

ANALYSIS OF A MIXED FINITE ELEMENT METHOD FOR A PHASE FIELD BENDING ELASTICITY MODEL OF VESICLE MEMBRANE DEFORMATION ^{*1)}

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Dedicated to the 70th birthday of Professor Lin Qun

Abstract

In this paper, we study numerical approximations of a recently proposed phase field model for the vesicle membrane deformation governed by the variation of the elastic bending energy. To overcome the challenges of high order nonlinear differential systems and the nonlinear constraints associated with the problem, we present the phase field bending elasticity model in a nested saddle point formulation. A mixed finite element method is then employed to compute the equilibrium configuration of a vesicle membrane with prescribed volume and surface area. Coupling the approximation results for a related linearized problem and the general theory of Brezzi-Rappaz-Raviart, optimal order error estimates for the finite element approximations of the phase field model are obtained. Numerical results are provided to substantiate the derived estimates.

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1. Introduction

Recent biological studies have demonstrated that biological membranes have very rich structures and play an integral part in cell functions. The usual vesicle membranes are formed by a bilayer of amphiphilic lipid molecules. The research on the structure, geometry, mechanics and function properties of membranes is thus of great interests in the emerging subject of lipidomics. The bending elasticity model for bilayer membranes, in particular, has been widely used to study the mechanical properties of vesicle membranes.

According to Helfrich [13, 26, 34], the elastic bending energy is formulated in the form of a surface integral on the membrane Γ :

$$E = \int_{\Gamma} \{a_1 + a_2(H - c_0)^2 + a_3G\} ds, \quad (1.1)$$

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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. The coefficient a_2 is the bending rigidity and a_3 the stretching rigidity, and 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 [17].

For brevity, we focus on the special case where the energy involves only the mean curvature square term, that is,

$$E_{elastic} = \int_{\Gamma} H^2 ds, \quad (1.2)$$

though much of our study here can be extended to work for (1.1) as well as other more general cases.

A classical method to study free interface computationally is to employ a mesh that has grid points on the interfaces, and deforms according to the motion of the boundary. Examples include the boundary integral and boundary element methods [27, 35]. An alternative is to employ fixed-grid methods that include the volume-of-fluid method, front-tracking method and level-set method [6, 12, 32, 33, 36]. The applications of these methods to the bending elasticity models can be found in, for example, [2, 29]. In recent works [17] and [15, 18, 19, 37], some phase field models have been developed based on a general energetic variation framework involving the above bending elastic energy. Extensions to coupled membrane and fluid interaction systems can be found in [1, 16].

A phase function $u = u(x)$, defined on the physical (computational) domain Ω containing the vesicle Γ , is a key ingredient of phase field modeling [5, 7, 8, 24]. We visualize that the level set $\{x : u(x) = 0\}$ gives the membrane, while $\{x : u(x) > 0\}$ represents the inside of the membrane and $\{x : u(x) < 0\}$ represents the outside of the membrane.

For the simplified energy (1.2), the corresponding phase field model is given by [17]

$$\mathcal{E}(u) = \int_{\Omega} \frac{1}{2\epsilon} (\epsilon \Delta u + \frac{1}{\epsilon} u(1-u^2))^2 dx. \quad (1.3)$$

The surface area and volume constraints can be specified as

$$A(u) = \int_{\Omega} u dx = \alpha, \quad (1.4)$$

$$B(u) = \int_{\Omega} \left(\frac{\epsilon}{2} |\nabla u|^2 + \frac{1}{4\epsilon} (u^2 - 1)^2 \right) dx = \beta. \quad (1.5)$$

Here, the parameter ϵ is a small regularization constant that determines the typical interfacial width of the phase field function u . The equilibrium phase field model is then defined by minimizing \mathcal{E} subject to the constraints (1.4-1.5). The consistency of the the phase field model energy (1.3) with the energy (1.2) in the sharp interface limit, that is, as $\epsilon \rightarrow 0$, has been demonstrated in [14].

In terms of algorithmic development, discrete finite difference, finite element and spectral approximations have all been developed [17, 19] for the phase field model presented above. Extensive numerical simulations have been carried out and different energetic bifurcation phenomena have been discussed in [17] and [15, 19], and they have demonstrated the effectiveness of the phase field approach in the modeling of vesicle membrane deformations. Although finite element analysis of phase field type models (largely for phase transition problems) have been studied by various authors, see for example [7, 10, 20, 23, 24], the analysis for the phase field bending elasticity model of vesicle membranes is still under development. In particular, it is a challenge to carry out rigorous error analysis due to the nonlinear nature of the variational

problem, the involvement of high order differential forms and the nonlinear constraints. So far, only basic convergence analysis has been given in [21] and no error estimate has been presented. In this paper, we study a mixed finite element method based on a new variational formulation of the phase field model. We present a complete analysis on the optimal order error estimates of the finite element solutions. Our basic approach is to derive an error estimate first for the mixed finite element approximation of a linearized problem by applying the abstract framework developed in [9] for nested linear saddle point problems. Then the optimal order error estimate is derived for the nonlinear phase field bending elasticity model (1.3-1.5) by applying the Brezzi-Rappaz-Raviart theory on the finite dimensional approximations of nonlinear problems [4]. The estimates are rigorous in the sense that we do not need to make any a priori assumption on the numerical solutions. Moreover, the theoretical results are further substantiated by the numerical experimental data. The reformulation as a nested saddle point problem and the subsequent analysis also shed light on the further algorithmic development for the phase field models.

The rest of this paper is organized as follows: in section 2, the phase field model is reformulated as a nonlinear nested saddle point variational system. In section 3, a related linear problem is formulated and analyzed based on the general framework of linear nested saddle point problem. In section 4, we discuss the mixed finite element approximation of the linear saddle point problem, then we derive error estimates for the nonlinear nested saddle point problem. Some preliminary numerical results are given in section 5 and finally, some conclusion remarks are presented in section 6.

2. A Saddle Point Formulation of the Phase Field Model

In this section, we first present the variational phase field model with prescribed surface area and volume as introduced in [17]. Then, we present its nested saddle point formulation based on the duality theory for variational problems and the corresponding Euler-Lagrange systems.

2.1. The Variational Phase Field Model

Let $\epsilon > 0$ be a small parameter that controls the width of the diffusive transition layer around the membrane, then as mentioned earlier, the original bending elastic energy model for vesicle membrane deformations under the prescribed surface area and bulk volume is formulated in a phase field setting as the following minimization problem with constraints [17]: find $u = u(x)$ such that it minimizes the elastic bending energy

$$\min \mathcal{E}(u) = \int_{\Omega} \frac{1}{2\epsilon} (\epsilon \Delta u + \frac{1}{\epsilon} (1 - u^2)u)^2 dx, \quad (2.1)$$

with subject to

$$A(u) = \alpha, \quad B(u) = \beta, \quad (2.2)$$

where the volume constraint functional $A = A(u)$ and the surface area constraint functional $B = B(u)$ are defined as in (1.4-1.5). We note that the variational problem (2.1-2.2) may be complemented with either a Dirichlet boundary condition $u|_{\partial\Omega} = -1$ or a Neumann boundary condition $\frac{\partial u}{\partial n}|_{\partial\Omega} = 0$. Additional variational (natural) boundary condition can also be derived. In a general ansatz, the consistency of the phase field elastic energy (2.1) with the sharp interface description (1.2) has been demonstrated [14] using the Dirichlet boundary condition. For $\epsilon \rightarrow 0$, there is little difference no matter which boundary condition is enforced. In fact, periodic boundary conditions may also be imposed if ϵ is small and the computational domain Ω is chosen to be sufficiently large. For convenience, we assume the homogeneous Neumann boundary condition in this paper. In the mixed formulation, this becomes a variational boundary condition, thus it is easy to implement numerically.

2.2. A Nested Min-max Variational Formulation

We consider the minimization problem with constraints (2.1-2.2) via the introduction of Lagrangian multipliers. Let the characteristic function $\delta(\cdot|0)$ be defined for any $\lambda_0 \in R$,

$$\delta(\lambda_0|0) = \begin{cases} 0, & \text{if } \lambda_0 = 0, \\ +\infty, & \text{otherwise.} \end{cases}$$

Obviously,

$$\delta(\lambda_0|0) = \sup_{\lambda \in R} \lambda \lambda_0.$$

Then,

$$\begin{aligned} \delta\left(\int_{\Omega} u dx - \alpha\right|0) &= \sup_{\lambda_1 \in R} \lambda_1 \left(\int_{\Omega} u dx - \alpha\right), \\ \delta\left(\int_{\Omega} \left[\frac{\epsilon}{2} |\nabla u|^2 + \frac{1}{4\epsilon} (u^2 - 1)^2\right] dx - \beta\right|0) &= \sup_{\lambda_2 \in R} \lambda_2 \left(\int_{\Omega} \left[\frac{\epsilon}{2} |\nabla u|^2 + \frac{1}{4\epsilon} (u^2 - 1)^2\right] dx - \beta\right). \end{aligned}$$

Now, the original constrained minimization problem can be transformed into the following saddle point problem.

$$\begin{aligned} \inf_{u \in \tilde{H}} \sup_{\lambda_1, \lambda_2 \in R} \quad & \left\{ \int_{\Omega} \frac{\epsilon}{2} |\Delta u - \frac{1}{\epsilon^2} (u^2 - 1)u|^2 dx + \lambda_1 \left(\int_{\Omega} u dx - \alpha\right) \right. \\ & \left. + \lambda_2 \left(\int_{\Omega} \left[\frac{\epsilon}{2} |\nabla u|^2 + \frac{1}{4\epsilon} (u^2 - 1)^2\right] dx - \beta\right) \right\}, \end{aligned} \quad (2.3)$$

where $\tilde{H} = H_n^2(\Omega)$ is the space of functions in $H^2(\Omega)$ with homogeneous Neumann boundary condition. On the other hand, by the duality theory,

$$\frac{\epsilon}{2} \int_{\Omega} |\Delta u - \frac{1}{\epsilon^2} (u^2 - 1)u|^2 dx = \sup_{p \in L^2(\Omega)} \left\{ \int_{\Omega} p \left(\Delta u - \frac{1}{\epsilon^2} (u^2 - 1)u\right) dx - \frac{1}{2\epsilon} \int_{\Omega} p^2 dx \right\}.$$

Thus, the problem (2.3) can be transformed into the following nested saddle point formulation

$$\begin{aligned} \inf_{u \in \tilde{H}} \sup_{p \in \tilde{M}} \sup_{\lambda_1, \lambda_2 \in R} \quad & \left\{ \int_{\Omega} p \left(\Delta u - \frac{1}{\epsilon^2} (u^2 - 1)u\right) dx - \frac{1}{2\epsilon} \int_{\Omega} p^2 dx \right. \\ & \left. + \lambda_1 \left(\int_{\Omega} u dx - \alpha\right) + \lambda_2 \left(\int_{\Omega} \left[\frac{\epsilon}{2} |\nabla u|^2 + \frac{1}{4\epsilon} (u^2 - 1)^2\right] dx - \beta\right) \right\}, \end{aligned} \quad (2.4)$$

where $\tilde{M} = L^2(\Omega)$.

2.3. A Weak Nested Saddle Point Formulation

Assume that the problem (2.4) has a saddle point $(u, p, \lambda_1, \lambda_2) \in \tilde{H} \times \tilde{M} \times R \times R$. Then $(u, p, \lambda_1, \lambda_2)$ is characterized by the following variational system:

$$\begin{cases} \int_{\Omega} \left[\left(\Delta u - \frac{1}{\epsilon^2} (u^2 - 1)u\right)q - \frac{1}{\epsilon} pq \right] dx = 0, & \forall q \in \tilde{M} \\ \int_{\Omega} \left[p \Delta v - \frac{1}{\epsilon^2} (3u^2 - 1)pv + \lambda_1 v + \lambda_2 \left(\frac{1}{\epsilon} (u^2 - 1)u - \epsilon \Delta u\right)v \right] dx = 0, & \forall v \in \tilde{H} \\ \mu_1 \left(\alpha - \int_{\Omega} u dx\right) = 0, & \forall \mu_1 \in R \\ \mu_2 \left(\int_{\Omega} \left[\frac{\epsilon}{2} |\nabla u|^2 + \frac{1}{4\epsilon} (u^2 - 1)^2\right] dx - \beta\right) = 0, & \forall \mu_2 \in R. \end{cases} \quad (2.5)$$

In terms of the first equation in (2.5), we can get

$$\Delta u = \frac{1}{\epsilon^2}(u^2 - 1)u + \frac{1}{\epsilon}p. \quad (2.6)$$

The last equation in (2.5) can be transformed via Green's formula into:

$$\mu_2 \left(\int_{\Omega} \left[-\frac{\epsilon}{2}u\Delta u + \frac{1}{4\epsilon}(u^2 - 1)^2 \right] dx + \frac{\epsilon}{2} \int_{\partial\Omega} \frac{\partial u}{\partial n} u ds - \beta \right) = 0, \quad \forall \mu_2 \in R. \quad (2.7)$$

Substituting (2.6) into (2.7) and in the second equation of (2.5), taking the test functions $v, q \in \hat{M} = H = H^1(\Omega)$ and applying integration by parts, we can get

$$\begin{cases} \int_{\Omega} \nabla u \cdot \nabla q dx + \int_{\Omega} \frac{1}{\epsilon^2}(u^2 - 1)uq dx + \frac{1}{\epsilon} \int_{\Omega} pq dx = 0, & \forall q \in \hat{M} \\ \int_{\Omega} \nabla v \cdot \nabla p dx + \int_{\Omega} \left[\frac{1}{\epsilon^2}(3u^2 - 1)p - \lambda_1 + \lambda_2 p \right] v dx = 0, & \forall v \in H \\ \mu_1 \left(\alpha - \int_{\Omega} u dx \right) = 0, & \forall \mu_1 \in R \\ \mu_2 \left(\int_{\Omega} \left[\frac{1}{2}up + \frac{1}{4\epsilon}(u^4 - 1) \right] dx + \beta \right) = 0, & \forall \mu_2 \in R. \end{cases} \quad (2.8)$$

The Neumann boundary condition of u is naturally implied from the weak form. It is easy to see that (2.8) is equivalent to the following variational formulation:

$$\begin{cases} \int_{\Omega} \nabla u \cdot \nabla q dx + \int_{\Omega} \frac{1}{\epsilon^2}(u^2 - 1)uq dx + \frac{1}{\epsilon} \int_{\Omega} pq dx = 0, & \forall q \in \hat{M} \\ \int_{\Omega} \nabla v \cdot \nabla p dx + \int_{\Omega} \left[\frac{1}{\epsilon^2}(3u^2 - 1)p v - \lambda_1 v + \lambda_2 p v \right] dx = 0, & \forall v \in H \\ \mu_1 \left(\alpha - \int_{\Omega} u dx \right) + \mu_2 \left(\int_{\Omega} \left[\frac{1}{2}up + \frac{1}{4\epsilon}(u^4 - 1) \right] dx + \beta \right) = 0, & \forall \mu_1, \mu_2 \in R. \end{cases} \quad (2.9)$$

Note that from the first equation in (2.9), we have (2.6) in the weak sense, and substituting into the second equation, we get the following strong form of the Euler-Lagrange equation in the distribution sense

$$-\Delta(\epsilon\Delta u + \frac{1}{\epsilon}(1 - u^2)u) + (\frac{1}{\epsilon^2}(3u^2 - 1) + \lambda_2)(\epsilon\Delta u + \frac{1}{\epsilon}(1 - u^2)u) - \lambda_1 = 0,$$

with appropriate boundary conditions. The system (2.9) may thus be viewed as a saddle point formulation of the above system. Similarly, we may also view the standard Galerkin finite element approximation of (2.9) as a mixed finite element approximation [3] of the above fourth order equation.

3. Analysis and Approximation of a Linear Problem

In this section, we first consider the theory and the mixed finite element approximation of a corresponding linear saddle point problem. The mixed finite element approximation of the nonlinear saddle point problem (2.9) is discussed in the next section.

3.1. A Linear Nested Saddle Point Problem

We extract the following linear part of the nonlinear problem (2.9): find $(p, u, \vec{\lambda}) \in X \times Q \times M$, where $X = Q = H^1(\Omega)$ and $M = R^2$, such that

$$\begin{cases} a(p, q) + b(u, q) = f(q), & \forall q \in X \\ b(v, p) + c(v, \vec{\lambda}) = g(v), & \forall v \in Q \\ c(u, \vec{\mu}) = \chi(\vec{\mu}), & \forall \vec{\mu} \in M \end{cases} \quad (3.1)$$

where the bilinear functionals are given by

$$\begin{aligned} a(p, q) &= \frac{1}{\epsilon} \int_{\Omega} pq dx, & \forall q \in X, \\ b(v, p) &= \int_{\Omega} \nabla p \cdot \nabla v dx, & \forall v \in Q, \\ c(u, \bar{\mu}) &= \int_{\Omega} (-\mu_1 + \mu_2 \rho(x)) u dx, & \forall \bar{\mu} \in M. \end{aligned} \quad (3.2)$$

Here, the function $\rho = \rho(x)$ is chosen so that the constraints $\int_{\Omega} u dx$ and $\int_{\Omega} u \rho(x) dx$ are independent. Without loss of generality, we let x_c denote the center of mass of Ω , that is,

$$x_c |\Omega| = \int_{\Omega} x dx,$$

then for simplicity, we may let $\rho(x) = e^T(x - x_c)$ where e is any given unit vector.

The terms $f(q)$, $g(v)$, and $\chi(\bar{\mu})$ on the right hand side of (3.1) are all taken to be some continuous linear functionals on X, Q, M respectively.

Using the abstract theory on the linear nested saddle point problem developed in [9], the existence and uniqueness of the solution of the continuous nested saddle point problem (3.1) can be proved along with the optimal error estimate of its finite element approximation.

3.2. Abstract Framework for Linear Nested Saddle Point Problems

Here, we recall a couple of results (Lemma 4.1 and Lemma 4.2 in [9]) on the nested saddle point problems and its finite element approximation.

Let X, Q and M be three real Hilbert spaces. Given three continuous bilinear functionals $a : X \times X \rightarrow R$, $b : X \times Q \rightarrow R$, and $c : Q \times M \rightarrow R$ and $f \in X'$, $g \in Q'$, and $\chi \in M'$, we consider the following problem:

Find $(u, p, \lambda) \in X \times Q \times M$, such that

$$\begin{cases} a(u, v) + b(v, p) = f(v), \quad \forall v \in X, \\ b(u, q) + c(q, \lambda) = g(q), \quad \forall q \in Q, \\ c(p, \mu) = \chi(\mu), \quad \forall \mu \in M. \end{cases} \quad (3.3)$$

Following [9], we define two subspaces $N_1 \subset Q$ and $N_2 \subset X$ as follows:

$$N_1 = \{q \in Q; c(q, \mu) = 0, \forall \mu \in M\}; \quad N_2 = \{v \in X; b(v, q) = 0, \forall q \in N_1\}. \quad (3.4)$$

We have the following results on the existence and uniqueness of the solution for the system (3.3) [9].

Lemma 3.1. *Assume that $a(\cdot, \cdot)$ is N_2 -coercive, i.e.*

$$a(v, v) \geq a_0 \|v\|_X^2, \quad \forall v \in N_2, \quad (3.5)$$

and the following inf-sup conditions hold:

$$\inf_{q \in N_1} \sup_{v \in X} \frac{b(v, q)}{\|v\|_X \|q\|_Q} \geq b_0 \quad (3.6)$$

$$\inf_{\mu \in M} \sup_{q \in Q} \frac{c(q, \mu)}{\|q\|_Q \|\mu\|_M} \geq c_0 \quad (3.7)$$

for some positive constants a_0, b_0, c_0 . Then the problem (3.3) has a unique solution $(u, p, \lambda) \in X \times Q \times M$.

Next let $X_h \subset X$, $Q_h \subset Q$, and $M_h \subset M$ be three finite dimensional subspaces. We introduce the corresponding approximation of (3.3) as follows. Find $(u_h, p_h, \lambda_h) \in X_h \times Q_h \times M_h$ such that

$$\begin{cases} a(u_h, v_h) + b(v_h, p_h) = f(v_h), \quad \forall v_h \in X_h, \\ b(u_h, q_h) + c(q_h, \lambda_h) = g(q_h), \quad \forall q_h \in Q_h, \\ c(p_h, \mu_h) = \chi(\mu_h), \quad \forall \mu_h \in M_h. \end{cases} \quad (3.8)$$

Similar as (3.4), we introduce two subspaces $N_{1h} \subset Q_h$ and $N_{2h} \subset X_h$ as follows:

$$N_{1h} = \{q_h \in Q_h; c(q_h, \mu_h) = 0, \quad \forall \mu_h \in M_h\}, \quad N_{2h} = \{v_h \in X_h; b(v_h, q_h) = 0, \quad \forall q_h \in N_{1h}\}. \quad (3.9)$$

We have the following results concerning the discrete problem (3.8).

Lemma 3.2. *Assume that $a(\cdot, \cdot)$ is N_{2h} -coercive, i.e.*

$$a(v_h, v_h) \geq a^* \|v_h\|_X^2 \quad \forall v_h \in N_{2h}, \quad (3.10)$$

and the following inf-sup conditions hold:

$$\inf_{q_h \in N_{1h}} \sup_{v_h \in X_h} \frac{b(v_h, q_h)}{\|v_h\|_X \|q_h\|_Q} \geq b^*, \quad (3.11)$$

$$\inf_{\mu_h \in M_h} \sup_{q_h \in Q_h} \frac{c(q_h, \mu_h)}{\|\mu_h\|_M \|q_h\|_Q} \geq c^* \quad (3.12)$$

for some positive constants a^*, b^*, c^* . Then the discrete problem (3.8) has a unique solution $(u_h, p_h, \lambda_h) \in X_h \times Q_h \times M_h$ with the following error estimate,

$$\begin{aligned} & \|u - u_h\|_X + \|p - p_h\|_Q + \|\lambda - \lambda_h\|_M \\ & \leq C \left\{ \inf_{v_h \in X_h} \|u - v_h\|_X + \inf_{q_h \in Q_h} \|p - q_h\|_Q + \inf_{\mu_h \in M_h} \|\lambda - \mu_h\|_M \right\}, \end{aligned} \quad (3.13)$$

where the constant C depends only on a^*, b^*, c^* , and on the operator norms $\|a\|, \|b\|$ and $\|c\|$ of the bilinear functional $a(\cdot, \cdot), b(\cdot, \cdot), c(\cdot, \cdot)$, respectively.

3.3. Application to the Linear Nested Saddle Point Problem

In order to get the existence and uniqueness of the solution for the continuous system (3.1), we need to prove (3.5-3.7) so that the lemma 3.1 can be applied.

For any given $\mu_1, \mu_2 \in \mathbb{R}$, notice that for $\rho(x) = e^T(x - x_c)$ where e is a given unit vector, we have $\int_{\Omega} \rho(x) dx = 0$, thus, by taking $v = -\mu_1 + \mu_2 \rho(x)$, we get

$$c(v, \vec{\mu}) = \|v\|_0^2 = \mu_1^2 |\Omega| + \mu_2^2 \int_{\Omega} \rho^2(x) dx \geq \min(|\Omega|, \int_{\Omega} \rho^2(x) dx) (\mu_1^2 + \mu_2^2),$$

and

$$\|v\|_1^2 = (\mu_1^2 + \mu_2^2) |\Omega| + \mu_2^2 \int_{\Omega} \rho^2(x) dx \leq \max(|\Omega|, \int_{\Omega} \rho^2(x) dx) (\mu_1^2 + \mu_2^2).$$

So,

$$\sup_{v \in Q} \frac{c(v, \vec{\mu})}{\|v\|_1} \geq \frac{\min(|\Omega|, \int_{\Omega} \rho^2(x) dx)}{[\max(|\Omega|, \int_{\Omega} \rho^2(x) dx)]^{\frac{1}{2}}} |\vec{\mu}|,$$

and this verifies (3.7).

Next, we prove the inf-sup condition (3.6). Note that by the definition (3.4), we easily get

$$N_1 = \{q \in Q; \int_{\Omega} q dx = 0 \text{ and } \int_{\Omega} \rho q dx = 0\} .$$

For $q \in N_1$, we may apply a standard Poincaré inequality

$$\|\nabla q\|_0^2 \geq c_1 \|q\|_1^2$$

for some constant $c_1 > 0$. So, we have

$$b(v, q) = \|\nabla q\|_0^2 \geq c_1 \|q\|_1^2$$

for some constant $c_1 > 0$. Then,

$$\sup_{v \in X} \frac{b(v, q)}{\|v\|_1} = \frac{\|\nabla q\|_0^2}{\|q\|_1} \geq c_1 \|q\|_1 . \tag{3.14}$$

The inf-sup condition (3.6) is thus verified.

Now, to prove the N_2 coercivity of $a(\cdot, \cdot)$, we first characterize the elements of N_2 . Given a smooth test function w defined in Ω , we define $q = w - \mu_1 - \mu_2 \rho(x)$ with

$$\mu_1 = \frac{1}{|\Omega|} \int_{\Omega} w(x) dx, \quad \mu_2 = \frac{\int_{\Omega} w(x) \rho(x) dx}{\int_{\Omega} \rho^2(x) dx} .$$

Then $q \in N_1$. So, for $v \in N_2$, we get from $b(v, q) = 0$ that

$$\int_{\Omega} \nabla v \cdot \nabla w dx = \mu_2 \int_{\Omega} \nabla v \cdot \nabla \rho dx = c_2 \int_{\Omega} w(x) \rho(x) ,$$

where c_2 is a constant. Applying integration by parts, we get

$$\int_{\partial\Omega} \frac{\partial v}{\partial n} w ds + \int_{\Omega} (-\Delta v - c_2 \rho) w dx = 0 .$$

This implies that v is a weak solution of $-\Delta v = c_2 \rho$ in Ω with the homogeneous Neumann boundary condition. This leads to:

$$N_2 = \{v \in X; -\Delta v = c_2 \rho, \text{ and } \frac{\partial v}{\partial n} = 0\} .$$

Let v_1 be the unique weak solution of

$$-\Delta v_1 = \rho, \quad \int_{\Omega} v_1 dx = 0, \quad \text{and} \quad \frac{\partial v_1}{\partial n} = 0 .$$

Then, for $v \in N_2$, we have $v = c_3 + c_2 v_1$, so, on one hand,

$$\|\nabla v\|_0^2 = c_2^2 \|\nabla v_1\|_0^2 ,$$

and on the other hand,

$$\int_{\Omega} |v|^2 dx = c_3^2 |\Omega| + c_2^2 \|v_1\|_0^2 \geq c_2^2 \|v_1\|_0^2 \geq c_2^2 \|\nabla v_1\|_0^2 \frac{\|v_1\|_0^2}{\|\nabla v_1\|_0^2} = \|\nabla v\|_0^2 \frac{\|v_1\|_0^2}{\|\nabla v_1\|_0^2} .$$

Thus, there exists a constant $c_4 > 0$ such that

$$a(v, v) = \int_{\Omega} v^2 dx \geq c_4 \|v\|_X^2 .$$

We thus have the coercivity of a in N_2 .

By the general abstract framework given in Lemma 3.1, we have

Theorem 3.1. *The linear continuous nested mixed variational system (3.1) has a unique solution $(p, u, \vec{\lambda}) \in X \times Q \times M$.*

3.4. The Mixed FEM of the Linear Problem

To construct the finite element approximation of the mixed formulation, we take the discrete function spaces as

$$X_h = Q_h = \{q_h \in C^0(\Omega) \cap H^1(\Omega) \mid q_{h|_e} \in P_k(e), \forall e \in J_h\}; \quad M_h = R^2 \quad (3.15)$$

where J_h is a triangulations of $\bar{\Omega}$ consisting elements K whose diameters are bounded above by the mesh parameter h , and P_k denotes the space of all polynomials of degree no bigger than k . For small $h \rightarrow 0$, we assume that the family J_h is uniformly regular in the sense that there exists two constants $\sigma, \tau > 0$, independent of h , such that

$$h_K \leq \sigma \rho_K, \quad \tau h \leq h_K \leq h,$$

where h_K is the diameter of K and ρ_K is the diameter of the inscribed sphere in K [11].

Then the mixed finite element approximation of the continuous mixed variational system (3.1) is: find $(p_h, u_h, \vec{\lambda}_h) \in X_h \times Q_h \times M_h$, such that

$$\begin{cases} a(p_h, q_h) + b(u_h, q_h) = f(q_h), \quad \forall q_h \in X_h, \\ b(v_h, p_h) + c(v_h, \vec{\lambda}_h) = g(v_h), \quad \forall v_h \in Q_h, \\ c(v_h, \vec{\mu}) = \chi(\vec{\mu}), \quad \forall \vec{\mu} \in M_h. \end{cases} \quad (3.16)$$

Here, the bilinear forms a , b and c are defined as in (3.2), $f(q)$, $g(v)$ and $\chi(\vec{\mu})$ again represent continuous linear functionals on X_h, Q_h, M_h .

We also define N_1^h and N_2^h as in (3.9) corresponding to the above bilinear forms. Following the same construction as in the continuous case, we can easily get that $b(\cdot, \cdot)$, $c(\cdot, \cdot)$ are bounded and satisfy the discrete inf-sup conditions (3.11) and (3.12). We may also prove the coercivity of $a(\cdot, \cdot)$ in N_2^h using argument similar to the continuous case. For instance, we may find a unique finite element function $v_1^h \in X_h$ that satisfies

$$\int_{\Omega} \nabla v_1^h \cdot \nabla w^h dx = \int_{\Omega} w^h(x) \rho(x), \quad \forall w^h \in X_h, \quad \text{and} \quad \int_{\Omega} v_1^h dx = 0.$$

Then, we also get a characterization of the subspace N_2^h as:

$$\begin{aligned} N_2^h &= \{v_h \in X_h \mid \int_{\Omega} \nabla v_h \cdot \nabla w_h dx = c_2 \int_{\Omega} w_h \rho(x), \forall w_h \in X_h\} \\ &= \{v_h = c_3 + c_2 v_1^h \mid c_2, c_3 \in R\}. \end{aligned}$$

Since v_1^h can be viewed as the finite element approximation of v_1 in X_h , by standard finite element theory, we get that

$$\lim_{h \rightarrow 0} \frac{\|v_1^h\|_0^2}{\|\nabla v_1^h\|_0^2} = \frac{\|v_1\|_0^2}{\|\nabla v_1\|_0^2}.$$

Thus, for h small, $\|v_1^h\|_0^2 / \|\nabla v_1^h\|_0^2$ is uniformly bounded, independent of h , thus, we again have a constant $c_5 > 0$ such that for h small, and for any $v_h \in N_2^h$,

$$a(v_h, v_h) = \frac{1}{\epsilon} \int_{\Omega} |v_h|^2 dx \geq c_5 \|v_h\|_X^2.$$

Then, following from Lemma 3.2, we have the following theorem

Theorem 3.2. *Assume the solution $(p, u, \vec{\lambda})$ of (3.1) is in $H^{k+1}(\Omega) \times H^{k+1}(\Omega) \times R^2$, then the mixed finite element approximation (3.16) corresponding to the linear nested saddle point system (3.1) has a unique solution $(p_h, u_h, \vec{\lambda}_h)$. And we have the following error estimate:*

$$\|p - p_h\|_1 + \|u - u_h\|_1 + |\vec{\lambda} - \vec{\lambda}_h| \leq Ch^k \{ \|u\|_{k+1} + \|p\|_{k+1} + |\vec{\lambda}| \}, \tag{3.17}$$

for some constant $C > 0$ independent of h and the solution u, p and $\vec{\lambda}$.

Note that similar to eigenvalue problems, the order of the error estimates for the Lagrange multipliers can often be higher than those given in the above. We leave the discussion on this and other type of error estimates to future works.

4. Error Estimate for FEM of the Phase Field Model

With the help of the error estimates for the linear problem, we now present the same estimates for the nonlinear saddle point problem. In this regard, we first recall some abstract theory on the finite dimensional approximations of nonlinear problems, then we apply it to the problem (2.9) which is the saddle point formulation of the phase field model for the vesicle membrane deformations.

4.1. BRR Theory

Let us recall some results on the finite dimensional approximations of the nonlinear problems due to Brezzi-Rappaz-Raviart [4].

Let V and W be two Banach spaces, Λ be a compact interval of the real line R . We introduce a C^1 mapping $G: \Lambda \times V \rightarrow W$ and a linear continuous mapping $T \in \mathcal{L}(W; V)$. We set:

$$F(\alpha, u) = u + TG(\alpha, u).$$

We consider the finite dimensional approximation of a solution pair $(\alpha, u) \in \Lambda \times V$ of the equation

$$F(\alpha, u) = 0. \tag{4.1}$$

Assume that for any $(\alpha, u) \in \Lambda \times V$, the operator $TD_uG(\alpha, u) \in \mathcal{L}(V, V)$ is compact, and there exists a branch $\{(\alpha, u(\alpha)), \alpha \in \Lambda\}$ of nonsingular solutions of the equation (4.1).

Next, for $h > 0$, we are given a finite-dimensional subspace V_h of the space V and an operator $T_h \in \mathcal{L}(W; V_h)$. We set for $\alpha \in \Lambda, u_h \in V_h$:

$$F_h(\alpha, u_h) = u_h + T_hG(\alpha, u_h).$$

The approximate problem consists of finding a solution $(\alpha, u_h) \in \Lambda \times V_h$ of the equation

$$F_h(\alpha, u_h) = 0. \tag{4.2}$$

Then, we have the following lemma [4].

Lemma 4.1. *Assume that G is a C^1 mapping from $\Lambda \times V$ into W with D^1G bounded on all bounded subsets of $\Lambda \times V, TD_uG(\alpha, u) \in \mathcal{L}(V, V)$ is compact, and (4.1) has a non-singular C^1 solution branch $\alpha \in \Lambda \rightarrow u(\alpha) \in V$. Assume in addition that*

$$\lim_{h \rightarrow 0} \|v - \Pi_h v\|_V = 0, \quad \forall v \in V \tag{4.3}$$

for some linear operator $\Pi_h \in \mathcal{L}(V; V_h)$ and

$$\lim_{h \rightarrow 0} \|T_h - T\|_{\mathcal{L}(W; V)} = 0. \tag{4.4}$$

Then, there exists a neighborhood ϑ of the origin in V and, for $h \leq h_0$ small enough, a unique C^1 function $\alpha \in \Lambda \rightarrow u_h(\alpha) \in V_h$ such that for all $\alpha \in \Lambda$

$$F_h(\alpha, u_h(\alpha)) = 0, \quad u_h(\alpha) - u(\alpha) \in \vartheta. \quad (4.5)$$

Furthermore, we have for some constant $K_0 > 0$, independent of h and α such that

$$\|u_h(\lambda) - u(\lambda)\|_V \leq K_0 \{ \|u(\lambda) - \Pi_h u(\lambda)\|_V + \|(T_h - T)G(\lambda, u(\lambda))\|_V \}. \quad (4.6)$$

4.2. A Mixed FEM of the Nonlinear Problem

Now we consider the mixed finite element approximation of nonlinear nested saddle point problem (2.9) by adopting the BRR framework quoted earlier.

We introduce the linear operator $T : g = (g_1, g_2, \vec{g}_3) \in \tilde{W} = H^{-1}(\Omega) \times H^{-1}(\Omega) \times R^2 \rightarrow \tilde{u} = (p, u, \vec{\lambda}) \in \tilde{V} = H^1(\Omega) \times H^1(\Omega) \times R^2$ defined by

$$\begin{cases} \int_{\Omega} p q dx + \epsilon \int_{\Omega} \nabla u \cdot \nabla q dx = \int_{\Omega} g_1 q dx, & \forall q \in H^1(\Omega), \\ \epsilon \int_{\Omega} \nabla v \cdot \nabla p dx - \lambda_1 \int_{\Omega} v dx + \lambda_2 \int_{\Omega} \rho v dx = \int_{\Omega} g_2 v dx, & \forall v \in H^1(\Omega), \\ -\mu_1 \int_{\Omega} u dx + \mu_2 \int_{\Omega} \rho u dx = \vec{\mu} \cdot \vec{g}_3, & \forall \vec{\mu} \in R^2. \end{cases} \quad (4.7)$$

Here, the mapping $G = (g_1, g_2, \vec{g}_3) = (g_1, g_2, g_{31}, g_{32})$ is given by

$$\begin{aligned} g_1(\tilde{u}) &= \frac{1}{\epsilon}(1 - u^2)u; \\ g_2(\tilde{u}) &= \lambda_2(p + \rho) + \frac{1}{\epsilon^2}(3u^2 - 1)p; \\ g_{31}(\tilde{u}) &= \alpha; \\ g_{32}(\tilde{u}) &= -\beta - \int_{\Omega} \left[\frac{1}{2}up + \frac{1}{4\epsilon}(u^4 - 1) \right] dx + \int_{\Omega} \rho u dx. \end{aligned}$$

By definition, $G = G(\tilde{u})$ depends on the parameter α (and also the parameter β). By normalization, we may always take $\beta = 1$ (or some other constant area), then the solution of (2.9) may be viewed as a solution branch of (4.7) with $G = G(\tilde{u})$ for the corresponding parameter α . Without causing confusion, we also adopt the notation $G = G(\alpha, \tilde{u})$ to emphasize on the dependence of G on the parameter α .

We use the standard notation for the Sobolev spaces to define

$$V = L^2(\Omega) \times L^2(\Omega) \times R^2,$$

so that $V \hookrightarrow \tilde{W}$ and the embedding is compact.

Given an element $G \in \tilde{W}$, we define the linear mapping T by $TG = -(p, u, \vec{\lambda})$ with $(p, u, \vec{\lambda})$ being the solution of (4.7) for the corresponding G . The nonlinear problem (2.9) is then equivalent to (4.1).

Now, set $V_h = X_h \times Q_h \times R^2$. A mixed finite element approximation of the nonlinear nested saddle point problem is then given by : find a solution $\tilde{u}_h = (p_h, u_h, \vec{\lambda}^h) \in V_h$ of the equation

$$\begin{cases} \int_{\Omega} p_h q_h dx + \epsilon \int_{\Omega} \nabla u_h \cdot \nabla q_h dx = \int_{\Omega} g_1(\tilde{u}_h) q_h dx, & \forall q_h \in X_h \\ \int_{\Omega} \nabla v_h \cdot \nabla p_h dx - \int_{\Omega} (\lambda_1^h v_h + \lambda_2^h \rho v_h) dx = \int_{\Omega} g_2(\tilde{u}_h) v_h dx, & \forall v_h \in Q_h \\ -\mu_1 \int_{\Omega} u_h dx + \mu_2 \int_{\Omega} \rho u_h dx = \vec{\mu} \cdot \vec{g}_3(\tilde{u}_h), & \forall \vec{\mu} \in R^2. \end{cases} \quad (4.8)$$

Similarly, for $G = (g_1(\tilde{u}_h), g_2(\tilde{u}_h), \vec{g}_3(\tilde{u}_h))$, we may define the linear operator $T_h : \tilde{W} \rightarrow V_h$ by $T_h G = -\tilde{u}_h = (p_h, u_h, \vec{\lambda}^h)$ which satisfies the equation (4.8) with a given element $G \in \tilde{W}$. Thus, the finite element approximation of (2.9) is equivalent to (4.2).

By the standard approximation properties of the finite element spaces, we obviously have (4.3). By the discussion on the linear problem, we have

$$\lim_{h \rightarrow 0} \|T - T_h\|_{\mathcal{L}(\tilde{W}, \tilde{V})} = 0$$

so that the condition (4.4) is satisfied. Moreover, assume that the solution \tilde{u} satisfies the full regularity estimates, that is, $\tilde{u} \in H^{k+1}(\Omega) \times H^{k+1}(\Omega) \times R^2$, where k is the degree of the piecewise polynomials used in the finite element spaces, we then have the estimate

$$\|(T - T_h)g\|_{\tilde{V}} \leq Ch^k \tag{4.9}$$

for some constant C , independent of h .

So, in order to apply the BRR theory, we need to check the bounds and differentiability of G and the compactness of $TD_{\tilde{u}}G$.

Lemma 4.2. *For any given α , G is a continuously differentiable mapping from \tilde{V} to V and the operator $\tilde{u} \rightarrow TD_{\tilde{u}}(G(\alpha, \tilde{u}))$ is a compact operator in $\mathcal{L}(\tilde{V}, \tilde{V})$.*

Proof. On one hand, we note that T is a linear continuous operator from \tilde{W} into \tilde{V} , and the imbedding $V \subset \tilde{W}$ is compact. Therefore, T is a compact operator from V into \tilde{V} . On the other hand, it is easy to check that for $\tilde{u} \in \tilde{V}$, by Sobolev imbedding theorem, $G(\tilde{u})$ is in V . So, in order to prove the lemma, it is sufficient to show that the operator $G : \tilde{V} \mapsto V$ is continuously differentiable. For $g_1(\tilde{u}) = \frac{1}{\epsilon}(1 - u^2)u$, we have

$$\begin{aligned} \|g_1(\tilde{u}_1) - g_1(\tilde{u}_2)\|_0 &= \frac{1}{\epsilon} \|(u_1^2 - 1)u_1 - (u_2^2 - 1)u_2\|_0 \\ &\leq c \|u_1 - u_2\|_{L^6} (\|u_1\|_{L^6}^2 + \|u_2\|_{L^6}^2) \\ &\leq c \|u_1 - u_2\|_1 (\|u_1\|_1^2 + \|u_2\|_1^2), \end{aligned}$$

for some generic constant $c > 0$. So g_1 is continuous in \tilde{V} . The continuity of g_2 and \vec{g}_3 can be similarly derived. Now, for any $\tilde{v} = (v, q, \vec{\mu}) \in \tilde{V}$,

$$\begin{aligned} D_{\tilde{u}}(g_1)\tilde{v} &= \frac{1}{\epsilon}(1 - 3u^2)v \\ D_{\tilde{u}}(g_2)\tilde{v} &= \frac{1}{\epsilon^2}(3u^2 - 1)q + \frac{6}{\epsilon^2}upv + \lambda_2q + \mu_2(p + \rho), \\ D_{\tilde{u}}(g_{31})\tilde{v} &= 0, \\ D_{\tilde{u}}(g_{32})\tilde{v} &= - \int_{\Omega} [\frac{1}{2}(uq + pv) + \frac{1}{\epsilon}u^3v]dx + \int_{\Omega} \rho v dx. \end{aligned}$$

By similar proof of the continuity of g_1 , we can show that $D_{\tilde{u}}G$ is also continuous with respect to \tilde{u} from \tilde{V} to V . In fact, G is a C^∞ mapping due to the fact that its components are all polynomial mappings from \tilde{V} to V and the norms of their derivatives all are bounded by a constant depending only on the norm of \tilde{u} in \tilde{V} . Therefore, we reach the conclusion of the lemma.

As a direct consequence of the BRR theory, and combining with the discussion on the linear problem, we have the following convergence properties of the mixed finite element approximation of the nonlinear variational problem.

Theorem 4.1. *Assume that Λ is a compact interval in R , and there exists a C^1 branch $\{\alpha, \tilde{u}(\alpha)\}$ of nonsingular solutions of the nonlinear variational problem (2.9). Then, there*

exists a neighborhood Θ of the origin in \tilde{V} , for $h \leq h_0$ small enough, there is a unique branch $\{\alpha, \tilde{u}_h(\alpha)\}$ of solutions of (2.9) such that $\tilde{u}_h(\alpha) - \tilde{u}(\alpha) \in \Theta$ for all $\alpha \in \Lambda$ with

$$\limsup_{h \rightarrow 0} \sup_{\alpha \in \Lambda} \|\tilde{u}(\alpha) - \tilde{u}_h(\alpha)\|_{\tilde{V}} = 0. \tag{4.10}$$

Moreover, if $\alpha \rightarrow \tilde{u}(\alpha)$ is a C^1 function from Λ into $U = H^{k+1}(\Omega) \times H^{k+1}(\Omega) \times R^2$, we have the error estimate

$$\|\tilde{u}(\alpha) - \tilde{u}_h(\alpha)\|_{\tilde{V}} \leq Ch^k, \tag{4.11}$$

where C is a constant independent of h .

The above estimates provide optimal order convergence of the finite element approximations to u and p in the standard $H^1(\Omega)$ norm. Of course, it would be of interests if estimates on the errors of the zero level set of u can also be obtained along with the estimates of the errors of u and p in other norms as well as superconvergence results for mixed methods [28]. We leave this as questions for future studies.

5. Numerical Results

The mixed finite element methods using continuous piecewise linear element spaces have been implemented. For simplicity, we report here only the case with 3d radial symmetry. This effectively reduces our computation to the case in a two dimensional domain.

Note that for most of the parameter values, the exact solutions of the nonlinear saddle point problem are not known analytically. Thus, in order to check the accuracy of the finite element approximation and in particular, to verify numerically the error estimates given in the above, we consider the following nonlinear system (5.1) which is obtained from (2.9) with extra forcing terms on the right hand side:

$$\begin{cases} \int_{\Omega} \nabla u \cdot \nabla q dx + \int_{\Omega} \frac{1}{\epsilon^2} (u^2 - 1) u q dx + \frac{1}{\epsilon} \int_{\Omega} p q dx = \int_{\Omega} f_1 q dx, & \forall q \in M \\ \int_{\Omega} \nabla v \cdot \nabla p dx + \int_{\Omega} [\frac{1}{\epsilon^2} (3u^2 - 1) p v - \lambda_1 v + \lambda_2 p v] dx = \int_{\Omega} f_2 q dx, & \forall v \in H \\ \mu_1 (\alpha - \int_{\Omega} u dx) + \mu_2 (\int_{\Omega} [\frac{1}{2} u p + \frac{1}{4\epsilon} (u^4 - 1)] dx + \beta) = \vec{\mu} \cdot \vec{f}_3, & \forall \vec{\mu} \in R^2. \end{cases} \tag{5.1}$$

The theoretical analysis made earlier in the paper naturally applies to the inhomogeneous system given in (5.1) also so we expected the finite element solutions would have the error estimates predicted in the theorem 4.1. But for (5.1), it is convenient to find an exact solution analytically. Here, we take the forcing terms properly so that an exact solution of the form

$$u(r, z) = \cos(\pi r) \cos(\pi z), \quad p(r, z) = \cos(\pi r) \cos(\pi z),$$

in the cylindrical coordinates can be obtained. The computational domain is taken as $[0, 1] \times [0, 1]$ which should be viewed as a cross section of a three dimensional cylinder in the (r, z) plane. The parameters are given as $\alpha = 0.0000$, $\beta = 5.6709$, and $\epsilon = 0.1$. Note that not all of these values correspond to some physically meaningful setting, in particular, for small ϵ , it is expected that for practical problems, the variable p often encounters larger variations than the variable u . However, the choice of the exact solution is taken for the convenience of verifying the error estimates. The errors of the computed finite element approximations using different mesh sizes are given in the table 1.

From the table 1, we can see that the errors of u and p in the H^1 -norm indeed show the convergence order is linear. This result confirms our theoretical analysis. In addition, second order errors in the L^2 -norm are also demonstrated, which match with the theoretical

mesh	$\ u - u_h\ _1$	$\ p - p_h\ _1$	mesh	$\ u - u_h\ _0$	$\ p - p_h\ _0$
8×8	0.314095	0.314140	8×8	0.006963	0.006963
16×16	0.155473	0.155496	16×16	0.001670	0.001670
32×32	0.077375	0.077398	32×32	0.000410	0.000409
64×64	0.038610	0.038618	64×64	0.000104	0.000101

Table 1: The numerical errors in the H^1 and L^2 norms

expectation based on the usual finite element error estimates for elliptic problems. Naturally, this also motivates further theoretical work in the future to confirm such an observation through rigorous derivation of L^2 error estimates.

6. Discussion and Conclusion

In this paper, we presented some studies on the mixed finite element approximation to a phase field model of vesicle membrane deformation under elastic bending energy, with prescribed volume and surface area. We focused on the theoretical analysis of the finite element approximation and provided rigorous error estimates using the abstract framework for nested saddle point formulation developed in [9] and the general Brezzi-Rappaz-Raviart theory for approximations of nonlinear problems [4]. The optimal order error estimate for the finite element approximation of the nonlinear phase field model has been demonstrated theoretically and verified numerically. There are various other numerical analysis and algorithmic issues to be studied further, for example, the nested saddle point reformulation of the phase field equations motivates the development of efficient and robust iterative schemes, in particular, Uzawa type algorithms, for such problems. Mixed finite element approximations to time dependent models can be considered as well, similar to the study in [30]. Adaptive finite element approximations of the nonlinear phase field models are now also under active investigation and will be reported elsewhere [22].

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