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CONVERGENCE OF NUMERICAL APPROXIMATIONS TO A PHASE FIELD BENDING ELASTICITY MODEL OF MEMBRANE DEFORMATIONS

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This paper is dedicated to Professor Max Gunzburger on the occasion of his 60th birthday

Abstract. We study numerical approximations of a recently proposed phase field model for the vesicle membrane deformations governed by the variation of the elastic bending energy. Both the spatial discretization for the equilibrium problem with given volume and surface area constraints and the time discretization of a dynamic problem via gradient flow are considered. Convergence results of the numerical approximations are proved.

Key Words. Numerical approximations, finite element, mixed finite element, phase field model, membrane deformation, elastic bending energy, gradient flow, convergence analysis

1. Introduction

The elastic bending energy model for bilayer membranes, first developed by Canham, Evans and Helfrich, has been widely used to study the mechanical properties of vesicle membranes. The elastic bending energy is formulated in the form of a surface integral on the membrane Γ [23, 26, 27]:

$$E = \int_\Gamma \left\{a_1 + a_2(H - c_0)^2 + a_3 G\right\}\, ds, \tag{1}$$

where a_1 represents the surface tension, $H = \frac{k_1+k_2}{2}$ is the mean curvature of the membrane surface, with k_1 and k_2 as the principle curvatures, and $G = k_1k_2$ is the Gaussian curvature. a_2 is the bending rigidity and a_3 the stretching rigidity. c_0 is the spontaneous curvature that describes the asymmetry effect of the membrane or its environment. The equilibrium membrane configurations are the minimizers of the energy subject to given surface area and volume constraints to account for the effects of density change and osmotic pressure[12].

In our recent works [12] and [10, 11, 13, 29], some phase field models have been developed based on a general energetic variational framework using the above bending elastic energy. In particular, for the simplified case of

$$E = \int_\Gamma (H - c_0)^2\, ds, \tag{2}$$

its corresponding form in the phase field model is given by

$$\mathcal{E}(\phi) = \int_\Omega \frac{1}{2\epsilon}\big(\epsilon\Delta\phi + (\frac{1}{\epsilon}\phi + c_0\sqrt{2})(1-\phi^2)\big)^2\, dx\ . \tag{3}$$

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The surface area and volume constraints can be specified as

$$A(\phi) = \int_\Omega \phi \, dx = \alpha \,, \tag{4}$$

$$B(\phi) = \int_\Omega \left[\frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{4\epsilon}(\phi^2-1)^2 \right] dx = \beta \,. \tag{5}$$

Here, Ω is a fixed computational domain containing the membrane surface Γ which is defined as the zero level set of the phase field function ϕ. The parameter ϵ is a small regularization constant that determines the typical interfacial width of ϕ. The spontaneous curvature c_0 is extended the whole domain Ω. For simplicity, we also define $C = \sqrt{2}c_0$ and sometimes just call C the spontaneous curvature. The equilibrium phase field model is then defined by minimizing $\mathcal{E}$ subject to the constraints (4-5). The consistency of the phase field model to the original sharp-interface bending elasticity model, as the interfacial width parameter $\epsilon \to 0$, has been analyzed in [9]. It is actually insightful to choose a special phase field function of the form $\phi(x) = \tanh(\frac{d(x,\Gamma)}{\sqrt{2}\epsilon)})$ where $d(x,\Gamma)$ is the signed distance from a point $x \in \Omega$ to the surface Γ, the geometric meanings of $\mathcal{E}$ and (4-5) would then become clear. In this paper, we also consider the dynamic problem governed by the constrained gradient flow of the energy $\mathcal{E}(\phi)$. We always assume either periodic boundary conditions or variational boundary conditions as those naturally derived from the variation of the energy $\mathcal{E}(\phi)$.

In [12, 13], numerous discretization schemes have been developed for the phase field model. They have been successfully implemented and used in the numerical simulation the membrane deformation. Various equilibrium solutions branches and energy diagrams have been obtained, including interesting new three dimensional solutions. The purpose of this paper is to give some theoretical analysis to the convergence of some of the numerical schemes used in earlier works. The theory given here relies only on the minimal regularity assumptions of the exact solution of the continuous models. Such convergence analysis not only provides firm mathematical foundation to the numerical methods, but also offers further theoretical understanding of the phase field models, as well as their physical and analytical properties. Over the years, there have been many works on the numerical analysis of phase field type of models for various physical problems, starting from [4, 22] to more recent works [21]. But to out knowledge, the work presented here represents the first collection of convergence results in the literature on the numerical approximations to the phase field bending elasticity models.

The paper is organized as follows. We first describe the numerical schemes used for the equilibrium phase field models. Some properties of the equilibrium problems and the convergence analysis of the numerical approximation are subsequently provided. The dynamic problems governed by the gradient flow and its discrete in time approximations are then presented, followed by a convergence analysis. Finally, we complement the analysis with some numerical experiments to conclude our discussion.

2. Spatial discretization of the equilibrium problem

We begin with the spatial discretizations of the equilibrium problem. The numerical schemes developed in [12] and subsequently in [10, 13] include standard finite difference, finite element and Fourier spectral methods, which were shown to have their own advantages and limitations in the practical implementation, depending on the boundary conditions and the problems to be simulated. Here, we focus mainly on a finite element spatial discretization on regular triangular meshes. We note that by using Voronoi triangulation meshes and mass lumping integrations, such a finite element approximation can also be interpreted as a finite volume scheme defined on the Voronoi-Delaunay pair [7, 16]. In the particular case of a uniform Cartesian grid, they also reduce to standard finite difference approximations.

The computational domain Ω is assumed to be a convex polyhedron. A family of regular Delaunay triangulations $\{T^h\}$ is defined on Ω, h corresponds to the mesh parameter of T^h given by $h = \max_{K\in T^h} \operatorname{diam}(K)$ where K denotes any tetrahedron in T^h. As usual, the regularity of the triangulation is defined by

Definition 2.1. *T^h is a family of* regular *triangulations of the domain Ω if there exists a constant $\tau \geq 1$ such that*

$$\max_{K\in T^h} \frac{h_K}{\rho_K} \leq \tau \qquad \forall h > 0$$

where $h_K := diam(K)$, $\rho(K) := \sup\{diam(S) | S \text{ is a ball contained in } K\}$.

We denote S^h the piecewise linear continuous functions defined on T^h [6]. We use $< \cdot, \cdot >$ to denote the standard L^2 inner product on Ω and $\|\cdot\|$ the corresponding norm.

In general, S^h does not belong to $H^2(\Omega)$, and the phase field energy $\mathcal{E}$ is not readily defined in this case. To resolve this problem, we may interpret the Δ operator on S^h in the weak sense, or, in the finite element jargon, we may employ a mixed weak formulation [3, 24] by introducing a new variable in the finite element space to represent the Laplacian of ϕ:

Definition 2.2. *Given $\phi^h \in S^h$, we define $\Delta_h \phi^h$ as an element in S^h such that*

$$< \nabla\phi^h, \nabla w^h >= - < \Delta_h \phi^h, w^h >, \quad \forall\, w^h \in S^h\ .$$

It is known that, if the mass lumping integration is applied to the right hand side of the above equation, such a definition coincides with the standard discretization of the Laplace operator using a co-volume technique (finite volume on the Voronoi-Delaunay pair) [16, 25]. From this definition, we can define the energy $\mathcal{E}$ for ϕ^h by

$$\mathcal{E}_h(\phi^h) = \frac{1}{2\epsilon}\|\big(\epsilon\Delta_h\phi^h + (\frac{1}{\epsilon}\phi^h + c_0\sqrt{2})(1-(\phi^h)^2)\|^2\ . \tag{6}$$

The constraints are given as

$$< \phi^h, 1 >= \alpha \tag{7}$$

and

$$\frac{\epsilon}{2}\|\nabla\phi^h\|^2 + \frac{1}{4\epsilon}\|\phi^{h2} - 1\|^2 = \beta\ . \tag{8}$$

The discrete approximation is then defined as minimizing $\mathcal{E}_h(\phi^h)$ for all $\phi^h \in S^h$ subject to the constraints (7)-(8).

3. Analysis and approximation of the equilibrium model

We now give some analytical results concerning the minimization of $\mathcal{E}$ and $\mathcal{E}_h$.

3.1. Existence of energy minimizers. First, we state a proposition on the existence of minimizer for the energy $\mathcal{E}$ which largely follows from the analysis in [9].

Proposition 3.1. *Let S denote the feasible set of $\phi \in H^2(\Omega)$ such that $A(\phi) = \alpha$ and $B(\phi) = \beta$, if for some suitable α and β, S is non-empty, then there is a $\phi^* \in S$ minimizing $\mathcal{E}(\phi)$.*

Proof. The energy functional is always non-negative and thus is bounded from below, and there is a minimizing sequence $\{\phi_n \in S\}_{n=1}^{\infty}$, such that

$$\lim_{n\to\infty} \mathcal{E}(\phi_n) = C^*,$$

where C^* is the infimum of $\mathcal{E}$. By the constraints, we know ϕ_n is uniformly bounded in $H^1(\Omega)$. Let $p(\phi) = \frac{1}{\epsilon^2}(\phi^2 - 1)(\phi + C\epsilon)$, then $\|p(\phi_n)\|_{L^2}$ is uniformly bounded. Coupling with the uniform bound $\mathcal{E}(\phi_n)$, we have $\Delta\phi_n$ is bounded uniformly in $L^2(\Omega)$. Invoking the H^2-regularity theory for elliptic problems, we have ϕ_n uniformly bounded in H^2. Thus, there exists a subsequence of $\{\phi_n\}$, denoted as $\{\phi_n\}$ again, weakly converging in H^2 to some ϕ^* in $H^2(\Omega)$. Using the compact imbedding and the lower-semicontinuity of norms, we easily get

$$\mathcal{E}(\phi^*) \leq \liminf \mathcal{E}(\phi_n) = C^*,$$

together with

$$A(\phi^*) = \lim_{n\to\infty} A(\phi_n) = \alpha \quad \text{and} \quad B(\phi^*) = \lim_{n\to\infty} B(\phi_n) = \beta\,.$$

Thus $\phi^* \in S$ is a minimizer of E, satisfying the constraints. $\square$

Let us make some clarification on the conditions on the parameters α and β for the nonemptyness of the feasible S. Since $(|\Omega| + \alpha)/2$ describes the volume and $3\sqrt{2}\beta/4$ describes the surface area [12] , similar to the constructive proof in the Appendix of [9], we have the following lemma,

Lemma 3.1. *If $\frac{|\Omega|+\alpha}{2} > \frac{4\pi}{3}(\frac{3\sqrt{2}\beta}{16\pi})^{\frac{3}{2}}$, there exist $\delta > 0$, $M > 0$ such that for all $0 < \epsilon < \delta$, there exists ϕ with $\mathcal{E}(\phi) < M$, $A(\phi) = \alpha$, $B(\phi) = \beta$.*

Note that when the spontaneous curvature term is absent, a constructive proof of the above lemma has been given in [9] which remains valid in the case corresponding to a bounded spontaneous curvature, we omit the details. This lemma gives a sufficient condition for assuring the feasible set S being not empty. Consequently, we have,

Corollary 3.1. *Under the condition*

$$\frac{|\Omega| + \alpha}{2} > \frac{4\pi}{3}(\frac{3\sqrt{2}\beta}{16\pi})^{\frac{3}{2}} \tag{9}$$

there exist $\delta > 0$, such that for all $0 < \epsilon < \delta$, there is a $\phi^* \in H^2(\Omega)$ minimizing $\mathcal{E}(\phi)$ while $A(\phi^*) = \alpha$ and $B(\phi^*) = \beta$.

The above condition on α and β is always assumed in our discussions.

3.2. A penalty formulation. Computationally, it is convenient to use a penalty formulation for the two constraints (4) and (5). We can use two penalty constants $M_1 > 0$, $M_2 > 0$ to get a modified Elastic bending energy

$$\mathcal{E}_M(\phi) = \mathcal{E}(\phi) + \frac{M_1}{2}\big(A(\phi) - \alpha\big)^2 + \frac{M_2}{2}\big(B(\phi) - \beta\big)^2\,. \tag{10}$$

For simplification of notation, let us take $M_1 = M_2 = M$, we then have the following existence theorem

Theorem 3.1. *For any given $M > 0$, there exists $\phi_M \in H^2(\Omega)$ such that*

$$\mathcal{E}_M(\phi_M) = \inf_{\phi \in H^2(\Omega)} \mathcal{E}_M(\phi).$$

The proof is essentially the same as that for the proposition 3.1 and we omit the details. To be more relevant to the numerical approximation, we now prove the following

Theorem 3.2. *With S non-empty, the minimum ϕ^* of $\mathcal{E}(\phi)$ in S can be approximated by the minimum ϕ_M of $\mathcal{E}_M(\phi)$, that is, there exists a sequence ϕ_{M_n}, which are minimizers of $\mathcal{E}_{M_n}(\phi)$, converging to some minimum ϕ^* of $\mathcal{E}(\phi)$ in $H^2(\Omega)$ and satisfying*

$$\mathcal{E}(\phi^*) = \lim_{M_n \to \infty} \mathcal{E}_{M_n}(\phi_{M_n}) \ .$$

Proof. Obviously, for any $M > 0$,

$$\mathcal{E}_M(\phi_M) = \min \mathcal{E}_M(\phi) \leq \mathcal{E}_M(\phi^*) = \mathcal{E}(\phi^*) \ .$$

Thus, $A(\phi_M)$, $B(\phi_M)$ and $\mathcal{E}(\phi_M)$ are uniformly bounded for large M. Similar to the proof of proposition 3.1, there exists a subsequence of ϕ_{M_n}, such that

$$\phi_{M_n} \rightharpoonup \hat{\phi} \quad \text{in} \quad H^2(\Omega) \quad \text{and strongly in} \quad H^1(\Omega)$$

such that

$$\alpha = \lim_{n \to \infty} A(\phi_{M_n}) = A(\hat{\phi}),$$
$$\beta = \lim_{n \to \infty} B(\phi_{M_n}) = B(\hat{\phi}),$$

thus $\hat{\phi} \in S$. Moreover, by the convergence and semi-lower continuity, we have

$$\mathcal{E}(\hat{\phi}) \leq \lim_{n \to \infty} \mathcal{E}(\phi_{M_n}) \leq \lim_{n \to \infty} \mathcal{E}_{M_n}(\phi_{M_n}) \leq \mathcal{E}(\phi^*) = \min_{\phi \in S} \mathcal{E}(\phi) \ .$$

So $\hat{\phi}$ reaches the minimum of $\mathcal{E}(\phi)$ with volume and surface area constraints. Moreover, the above inequality becomes equality which implies the strong convergence of ϕ_{M_n} to $\hat{\phi}$. □

3.3. Convergence of the numerical Approximation. We now first prove the convergence of the numerical approximations of minimizer of $\mathcal{E}_M$ for any $M > 0$.

We consider the following functional

$$\mathcal{E}_{M,h}(\phi^h) = \mathcal{E}_h(\phi^h) + \frac{M}{2}\left(A(\phi^h) - \alpha\right)^2 + \frac{M}{2}\left(B(\phi^h) - \beta\right)^2 \ . \tag{11}$$

Let us consider $\phi^h_M \in S_h$ which gives that $\mathcal{E}_{M,h}(\phi^h_M) = \inf_{\phi^h \in S_h} \mathcal{E}_{M,h}(\phi^h)$. For given h, the existence of the minimizer is easy to get as S_h is a finite dimensional space. First, we show that

Lemma 3.2. *Let ϕ be a minimizer of $\mathcal{E}_M$ in $H^2(\Omega)$, and let $p = \Delta\phi$, there exists a sequence $\phi^h \in S_h$ such that as $h \to 0$, ϕ^h converges to ϕ in H^1, $\Delta_h \phi^h$ converges to p in L^2, and moreover $\mathcal{E}_h(\phi^h)$ converges to $\mathcal{E}(\phi)$.*

Proof. Let us take ϕ_δ to be a mollified version of ϕ, such that ϕ_δ is smooth and ϕ_δ converges to ϕ in H^2 as $\delta \to 0$. For ϕ_δ, we define ϕ^h_δ to be the solution of

$$< \nabla\phi^h_\delta, \nabla w^h > = < \nabla\phi_\delta, \nabla w^h > \ , \quad \forall w^h \in S_h$$

with the constraint

$$< \phi^h_\delta, 1 > = < \phi_\delta, 1 > \ .$$

We then have that ϕ_δ^h converges to ϕ_δ in H^1 as $h \to 0$.

Moreover, by the definition of the Δ_h, we have

$$< \Delta_h \phi_\delta^h, w^h >=< \Delta\phi_\delta, w^h > , \quad \forall w^h \in S_h \ .$$

That is, $p^h = \Delta_h \phi_\delta^h$ is the L^2 projection of $\Delta\phi_\delta$ in S_h. By the smoothness of $\Delta\phi_\delta$, we have p^h converges to $\Delta\phi_\delta$ in L^2 as $h \to 0$. Thus, by a diagonal selection principle, with $\delta \to 0$ and $h \to 0$, we can find a sequence of $h \to 0$ such that the corresponding ϕ^h satisfies the above lemma. □

Note that from the proof, we can see that for any sequence $h_n \to 0$ as $n \to \infty$, there exists a subsequence satisfying the above lemma. We next state a convergence results.

Theorem 3.3. *Given $M > 0$, there exists a sequence ϕ^h, the minimizers of $\mathcal{E}_{M,h}(\phi^h)$ in S_h such that ϕ^h converges in H^1 to a minimizer of $\mathcal{E}_M$ in H^2.*

Proof. Let ϕ^* be a minimizer of $\mathcal{E}_M$ in $H^2(\Omega)$, and let $p^* = \Delta\phi^*$. By lemma 3.2, we can find a sequence of approximation $\psi^h \in S_h$ with $h \to 0$, such that ψ^h converges to ϕ^* in H^1 and moreover, $\Delta_h\psi^h$ converges to p^* in L^2. Thus, we have $\mathcal{E}_{M,h}(\psi^h)$ bounded uniformly by $\mathcal{E}_M(\phi^*)+\sigma$ as $h \to 0$. Here, the constant $\sigma > 0$ can be made arbitrarily small as $h \to 0$. For the corresponding minimum $\phi^h \in S_h$ with

$$\mathcal{E}_{M,h}(\phi^h) = \inf_{w^h \in S_h} \mathcal{E}_{M,h}(w^h) \ ,$$

it follows that $\mathcal{E}_{M,h}(\phi^h)$ is uniformly bounded above by $\mathcal{E}_M(\phi) + \sigma$ as $h \to 0$. It follows that we have ϕ^h bounded uniformly in H^1 and $\Delta_h\phi^h$ bounded uniformly in L^2. By compact imbedding of Sobolev spaces, we have a subsequence (denoted still by $\{\phi^h\}$), satisfying

$$\begin{array}{lll} \phi^h \rightharpoonup \hat{\phi} & \text{in} & H^1 \ , \\ \phi^h \to \hat{\phi} & \text{in} & L^p \ (p < 6) \ , \\ \Delta_h\phi^h \rightharpoonup \hat{p} & \text{in} & L^2 \ . \end{array}$$

From the boundary condition, it is easy to deduce that $< \hat{p}, 1 >= 0$, thus, we can find $\tilde{\phi} \in H^2$ such that

$$< \nabla\tilde{\phi}, \nabla v >= - < \hat{p}, v > \ , \quad \forall \ v \in H^1(\Omega) \ ,$$

and $< \tilde{\phi}, 1 >=< \hat{\phi}, 1 >$.

So for any $v \in S_h \subset H^1$

$$\lim_{h\to 0} < \nabla(\tilde{\phi} - \phi^h), \nabla v >= \lim_{h\to 0}\{- < \Delta_h\phi^h, v > - < \nabla\phi^h, \nabla v >\} = 0 \ .$$

But, $\tilde{\phi} - \phi^h$ is uniformly bounded in H^1, using the density of S_h in $H^1(\Omega)$ as $h \to 0$, we get

$$< \nabla(\tilde{\phi} - \hat{\phi}), \nabla v >= \lim_{h\to 0} < \nabla(\tilde{\phi} - \phi^h), \nabla v >= 0 \ , \quad \forall v \in H^1(\Omega) \ .$$

This together with $< \tilde{\phi}, 1 >=< \hat{\phi}, 1 >$ implies that $\hat{\phi} = \tilde{\phi} \in H^2(\Omega)$.

Moreover, $\hat{p} = \Delta\hat{\phi}$. Then using the lower semi-continuity of norms and the strong convergence, we get

$$\mathcal{E}_M(\hat{\phi}) \le \liminf_{h\to 0} \mathcal{E}_{M,h}(\phi^h) \le \mathcal{E}_M(\phi^*) + \sigma$$

for any $\sigma > 0$. As σ is arbitrary, we have

$$\mathcal{E}_M(\hat{\phi}) = \mathcal{E}_M(\phi^*) = \inf_{\phi \in H^2(\Omega)} \mathcal{E}_M(\phi).$$

That is, $\hat{\phi}$ is a minimizer of $\mathcal{E}_M$ and we also have the convergence of the ϕ^h and $\Delta_h \phi^h$ to $\hat{\phi}$ and $\Delta\hat{\phi}$ respectively, as well as the convergence of the energy $\mathcal{E}_{M,h}(\phi^h)$ to $\mathcal{E}_M(\hat{\phi})$. □

The above proof in fact implies that in the above theorem as $h \to 0$, every convergent subsequence $\{\phi^h\}$ has its weak limit being a minimizer of $\mathcal{E}_M$, moreover, such a sequence satisfies strong convergence properties, as stated in the following corollary.

Corollary 3.2. *With respect to the weak H^1 topology, let $\hat{\phi}$ be in the limit set of $\{\phi^h\}$, the minimizers of $\mathcal{E}_M$ in S_h, then $\hat{\phi} \in H^2(\Omega)$ is a minimizer of $\mathcal{E}_M$ and*

$$\phi^h \to \hat{\phi} \quad in \quad H^1 , \qquad and \quad \Delta_h \phi^h \to \Delta\hat{\phi} \quad in \quad L^2 .$$

In addition, by triangle inequality, we can now conclude:

Theorem 3.4. *There exists a sequence ϕ^n, the minimizers of $\mathcal{E}_{M_n,h_n}$ in S_h, such that as $n \to \infty$, $h_n \to 0$ and $M_n \to \infty$, and ϕ^n converges strongly in H^1 to ϕ, a minimizer of $\mathcal{E}$ in H^2. Moreover, $\Delta_{h_n}\phi^n$ converges to $\Delta\phi$ in L^2.*

Proof. The result follows from theorems 3.2 and 3.3 and corollary 3.2. □

In addition to the above convergence result under minimal regularity assumption on the exact solution, it is also possible to derive an error estimate for the finite element approximations to those exact solutions having higher regularity, we refer to [18] for further discussions.

4. Gradient flow

Gradient flow may be used as an approach to compute the minimizers of the energies [1]. Meanwhile, they also illustrate interesting dynamic transformations of the cell membranes. For brevity, we focus on the Allen-Cahn type dynamics, corresponding to the standard L^2 gradient flow. Another popular dynamics to be studied elsewhere is the Cahn-Hilliard type conservative dynamics corresponding to the H^{-1} gradient flow.

As in [13], let us denote

$$\left\{ \begin{array}{l} f(\phi) = \epsilon\Delta\phi - \dfrac{1}{\epsilon}(\phi^2 - 1)\phi \ , \\ f_c(\phi) = \epsilon\Delta\phi - \dfrac{1}{\epsilon}(\phi^2 - 1)(\phi + C\epsilon) \ , \\ g(\phi) = \Delta f_c(\phi) - \dfrac{1}{\epsilon^2}(3\phi^2 + 2C\epsilon\phi - 1) f_c(\phi) \ . \end{array} \right. \tag{12}$$

To preserve the surface area and volume constraints in time, we may consider the constrained gradient flow for the energy $\mathcal{E}$ that incorporates Lagrange multipliers or again employ a penalty formulation.

The gradient flow with Lagrange multipliers λ_1 and λ_2 is given as

$$\phi_t = -\gamma g(\phi) + \lambda_1 + \lambda_2 f(\phi) \tag{13}$$

where the constant $\gamma > 0$ is a time relaxation parameter, λ_1, λ_2 are Lagrange multipliers which are time dependent constants, they are determined through additional equations to enforce the constraints [13]. On the other hand, the gradient flow with the penalty constants $M_1 = M_2 = M$ is given by

$$\phi_t = -\gamma \frac{\delta\mathcal{E}_M(\phi)}{\delta\phi} = -\gamma\big(g(\phi) + M(A - \alpha) + M(B - \beta) f(\phi)\big). \tag{14}$$

Here, either periodic boundary conditions or variational boundary conditions as those naturally derived from the variation of the energy $\mathcal{E}$ are assumed. We specify the initial condition as $\phi(\mathbf{x},0)=\phi_0(\mathbf{x})$ for any $\mathbf{x}\in\Omega$.

Similar to the discussion in [11], both gradient flows have their respective energy laws:

Lemma 4.1. *The solution of (13) satisfies*

$$\frac{d}{dt}\mathcal{E}(\phi)+\gamma\|\phi_t\|^2=0\ , \tag{15}$$

while the solution of (14) satisfies

$$\frac{d}{dt}\mathcal{E}_M(\phi)+\gamma\|\phi_t\|^2=0\ . \tag{16}$$

Let us define the function space $\mathcal{V}$ by

$$\mathcal{V}=H^1(0,T;L^2(\Omega))\cap L^2(0,T;H^2(\Omega))\ .$$

With the energy laws, it is easy to show the well-posedness of the gradient flow equations:

Theorem 4.1. *For any $T>0$ and $\phi_0\in H^2(\Omega)$, each of the equations (13) and (14) has a unique weak solution in $\mathcal{V}$ satisfying the respective energy laws (15) or (16).*

The proof can be constructed via a standard Galerkin argument. With both estimates on the time and spatial derivatives given by the energy laws, one can apply standard compactness results to get the local existence and then apply uniform bounds to extend the solution globally. The uniqueness is also easy to obtain. In later discussion, we provide another proof of the well posedness via a time discretization.

4.1. Semi-discrete implicit scheme. In [13], we derived the following fully implicit scheme that preserves a discrete energy law and thus ensures the monotone decreasing of the energy while preserving the constraints. First, without any confusion, we redefine (or extend) the functions f and g as

$$f(\phi,\eta)=\frac{\epsilon}{2}\Delta(\phi+\eta)-\frac{1}{4\epsilon}[(\phi)^2+(\eta)^2-2](\phi+\eta)\ ,$$

and

$$\begin{aligned}g(\phi,\eta)=&\frac{1}{2}\Delta[f_c(\phi)+f_c(\eta)]\\&-\frac{1}{2\epsilon^2}\left[(\phi)^2+\phi\eta+(\eta)^2-1+C\epsilon(\phi+\eta)\right](f_c(\phi)+f_c(\eta))\end{aligned}$$

where f_c is still as defined in (12). Note that the two redefined functions f and g are symmetric with respect to the two arguments and we have the consistency with the original functions defined in (12) when the two arguments coincide. Such generalized definitions of nonlinear terms have been used in, for example [15], to derive discrete energy laws. They are convenient to use in our discussion here as well.

With f and g specified as in the above, and k being the time step size, an implicit numerical scheme may be introduced as follows:

$$\left\{\begin{array}{rcl} \dfrac{\phi^{n+1}-\phi^n}{k}+\gamma g(\phi^{n+1},\phi^n)-\lambda_1^{(n+1)}-\lambda_2^{(n+1)}f(\phi^{n+1},\phi^n) &=& 0, \\ \lambda_1^{(n+1)}|\Omega|+\lambda_2^{(n+1)}\displaystyle\int_\Omega f(\phi^{n+1},\phi^n)\,dx-\gamma\int_\Omega g(\phi^{n+1},\phi^n)\,dx &=& 0, \\ \lambda_1^{(n+1)}\displaystyle\int_\Omega f(\phi^{n+1},\phi^n)\,dx+\lambda_2^{(n+1)}\int_\Omega f(\phi^{n+1},\phi^n)^2\,dx && \\ -\gamma\int_\Omega f(\phi^{n+1},\phi^n)g(\phi^{n+1},\phi^n)\,dx &=& 0\,. \end{array}\right. \tag{17}$$

Based on the first two equations of the above system, we can easily show

$$\begin{aligned} A(\phi^{n+1})-A(\phi^n) &= \int_\Omega \phi^{n+1}\,dx-\int_\Omega \phi^n\,dx \\ &= -k\int_\Omega[\gamma g(\phi^{n+1},\phi^n)-\lambda_1^{(n+1)}-\lambda_2^{(n+1)}f(\phi^{n+1},\phi^n)]\,dx=0\,. \end{aligned}$$

By the first and the third equations, we have

$$\begin{aligned} B(\phi^{n+1})-B(\phi^n) &= \int_\Omega(\phi^{n+1}-\phi^n)f(\phi^{n+1},\phi^n)\,dx \\ &= -k\int_\Omega\big[\gamma g(\phi^{n+1},\phi^n)-\lambda_1^{(n+1)}-\lambda_2^{(n+1)}f(\phi^{n+1},\phi^n)\big]f(\phi^{n+1},\phi^n)\,dx=0\,. \end{aligned}$$

Furthermore, we also obtain

Lemma 4.2. *The solution of (17) satisfies*

$$\begin{aligned} \mathcal{E}(\phi^{n+1})-\mathcal{E}(\phi^n) &= \int_\Omega(\phi^{n+1}-\phi^n)g(\phi^{n+1},\phi^n)\,dx \\ &= -k\int_\Omega g(\phi^{n+1},\phi^n)\big[\gamma g(\phi^{n+1},\phi^n)-\lambda_1^{(n+1)}-\lambda_2^{(n+1)}f(\phi^{n+1},\phi^n)\big]\,dx \\ &= -\frac{k}{\gamma}\int_\Omega\big[\gamma g(\phi^{n+1},\phi^n)-\lambda_1^{(n+1)}-\lambda_2^{(n+1)}f(\phi^{n+1},\phi^n)\big]^2\,dx \\ &= -\frac{1}{\gamma k}\int_\Omega(\phi^{n+1}-\phi^n)^2\,dx\,. \end{aligned}$$

The equation in the above lemma is the discrete analog of the energy law. Note that at each time step, predictor-corrector type schemes can be used to iteratively solve the system (17) for ϕ^{n+1}, $\lambda_1^{(n+1)}$ and $\lambda_2^{(n+1)}$.

For the penalty formulation, we have a similar but simpler fully implicit scheme given as follows:

$$\begin{aligned} \frac{\phi^{n+1}-\phi^n}{k} &= -\gamma\big\{g(\phi^{n+1},\phi^n)+\frac{M}{2}(A(\phi^{n+1})+A(\phi^n)-2\alpha) \\ &\quad +\frac{M}{2}(B(\phi^{n+1})+B(\phi^n)-2\beta)f(\phi^{n+1},\phi^n)\big\}\,. \end{aligned} \tag{18}$$

For the solution of (18), we have

$$\mathcal{E}(\phi^{n+1})-\mathcal{E}(\phi^n) = \int_\Omega(\phi^{n+1}-\phi^n)g(\phi^{n+1},\phi^n)\,d\mathbf{x} \tag{19}$$

and

$$\begin{aligned} &\frac{M}{2}(A(\phi^{n+1})-\alpha)^2-\frac{M}{2}(A(\phi^n)-\alpha)^2 \\ &\quad = \frac{M}{2}\big(A(\phi^{n+1})+A(\phi^n)-2\alpha\big)\big(A(\phi^{n+1})-A(\phi^n)\big) \\ &\quad = \frac{M}{2}\big(A(\phi^{n+1})+A(\phi^n)-2\alpha\big)\int_\Omega(\phi^{n+1}-\phi^n)\,dx\,. \end{aligned} \tag{20}$$

Also, since

$$B(\phi^{n+1}) - B(\phi^n) = \int_\Omega (\phi^{n+1} - \phi^n) f(\phi^{n+1}, \phi^n)\, dx\,,$$

we have

$$\begin{aligned}
&\frac{M}{2}(B(\phi^{n+1}) - \beta)^2 - \frac{M}{2}(B(\phi^n) - \beta)^2 \\
&\quad = \frac{M}{2}\big(B(\phi^{n+1}) + B(\phi^n) - 2\beta\big)\big(B(\phi^{n+1}) - B(\phi^n)\big) \\
&\quad = \frac{M}{2}\big(B(\phi^{n+1}) + B(\phi^n) - 2\beta\big) \int_\Omega (\phi^{n+1} - \phi^n) f(\phi^{n+1}, \phi^n)\, dx\,. \qquad (21)
\end{aligned}$$

Putting together (19), (20) and (21), we have the discrete energy law for the numerical solution corresponding to the penalty formulation:

Lemma 4.3. *The solution of (18) satisfies*

$$\mathcal{E}_M(\phi^{n+1}) - \mathcal{E}_M(\phi^n) + \frac{1}{\gamma k}\int_\Omega (\phi^{n+1} - \phi^n)^2\, dx = 0\,. \qquad (22)$$

Notice that, to discretize the penalty formulation of the gradient flow in time, we may also adopt a full backward Euler scheme:

$$\frac{\phi^{n+1} - \phi^n}{k} = -\gamma\big(g(\phi^{n+1}) + M(A(\phi^{n+1}) - \alpha) + M(B(\phi^{n+1}) - \beta) f(\phi^{n+1})\big)\,. \qquad (23)$$

In this case, the discrete energy law no longer holds strictly, instead, we have

Proposition 4.1. *For all $k > 0$ and a given $\phi^n \in H^2(\Omega)$, there exists a solution ϕ^{n+1} satisfying the backward Euler scheme (23). Moreover, ϕ^{n+1} may be given by the minimizer in $H^2(\Omega)$ of the modified energy functional*

$$\mathcal{E}_M(\phi) + \frac{1}{2\gamma k}\int_\Omega (\phi - \phi^n)^2\, dx\,.$$

Furthermore,

$$\mathcal{E}_M(\phi^{n+1}) - \mathcal{E}_M(\phi^n) + \frac{1}{2\gamma k}\int_\Omega (\phi^{n+1} - \phi^n)^2\, dx \le 0\,. \qquad (24)$$

Proof. The proof of the existence of above modified energy minimizer is the almost the same as the proof of Theorem 3.1, we omit the details. It is also easy to verify that the Euler-Lagrange equation of the functional

$$\mathcal{E}_M(\phi) + \frac{1}{2\gamma k}\int_\Omega (\phi - \phi^n)^2\, dx$$

is equivalent to (23), thus, we have the existence of solution to (23). Moreover, since ϕ^n is a feasible function for the above energy minimization, we have

$$\mathcal{E}_M(\phi^{n+1}) + \frac{1}{2\gamma k}\int_\Omega (\phi^{n+1} - \phi^n)^2\, dx \le \mathcal{E}_M(\phi^n)\,.$$

The results of the proposition are all proved. $\square$

4.2. Analysis of the semi-discrete approximation. In this section, we prove the numerical approximation for the gradient flows. We focus on the scheme (18). The conclusions for the Lagrange multiplier formulation and the backward Euler schemes are similar.

First, we have

Proposition 4.2. *Given $\phi_0 \in H^2(\Omega)$, for small enough $k > 0$, there exists a unique $\phi^{n+1} \in H^2(\Omega)$ satisfying the fully implicit scheme (18) for a given $\phi^n \in H^2(\Omega)$.*

Proof. For convenience, let

$$p(x) = \frac{1}{\epsilon}(x^2-1)(x+C\epsilon), \quad q(x) = p'(x), \qquad r(x) = p''(x)\ . \tag{25}$$

Given $\zeta = \phi^n$, we define a nonlinear map P from $H^2(\Omega)$ to itself by $\rho = P\omega$ with ρ satisfying:

$$\frac{\rho-\zeta}{\gamma k} = -\frac{1}{2}\Delta[\epsilon\Delta(\rho) + f_c(\zeta)] - \varphi(\omega) \tag{26}$$

where

$$\begin{aligned}\varphi(\omega) = &-\frac{1}{2}q(\omega)\Delta\omega - \frac{1}{2}r(\omega)|\nabla\omega|^2\\ &-\frac{1}{2\epsilon^2}\left[\omega^2+\omega\zeta+(\zeta)^2+C\epsilon(\zeta+\omega)-1\right](f_c(\zeta)+f_c(\omega))\\ &+\frac{M}{2}(A(\omega)+A(\zeta)-2\alpha)+\frac{M}{2}(B(\omega)+B(\zeta)-2\beta)f(\omega,\zeta)\ .\end{aligned} \tag{27}$$

The map P is obviously well-defined for any $\zeta, \omega \in H^2(\Omega)$. Moreover, direct calculation shows that a solution to (18) is the same as a fixed point of P.

For given parameters α, β, γ, ϵ, M and $\zeta \in H^2(\Omega)$, we define a set

$$U = \{u \in H^2(\Omega) \ \mid \ \|u\|_{H^2} \le C\}$$

for some suitably chosen constant $C > 0$ to be specified later. We now show that for k small, P is a contraction from U into itself, thus it has a unique fixed point.

First, by the continuous embedding of $H^2(\Omega)$ into $C(\overline{\Omega})$, we easily get $\varphi(\omega)$ is a continuous map from $H^2(\Omega)$ to $L^2(\Omega)$ and the it is uniformly continuous for $\omega \in U$, that is, we have for any $\omega, \hat\omega \in U$,

$$\|\varphi(\omega)\|_{L^2} \le c_1\ , \quad \|\varphi(\omega)-\varphi(\hat\omega)\|_{L^2} \le c_2\|\omega-\hat\omega\|_{H^2}$$

for some constants c_1 and c_2 depending on C.

Then, multiplying $\rho - \zeta$ on both sides of (26), integrating over Ω and using integration by parts, we get

$$\frac{1}{\gamma k}\|\rho-\zeta\|_{L^2}^2 + \frac{\epsilon}{2}\|\Delta(\rho-\zeta)\|_{L^2}^2 = \frac{1}{2}\int_\Omega \Delta(\zeta-\rho)(f_c(\zeta)+\epsilon\Delta\zeta)dx - \int_\Omega(\rho-\zeta)\varphi(\omega)dx\ .$$

By Cauchy-Schwartz, the bound on $\varphi(\omega)$ and the fact that $f_c(\zeta) + \epsilon\Delta\zeta$ is bounded in L^2 for $\zeta \in H^2$, we get

$$\frac{1}{2\gamma k}\|\rho-\zeta\|_{L^2}^2 + \frac{\epsilon}{4}\|\Delta(\rho-\zeta)\|_{L^2}^2 \le \frac{1}{4\epsilon}\|f_c(\zeta)+\epsilon\Delta\zeta\|_{L^2}^2 + 2\gamma k\|\varphi(\omega)\|_{L^2}^2\ .$$

In turn, this implies that

$$\|\rho\|_{H^2} \le C' + \sqrt{k}c_3$$

for some constant C' independent of k and C and constant c_3 dependent on C but independent of k. Hence, if we take $C = C' + 1$ (thus determining c_3) and let k

be small such that $\sqrt{k}c_3 \le 1$, then we have P maps U into itself. Now, for any $\omega_1, \omega_2 \in U$, let $\rho_i = P\omega_i$ for $i = 1, 2$, we can get

$$\frac{\rho_1 - \rho_2}{\gamma k} + \frac{\epsilon}{2}\Delta^2(\rho_1 - \rho_2) = \varphi(\omega_2) - \varphi(\omega_1) \ .$$

Again, multiplying $\rho_1 - \rho_2$, integrating in Ω and applying integration by parts, we have

$$\begin{aligned}\frac{1}{\gamma k}\|\rho_1 - \rho_2\|_{L^2}^2 + \frac{\epsilon}{2}\|\Delta(\rho_1 - \rho_2)\|_{L^2}^2 &\le \|\rho_1 - \rho_2\|_{L^2}\|\varphi(\omega_2) - \varphi(\omega_1)\|_{L^2} \\ &\le \frac{1}{2\gamma k}\|\rho_1 - \rho_2\|_{L^2}^2 + \frac{\gamma k c_2^2}{2}\|\omega_1 - \omega_2\|_{H^2}^2 \ .\end{aligned}$$

We easily see that if k is small enough, we get from elliptic regularity theory that there exists a constant $c > 0$ such that

$$\|\rho_1 - \rho_2\|_{H^2}^2 \le c\Big\{\frac{1}{2\gamma k}\|\rho_1 - \rho_2\|_{L^2}^2 + \frac{\epsilon}{2}\|\Delta(\rho_1 - \rho_2)\|_{L^2}^2\Big\} \le \frac{\gamma k c c_2^2}{2}\|\omega_1 - \omega_2\|_{H^2}^2 \ .$$

Therefore, if k is also small enough to have $\frac{\gamma k c c_2^2}{2} < 1$, then we get P as a contraction from U to U.

Finally, note that the discrete energy law gives a uniform bound on ϕ^n for all n, thus, the smallness of k depends only on the initial data when other parameters are are fixed. The proposition is proved.

□

Note that the existence of solution may also be obtained via Schauder fixed point theorem using argument similar to the above.

Now, we denote the linear interpolation in time of the discrete solution by ϕ^k, that is,

$$\phi^k(t) = \frac{1}{k}\left[(t - nk)\phi^{n+1} + ((n+1)k - t)\phi^n\right] \ ,$$

for $nk \le t \le (n+1)k$. Then, we have

Theorem 4.2. *Given $T > 0$, $Nk = T$, the solution of (18) satisfies*

$$\phi^k \rightharpoonup \phi^* \quad in \quad \mathcal{V} \ , \qquad as \qquad k \to 0,$$

where ϕ^* is a weak solution of the gradient flow (14). Moreover, this weak solution ϕ^* is unique.

Proof. From the discrete energy law, we know that $\mathcal{E}_M(\phi^n)$ is uniformly bounded. Therefore, $A(\phi^n)$, $B(\phi^n)$ and $\mathcal{E}(\phi^n)$ are uniformly bounded. Same as in the first part proof of proposition 3.1, we have $\phi^n \in H^2(\Omega)$ being uniformly bounded in $H^2(\Omega)$, and this implies that ϕ^k is uniformly bounded in $L^2(0, T; H^2(\Omega))$.

Denote

$$\begin{aligned}G(\phi^n, \phi^{n+1}) \quad &= \quad -\gamma\big\{g(\phi^{n+1}, \phi^n) + \frac{1}{2}M(A(\phi^{n+1}) + A(\phi^n) - 2\alpha) \\ &\qquad + \frac{1}{2}M(B(\phi^{n+1}) + B(\phi^n) - 2\beta)f(\phi^{n+1}, \phi^n)\big\} \ ,\end{aligned} \tag{28}$$

we have $\phi^k_t = G(\phi^n, \phi^{n+1})$ for $t \in (nk, (n+1)k)$ and

$$\begin{aligned}\mathcal{E}_M(\phi^{n+1}) - \mathcal{E}_M(\phi^n) &= -\frac{1}{\gamma k}\int_\Omega (\phi^{n+1}-\phi^n)^2\,dx \\ &= -\frac{k}{\gamma}\int_\Omega G(\phi^n,\phi^{n+1})^2\,dx \\ &= -\frac{1}{\gamma}\int_{nk}^{(n+1)k}\int_\Omega G(\phi^n,\phi^{n+1})^2\,dx\,dt\,.\end{aligned}$$

Thus for finite $T>0$,

$$\int_0^T\int_\Omega G(\phi^n,\phi^{n+1})^2\,dx\,dt = \gamma(\mathcal{E}_M(\phi^0) - \mathcal{E}_M(\phi^N))\,,$$

and we see that ϕ^k_t is uniformly bounded in $L^2(0,T;L^2(\Omega))$ by $\mathcal{E}_M(\phi^0)$.

Together, we get that ϕ^k is uniformly bounded in $\mathcal{V}$. Consequently there exists a subsequence of ϕ^k, denoted as $\{\phi^k\}$ again, and a function $\phi^* \in \mathcal{V}$ such that

$$\phi^k \rightharpoonup \phi^* \quad \text{in} \quad L^2(0,T;H^2(\Omega)) \qquad \text{and} \qquad \phi^k_t \rightharpoonup \phi^*_t \quad \text{in} \quad L^2(0,T;L^2(\Omega)).$$

Thus, using compact imbedding results [28], we get the strong convergence of ϕ^k to ϕ^* in $L^2(0,T;H^1(\Omega))$ (possibly after selecting a subsequence) as $k \to 0$.

Without any confusion, we now denote ϕ_+ as a step-wise function

$$\phi_+(t) = \phi^n \quad \text{for} \quad t \in [nk,(n+1)k)\,.$$

We have

$$\phi^k(t) - \phi_+(t) = \frac{1}{k}((n+1)k - t)(\phi^{n+1}-\phi^n) = ((n+1)k-t)G(\phi^n,\phi^{n+1}) \to 0\,,$$

in $L^\infty(0,T;L^2(\Omega))$ as $k \to 0$. Similarly, we denote

$$\phi_-(t) = \phi^n \quad \text{for} \quad t \in [(n-1)k, nk)\,.$$

Then, $\phi^k(t) - \phi_-(t) \to 0$ in $L^\infty(0,T;L^2(\Omega))$.

Furthermore, as $\mathcal{E}_M(\phi^n)$ is uniformly bounded by $\mathcal{E}_M(\phi^0)$, we get $\mathcal{E}_M(\phi^k)$ uniformly bounded by $\mathcal{E}_M(\phi^0)$ for all $t \in (0,T)$. This, in turn, implies that $\mathcal{E}(\phi^n)$ is uniformly bounded and $\mathcal{E}(\phi^k)$ is uniformly bounded in $(0,T)$. Same as in the first part proof of proposition 3.1, we have ϕ^k uniformly bounded in $L^\infty(0,T;H^2(\Omega))$ as $k \to 0$ and $\Delta\phi^k$ uniformly bounded in $L^\infty(0,T;L^2(\Omega))$. Meanwhile, for the step-wise function we have also $\phi_\pm(t) \in L^\infty(0,T;H^2(\Omega))$ and $\Delta\phi_\pm \in L^\infty(0,T;L^2(\Omega))$ with

$$\Delta\phi_\pm \rightharpoonup \Delta\hat{\phi}$$

in $L^2(0,T;L^2(\Omega))$ for some $\hat{\phi} \in L^2(0,T;H^2(\Omega))$. Now using the uniqueness of the weak limit and the convergence properties of ϕ^k along with the fact that $\phi^k(t) - \phi_\pm(t) \to 0$ in $L^\infty(0,T;L^2(\Omega))$ as discussed in the above, we get $\phi^* = \hat{\phi}$.

As ϕ^k satisfies $\phi^k_t = G(\phi_+,\phi_-)$, we have

$$\begin{aligned}&< \phi^k_t, v > + \gamma < \frac{1}{2}(f_c(\phi_-) + f_c(\phi_+)), \Delta v > \\ &\quad + \gamma < -\frac{1}{2\epsilon^2}\left[(\phi_-)^2 + \phi_-\phi_+ + (\phi_+)^2 - 1\right](f_c(\phi_-)+f_c(\phi_+)), v > \\ &\quad + \gamma < C\epsilon(\phi_- + \phi_+)(f_c(\phi_-)+f_c(\phi_+)), v > \\ &\quad + \gamma < \frac{1}{2}M(A(\phi_-) + A(\phi_+) - 2\alpha), v > \\ &\quad + \gamma < \frac{1}{2}Mf(\phi_+,\phi_-)(B(\phi_-)+B(\phi_+) - 2\beta), v >= 0\,,\end{aligned} \tag{29}$$

for each $v \in H_0^2(\Omega)$ and time $0 \le t \le T$.

Now we claim $f(\phi_+, \phi_-) \rightharpoonup f(\phi^*)$ in $L^2(0,T;L^2(\Omega))$.

In fact, by the continuous embedding of $H^2(\Omega)$ into $C(\overline{\Omega})$, we get $\phi_\pm(t)$, $\phi^k(t)$ and $\phi^*(t)$ are uniformly bounded in $L^\infty((0,T)\times\Omega)$. On the other hand, from

$$\phi^k \to \phi^* \quad \text{in} \quad L^2(0,T;H^1(\Omega)) \quad \text{and} \quad \phi^n - \phi^k \to 0 \quad \text{in} \quad L^\infty(0,T;L^2(\Omega)),$$

we have

$$\phi_\pm \to \phi^* \quad \text{in} \quad L^2(0,T;L^2(\Omega)).$$

Thus

$$|(\phi_\pm)^3 - (\phi^*)^3| = |\phi_\pm - \phi^*||(\phi_\pm)^2 + \phi_\pm\phi^* + (\phi^*)^2| \le C|\phi_\pm - \phi^*|,$$

and we get $(\phi_\pm)^3 \to (\phi^*)^3$ in $L^2(0,T;L^2(\Omega))$. Also,

$$|(\phi_+)^2\phi_- - (\phi^*)^3| \le |(\phi_+)^3 - (\phi^*)^3| + |(\phi_+)^2(\phi_- - \phi_+)| \to 0\ ,$$

so we finally have

$$\frac{1}{4\epsilon}[(\phi_-)^2 + (\phi_+)^2 - 2](\phi_- + \phi_+) \to \frac{1}{\epsilon}((\phi^*)^2 - 1)\phi^* \quad \text{in} \quad L^2(0,T;L^2(\Omega))\ .$$

Together with $\Delta\phi_\pm \rightharpoonup \Delta\phi^*$, we have

$$f(\phi_-, \phi_+) \rightharpoonup f(\phi^*) \ \text{ and } \ f_c(\phi_+), f_c(\phi_-) \rightharpoonup f_c(\phi^*)$$

in $L^2(0,T;L^2(\Omega))$. Denote, for $t \in [nk,(n+1)k)$,

$$u_n = \frac{1}{2\epsilon^2}\left[(\phi_-)^2 + \phi_-\phi_+ + (\phi_+)^2 - 1 + C\epsilon(\phi_- + \phi_+)\right]\ ,$$

$$u^* = \frac{1}{\epsilon^2}(3(\phi^*)^2 + 2C\epsilon\phi^* - 1)\ ,$$

and

$$v_n = f_c(\phi_-^n) + f_c(\phi_+^n)\ , \quad v^* = f_c(\phi^*).$$

We have

$$u_n \to u^* \quad \text{and} \quad v_n \rightharpoonup v^* \quad \text{in} \quad L^2(0,T;L^2(\Omega))\ .$$

Since u_n and u^* are uniformly bounded in $L^\infty((0,T)\times\Omega)$, we have

$$|< u_n v_n - u^* v^*, w >| \le |< (v_n - v^*)u^*, w >| + |< (u_n - u^*)v_n, w >| \to 0$$

for any $w \in L^\infty((0,T;L^2(\Omega))$. Thus

$$u_n v_n \rightharpoonup u^* v^* \quad \text{in} \quad L^2(0,T;L^2(\Omega))\ .$$

Following from $\phi_\pm \to \phi^*$ in $L^2(0,T;L^2(\Omega))$, we have

$$A(\phi_\pm) \to A(\phi^*) \quad \text{in} \quad L^2(0,T).$$

Also it is obvious that

$$B(\phi_\pm) \to B(\phi^*) \quad \text{in} \quad L^2(0,T).$$

All together, from (29), we have

$$\int_0^T \Big\{ < \phi_t^*, v > + \gamma < f_c(\phi^*), \Delta v > - \gamma < \frac{1}{\epsilon^2}(3(\phi^*)^2 + 2C\epsilon\phi^* - 1)f_c(\phi^*), v > \\ + \gamma < M(A-\alpha), v > + \gamma < Mf(B-\beta), v > \Big\}\, dt = 0$$

for all $v \in L^2(0,T;H_0^2(\Omega))$. Thus ϕ^* is a weak solution of the gradient flow (14). And the weak solution ϕ^* actually belongs to $C(0,T;L^2(\Omega))$. Then the initial phase field function of the gradient flow $\phi(0) = \phi_0$ makes sense.

We finally prove the uniqueness of ϕ^* for a given initial phase field function ϕ_0. Suppose there are two weak solutions ϕ_1, ϕ_2 in $\mathcal{V}$ of the gradient flow (14), then from the energy estimates, we can easily get first that ϕ_1 and ϕ_2 are uniformly bounded in $C(\overline{\Omega})$.

Then letting $u = \phi_1 - \phi_2$, we have

$$\frac{1}{\gamma} < u_t, v > + < f_c(\phi_1) - f_c(\phi_2), \Delta v > - < q(\phi_1) f_c(\phi_1) - q(\phi_2) f_c(\phi_2), v >$$
$$+ < M(A(\phi_1) - A(\phi_2)), v > + < M(f(\phi_1)B(\phi_1) - f(\phi_2)B(\phi_2)), v >= 0 \, .$$

where the polynomial q is defined as in (25).

It is obvious that $A(\phi_i)$, $B(\phi_i)$ are uniformly bounded for $i = 1, 2$. As ϕ_1, ϕ_2 are uniformly bounded in $C(\overline{\Omega})$, taking the formulae of f_c and f, and setting $v = u$, we finally have

$$\frac{d}{dt}\|u\|_{L_2}^2 + \gamma\epsilon\|\Delta u\|_{L_2}^2 \le \tilde{M}\|u\|_{H_2}\|u\|_{L^2}$$

where $\tilde{M}$ is a constant independent of u. Thus, we have for a suitable constant $\hat{M} > 0$,

$$\frac{d}{dt}\|u\|_{L_2}^2 \le \hat{M}\|u\|_{L^2}^2 \, .$$

As $u|_{t=0} = 0$, we have $\|u\|_{L_2}^2 = 0$ for all $t > 0$. Thus $\phi_1 = \phi_2$. Finally, due to the uniqueness of ϕ^*, we actually get that the convergence of the whole sequence $\phi^k \rightharpoonup \phi^*$ as $k \to 0$.

□

By similar argument, we can also get the following convergence results for the backward Euler scheme and the formulation in Lagrange multipliers, the proofs are omitted.

Theorem 4.3. *Given $T > 0$, $Nk = T$, the solution of (17) satisfies*

$$\phi^k \rightharpoonup \phi^* \quad in \quad \mathcal{V} \, , \quad as \quad k \to 0,$$

where ϕ^* is the weak solution of the gradient flow (13).

Theorem 4.4. *Given $T > 0$, $Nk = T$, the solution of (23) satisfies*

$$\phi^k \rightharpoonup \phi^* \quad in \quad \mathcal{V} \, , \quad as \quad k \to 0,$$

where ϕ^* is the weak solution of the gradient flow (14).

5. Numerical simulation results

Here, we briefly present a few sample numerical experiments, one for the equilibrium problem, and the other for the gradient flow. These experimental results confirm the convergence analysis presented earlier in the paper. Equilibrium state of the vesicle shape can also be computed via (14), the gradient flow of the penalty formulation. We use the implicit numerical scheme (17) for the time discretization. For the spatial discretizations, we may use any of the Finite Difference, Finite Element and spectral methods. Due to the periodic boundary condition we assume here, the spectral Fourier method is used for the results documented here.

In our experiments, the computational domain is taken as $[-\pi, \pi]^3$. The other parameter values are: volume parameter $\alpha = -202.67$, surface area parameter $\beta = 45.43$ and $\epsilon = 0.255254$. In addition, we set bending rigidity to be 10.0 and we do not consider the spontaneous curvature, that is, we let $c_0 = 0.0$.

The first experiment is to test the computation of the equilibrium shape with fixed volume and surface area. We use a penalty constant $M = 10000$ which is sufficiently large to enforce the volume and surface area constraints. The time step k is dynamically adjusted to balance the stability and the fast computation of the steady state [12]. To verify the convergence of the numerical approximations, we repeat the same experiment with four different spatial meshes: $16 \times 16 \times 16$, $32 \times 32 \times 32$, $48 \times 48 \times 48$ and $64 \times 64 \times 64$. The initial starting shape of the membrane is a flat elliptic shaped disk (see left most picture of figure 1), which, for the given volume and surface area, is not an equilibrium shape. As time increases, it pinches off to be a torus, which is the final equilibrium shape. The detailed dynamic process computed with a $64 \times 64 \times 64$ grid is depicted in figure 1.

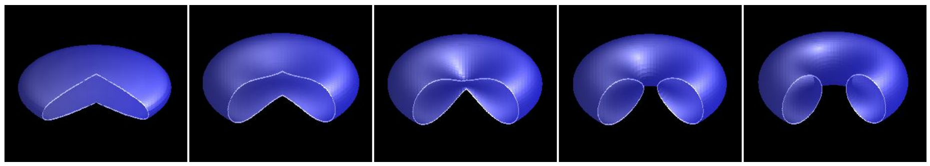

FIGURE 1. The pinch-off of a disk to a torus (cut view).

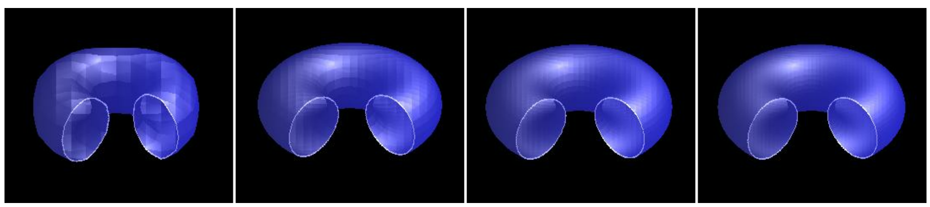

FIGURE 2. Final equilibrium shapes (cut view) on $16 \times 16 \times 16$, $32 \times 32 \times 32$, $48 \times 48 \times 48$ and $64 \times 64 \times 64$ meshes.

Comparisons of the final equilibrium shapes computed with different spatial meshes are made in figure 2, which provide verification to the convergence of our numerical simulation. Table 1 illustrates the final elastic bending energy $\mathcal{E}(\phi)$, from which we see the convergence of the energy. Note that the energy values computed on the coarse grids have additional errors from numerical quadratures whose effects diminish on the finer grids.

Mesh sizes	$16 \times 16 \times 16$	$32 \times 32 \times 32$	$48 \times 48 \times 48$	$64 \times 64 \times 64$
Energy	409.22535	423.20807	423.20086	423.20087

TABLE 1. Energy comparison of the experiments in Figure 2

The second experiment is to test the convergence for the gradient flow. We repeat the same experiment with a spatial mesh size $64 \times 64 \times 64$ but with different time step sizes. Two different constant step sizes were adopted: 6.0×10^{-8} and 3.0×10^{-8}. Figure 3 gives the plot of the decreasing energy for the gradient flows. As the energy decays very fast, we draw the energy in a log scale against the time, that is, the curves in the figure are for $\log(\mathcal{E}_M - 423.20)$ against time, where the number 423.20 is nearly the value of the energy minimum.

The plot again confirms the numerical convergence of the simulation results with the different time step sizes. The agreement remained excellent even after 3.7 million steps. More numerical simulation results can be found in [12] and [10, 13] and our subsequent works.

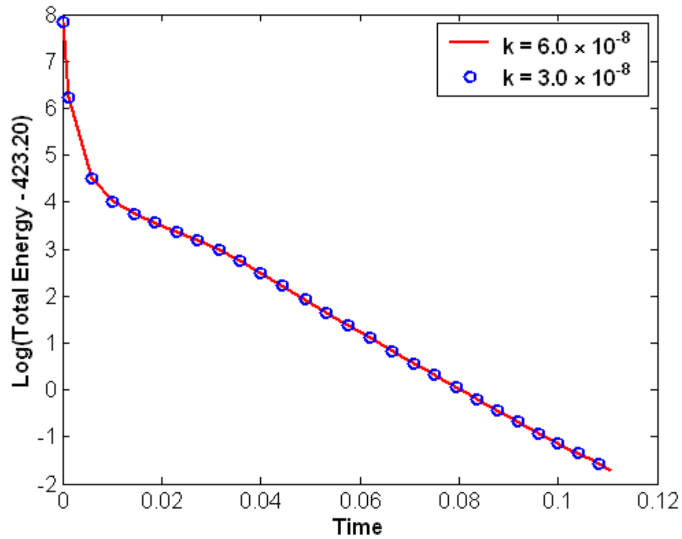

FIGURE 3. Energy of gradient flows for different time steps.

6. Conclusion

The phase field models developed in [12, 13] and [10, 11] for the equilibrium and dynamic vesicle deformations have been shown to be very effective tools to study the mechanical properties of the cell membranes and their interactions with external fields, through extensive computational studies. In this paper, some rigorous mathematical analysis on the equilibrium phase field model, its gradient flow, and their numerical approximations has been carried out to make the numerical simulations on a more solid theoretical ground. For the equilibrium problems, the focus is on finite element spatial discretizations, while for the gradient flow, the attention is given to a time-discretization preserving the energy law at the discrete level. The convergence analysis of the numerical approximations further substantiates the reliability of the experimental results. Our theory relies only on the minimal regularity assumptions of the exact solutions of the continuous models, but it is also limited to the simple case where no external field is introduced. In the future, the convergence of fully discrete schemes for the time-dependent problem, being either the Allen-Cahn type dynamics considered here or the Cahn-Hilliard dynamics, may be analyzed, similar to the studies given in [15, 19, 20]. The extension to more general settings such as those involving membrane fluid interactions (see discussions in [2, 8] and a more rigorously derived model in [11]) may also be considered. Extension may also include the study of models for multicomponent and open membranes studied in [30]. Other possible directions of study include a more careful examination on the order of convergence when more regularity of the solutions can be postulated [18] and adaptive schemes based on a posterior error estimates [17]. Convergence analysis of the discretization in the sharp interface limit, that is, as $\epsilon \to 0$, will also be of practical interests [21]. Naturally, more numerical simulations may be carried out to provide more insight into the interesting properties of the membrane vesicles.

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