfaces may involve singularities and/or may evolve together with the phase field variables.

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References

[1] J. Barrett, J. Blowey, An error bound for the finite element approximation of the Cahn–Hilliard equation with logarithmic free energy, Numer. Math. 72 (1995) 1–20.

[2] J. Barrett, J. Blowey, H. Garcke, On fully practical finite element approximations of degenerate Cahn–Hilliard systems, M2AN 35 (2001) 713–748.

[3] T. Baumgart, S. Hess, W. Webb, Imaging coexisting fluid domains in biomembrane models coupling curvature and line tension, Nature 425 (2003) 821–824.

[4] A. Bausch et al., Grain boundary scars and spherical crystallography, Science 299 (2003) 1716–1718.

[5] G. Caginalp, Stefan and Hele–Shaw type models as asymptotic limits of the phase field equations, Phys. Rev. A 39 (1989) 5887–5896.

[6] J. Cahn, On spinodal decomposition, Acta Metall. 9 (1961) 795–801.

[7] J. Cahn, J. Hilliard, Free energy of a non-uniform system. I. interfacial free energy, J. Chem. Phys 28 (1958) 258–267.

[8] L.-Q. Chen, J. Shen, Applications of semi-implicit fourier-spectral method to phase field equations, Comput. Phys. Commun. 108 (1996) 147–158.

[9] P. Ciarlet, The Finite Element Method For Elliptic Problems, North Holland, Amsterdam, 1978.

[10] L. Cueto-Felgueroso, J. Peiraire, A time-adaptive finite volume method for the Cahn–Hilliard and Kuramoto–Sivashinsky equations, J. Comput. Phys 227 (2008) 9985–10017.

[11] A. Demlow, Higher-order finite element methods and pointwise error estimates for elliptic problems on surfaces, SIAM J. Numer. Anal. 47 (2009) 805–827.

[12] A. Demlow, G. Dziuk, An adaptive finite element method for the Laplace–Beltrami operator on implicitly defined surfaces, SIAM J. Numer. Anal 45 (2007) 421–442.

[13] I. Dolcetta, S. Vita, R. March, Area-preserving curve-shortening flows: from phase separation to image processing, Interfaces Free Bound. 4 (2002) 325–343.

[14] Q. Du, V. Faber, M. Gunzburger, Centroidal Voronoi tessellations: applications and algorithms, SIAM Rev. 41 (1999) 37–676.

[15] Q. Du, M. Gunzburger, L. Ju, Constrained centroidal Voronoi tessellations on general surfaces, SIAM J. Sci. Comput. 24 (2003) 1488–1506.

[16] Q. Du, L. Ju, Approximations of a Ginzburg–Landau model for superconducting hollow spheres based on spherical centroidal voronoi tessellations, Math. Comput. 74 (2005) 1257–1280.

[17] Q. Du, L. Ju, L. Tian, Analysis of a mixed finite-volume discretization of fourth-order equations on general surfaces, IMA J. Numer. Anal. 29 (2009) 376–403.

[18] Q. Du, R. Nicolaides, Numerical analysis of a continuum model of phase transition, SIAM J. Numer. Anal. 28 (1988) 1310–1322.

[19] Q. Du, D. Wang, Anisotropic centroidal Voronoi tessellations and their applications, SIAM J. Sci. Comput. 26 (2005) 737–761.

[20] G. Dziuk, Finite elements for the Beltrami operator on arbitrary surfaces, in: S. Hildebrandt, R. Leis (Eds.), Partial differential equations and calculus of variations, Lecture Notes in Mathematics, vol. 1357, Springer, Berlin, 1988, pp. 142–155.

[21] G. Dziuk, C. Elliott, Surface finite elements for parabolic equations, J. Comput. Math. 25 (2007) 385–407.

[22] G. Dziuk, C. Elliott, Eulerian finite element method for parabolic PDEs on implicit surfaces, Interfaces Free Bound. 10 (2008) 119–138.

[23] C. Elliott, The Cahn–Hilliard model for the kinetics of phase separation, in: J.F. Rodrigues (Ed.), Mathematical models for phase change problems, Int. Ser. Numer. Math., vol. 88, Birkhauser-Verlag, Basel, 1989, pp. 35–73.

[24] C. Elliott, D.A. French, A nonconforming finite element method for the two-dimensional Cahn–Hilliard equation, SIAM J. Numer. Anal 26 (1989) 884–903.

[25] D.J. Eyre. Unconditionally gradient stable time marching the Cahn–Hilliard equation. Mater. Res. Soc. Sympos. Proc., 529:3946, Warrrndale, PA, 1998.

[26] X. Feng, A. Prohl, Analysis of a fully-discrete finite element method for the phase field model and approximation of its sharp interface limits, SIAM J. Numer. Anal 73 (246) (2003) 541–567.

[27] X. Feng, A. Prohl, Error analysis of a mixed finite element method for the Cahn–Hilliard equation, Numer. Math. 99 (2004) 47–84.

[28] I. Fonseca, M. Morini, Surfactants in foam stability: a phase field model, Arch. Ration. Mech. 183 (2007) 411–456.

[29] D. Furihata, A stable and conservative finite difference scheme for the Cahn–Hilliard equation, Numer. Math. 87 (2001) 675–699.

[30] D. Gilbarg, N. Trudinger, Elliptic Partial Differential Equations of Second Order, Springer-Verlag, Berlin, Heidelberg, New York, Tokyo, 1983.

[31] J.B. Greer, A.L. Bertozzi, G. Sapiro, Fourth order partial differential equations on general geometries, J. Comput. Phys. 216 (1) (2006) 216–246.

[32] M.E. Gurtin, On the two-phase stephan problem with interfacial energy and entropy, Acta Rat. Mech. Anal. 96 (1988) 199–243.

[33] Y. He, Y. Liu, T. Tang, On large time-stepping methods for the Cahn–Hilliard equation, Appl. Numer. Math. 57 (2007) 616–628.

[34] E. Hebey, Nonlinear Analysis on Manifolds: Sovolev Spaces and Inequalities, AMS, 2000.

[35] J.-H. Jeong, N. Goldenfeld, J. Dantzig, Phase field model for three-dimensional dendritic growth with fluid flow, Phys. Rev. E 64 (2001) 1–14.

[36] A. Kassam, L. Trefethen, Fourth-order time-stepping for stiff pdes, SIAM J. Sci. Comput. 26 (2005) 1214–1233.

[37] B. Nicolaenko, B. Scheure, R. Temam, Inertial manifold for the Cahn–Hilliard model of phase transition, in: Ordinary and Partial Differential Equations, Longman Scientific and Technical, 1987, pp. 147–160.

[38] R.L. Pego, Front migration in the nonlinear Cahn–Hilliard equation, Proc. Roy. Soc. Lond. A 422 (1989) 261–278.

[39] A. Ratz, A. Voigt, Pdes on surfaces a diffuse interface approach, Commun. Math. Sci. 4 (2006) 575–590.

[40] A.M. Stuart, A.R. Humphries, Model problems in numerical stability theory for initial value problems, SIAM Rev. 36 (1994) 226–257.

[41] P. Sens, S.A. Safran, Inclusion induced phase separation in mixed lipid film, EuroPhys. J. E 1 (2000) 237.

[42] P. Tang, F. Qiu, H. Zhang, Y. Yang, Phase separation patterns for diblock copolymers on spherical surfaces: a finite volume method, Phys. Rev. E 72 (2005) 016710.

[43] S. Tremaine, On the origin of irregular structure in Saturn's rings, Astron. J. 125 (2003) 894–901.

[44] G. Wells, E. Kuhl, K. Garikipati, A discontinuous galerkin method for the Cahn–Hilliard equation, J. Comput. Phys. 218 (2006) 860–877.

[45] S.M. Wise, C. Wang, J.S. Lowengrub, An energy-stable and convergent finite-difference scheme for the phase field crystal equation, SIAM J. Numer. Anal. 47 (2009) 2269–2288.

[46] Y. Xia, Y. Xu, C.-W. Shu, Local discontinuous Galerkin methods for the Cahn–Hilliard type equations, J. Comput. Phys. 227 (2007) 472–491.

[47] J. Zhu, L.-Q. Chen, J. Shen, V. Tikare, Coarsening kinetics from a variable-mobility Cahn–Hilliard equation: application of a semi-implicit fourier spectral method, Phys. Rev. E 60 (1999) 3564–3572.