PHASE FIELD MODELS AND SIMULATIONS OF VESICLE BIO-MEMBRANES

A Thesis in
Mathematics

by
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Abstract

Recently, we begin to systematically study the shape deformation of vesicle membranes by numerical simulations, sometimes under external fluid fields, using a unified energetic variational formulation with phase field methods based on the minimization of elastic bending energy with volume and surface area constraints ([21, 19, 20, 22, 23, 24]). Analysis and numerical methods in both static and dynamic are developed to solve the phase field models.

Phase field approach is a global method, allowing topological changes of the interface. And complex interfaces may be described as a relatively simple phase function within the phase field approach. Compare to other numerical methods, phase field method is more unified, global, and relatively easier for implementation.

First we build the phase field theory for finding the equilibrium vesicle shapes. Theoretically, we build the phase field model for the biological elastic bending energy model. And the consistency of our phase field model with the general sharp interface model is verified. Further, we develop a serial methods including the Euler-Lagrange and penalty constraints methods to solving the phase field model. In guiding the numerical simulations, we prove the convergence of our numerical simulation results to the analytical phase field energy minimizers.

Many simulations are carried out to find the equilibrium shapes of vesicle membranes in the axial symmetrical and the truly 3D cases. Different energetic bifurcation phenomena are discussed. We also plot a relatively complete energy diagram. The effect
of the spontaneous curvature is also discussed for both constant and variable cases. In
the 3D non-symmetrical case, some non-symmetrical examples are found and compared
with biological experiments.

The study of the vesicle transformations within fluid fields is another important
contribution of this work. We successfully couple the phase field transformation with the
fluid dynamics. Theoretically analysis of the extra stress term caused by the membrane
to the fluids is carried out and further compared with the Euler-Lagrangian equation of
Willmore’s problem. Energy laws within the coupled systems ensure the similar asymp-
totic limit of the phase field formulation to the equilibrium system. Extensive three
dimensional numerical simulations are carried out guiding by a set of numerical schemes
for both the phase field transformation and fluid dynamics.

The last contribution of this work is that a series of new formulae is used in
detecting the topological changes in vesicle membrane transformations. More important,
some of the formulae are developed in a very general frame work and can be applied
to other problems and potentially can be used in controlling the structure of vesicle
membranes. Numerical simulations are carried out to check those formulae in all kinds
of cases involving the topological events.

For biology, this work gives the mathematical simulation to study the physics of
vesicle membranes. For mathematics, this work verifies the power of phase field method
and further develops this methods by combining with the fluid mechanics and topology.
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Chapter 1

Overview

1.1 Prologue

The study of the physics of biological membranes of vesicles such as cells is very important. Most part of the membranes is composed by lipid (Figure 1.1), a molecule with one polar (hydrophilic) head and one or more hydrophobic tails. On a cell membrane lipids form a bilayer structure, inside which the tails gather together protected from water by the outer headers. This lipid bilayer structure is a basic building block of almost all the cell membranes. Put the isolated lipids from cellular membranes in water, they will spontaneously form a variety of structures such as micelles and liposomes. Those structures has very important applications, for example, liposome, a special self-closing lipid bilayer, is designed to delivery drugs, DNA’s to cells.

Our goal is to study, together with bio-scientists, the deformation and interaction of vesicle membranes in equilibrium shapes or under external fields such as fluid fields, electric and magnetic fields. The vesicles we study here are those self closing lipid bilayer structures, such as cells, liposomes, etc.

1.2 Biological elastic bending energy model

Vesicle membranes are fluid like, because the lipids have rapid lateral movement and even relatively slower flip-flop movement. It turns out one simplistic model, first
Fig. 1.1. The lipid bilayer structure and the micelle, vesicle.

studied by Canham, Evans and Helfrich [12, 13], in which the equilibrium shape of bio-
membranes is mainly determined by the curvature of the surface, formed by double layer
lipids.

The basic assumption in this model is that the equilibrium shape of such an membrane is determined by minimizing the elastic bending energy:

\[
E = \int_\Gamma a_1 + a_2(H - c_0)^2 + a_3K ds,
\]

where \( H = \frac{k_1 + k_2}{2} \) is the mean curvature of the membrane surface, with \( k_1 \) and \( k_2 \) as the principle curvatures, \( K = k_1 k_2 \) is the Gaussian curvature, \( a_1 \) is the surface tension, \( a_2, a_3 \) are the bending rigidities that can depend on the local heterogeneous concentration of the species (such as protein molecules on the blood cells), \( c_0 \) is the spontaneous curvature
that describes the asymmetry effect of the membrane or its environment. With two constant valued $a_1$ and $a_3$, the first term and the last term may be neglected as they remain constants for vesicles with a given surface area and preserving a topological structure due to the Gauss-Bonnet formula. In this sense, we start from the elastic bending energy written by:

$$E = \int \frac{k}{2} (H - c_0)^2 ds$$

(1.2)

where $k$ is the bending rigidity and $c_0$ is the spontaneous curvature.

The problem here is to minimize the elastic bending energy with prescribed volume and surface area constraints. In the isotropic case with zero spontaneous curvature $c_0$, the elastic bending energy is usually written by [12, 13]:

$$E = \int \frac{k}{2} H^2 ds,$$

(1.3)

The Euler-Lagrangian equation of (1.3) (without the volume and area constraints) can be shown to be:

$$\Delta_\Gamma H + 2H(H^2 - K) = 0.$$  

(1.4)

Notice the above variational problem is closely related to the Willmore’s problem [57, 4, 30]. Energies of (1.3) types can also be found in the study of the configurations of smectic-A liquid crystals [16, 34], with connection to the Dupin cyclides [31, 34].

One classical method to study the moving interfaces is to employ a mesh that has grid points on the interfaces, and deforms according to the motion of the boundary, such as the boundary integral and boundary element methods (cf. [14, 55, 33] and their
Keeping track of the moving mesh may entail computational difficulties and large displacement in internal domains may cause mesh entanglement. Typically, sophisticated remeshing schemes have to be used in these cases.

As an alternative, fixed-grid methods that regularize the interface have been highly successful in treating deforming interfaces. These include the volume-of-fluid (VOF) method [39, 40], the front-tracking method [27, 28] and the level-set method [10, 46, 45]. Instead of formulating the flow of two domains separated by an interface, these methods represent the interfacial tension as a body-force or bulk-stress spreading over a narrow region covering the interface. Then a single set of governing equations can be written over the entire domain, and solved on a fixed grid in a purely Eulerian framework.

The energetic phase field model can be viewed as a physically motivated level-set method. Instead of choosing an artificial smoothing function for the interface, the diffuse-interface model describes the interface by a mixing energy. This idea can be traced to van der Waals [56], and is the foundation for the phase-field theory for phase transition and critical phenomena (see [25, 8, 7, 43, 44, 9] and the references therein). The phase field models allow topological changes of the interface [42] and over the years, they have attracted a lot of interests in the field of nonlinear analysis (cf. [1, 6, 11, 50, 54]). Similar to the popular level set formulations (see [46] for an extensive discussion), they have many advantages in numerical simulations of the interfacial motion (cf. [10]). When the transition width approaches zero, the phase field model with diffuse-interface becomes identical to a sharp-interface level-set formulation and it can also be reduced properly to the classical sharp-interface model.
1.3 Content of this work

In Chapter 2, we build the theoretical framework of phase field model for solving the equilibrium vesicle shapes. In section 2.2, our first step is to formulate the elastic bending energy given by (1.2) in the phase field framework. And we further build our phase field model for equilibrium vesicle shapes in section 2.3. Preliminary analysis is already done through asymptotic expansions, the convergence of the phase field formulation to the sharp interface model surfaces minimizing elastic bending energy with volume and surface area constraints (section 2.4). Under the assumption of the existence of a smooth limiting surface, it is shown that the interface of a phase field which is a critical point of the elastic bending energy converges to a critical point of the surface energy. Further in the section 2.5 the elastic bending energy of the phase field converges to the surface energy and the Lagrange multipliers associated with the volume and surface area constraints remain uniformly bounded. Computationally, it is convenient to use the penalty formulation (section sec:penal). In section 2.7, we build the theory of numerical approximation of phase field function. And we verify the convergence of our numerical simulation results to the analytical phase field energy minimizers.

Our phase field formulation in Chapter 2 provide a basic tool for systematically simulation the transformation of equilibrium vesicle membranes. In Chapter 3, we carry out the numerical simulations in three dimensional axis-symmetrical cases. Numerical scheme and algorithms are discussed in details. Based on the numerical results of three dimensional z-axial symmetric cases, we are able to identify many possible solution branches (3.3). Some of the configurations, to our knowledge, are obtained for the first
time using the numerical simulations. An energy diagram characterizing the solution bifurcation and the hysteresis phenomena are also presented. Such bifurcation studies have not been done systematically in the literature before (cf. [52]). Section 3.4 gives another contribution of us that the study of the spontaneous curvature $c_0$ used in the energy (1.2). The spontaneous curvature can be a constant, it can also be variable. A set of new and much more complex shapes are found in this section. Especially we illustrate how the spontaneous curvature works on surface structure by studying the non-constant spontaneous curvature cases.

We also developed the truly three dimensional scheme in Chapter 4. First the numerical scheme using the Lagrange multipliers is in section 4.2. And then in section 4.4, we first show some convergence test for our method, then we made a lot of interesting experiments to show a beautiful truly 3-d vesicles world. Besides the 3-d axis-symmetrical shapes, we also show some non-axis-symmetrical vesicles. More examples are designed to illustrate how the spontaneous curvature works on a vesicle surface. Finally, we give some experiments showing the emerging, splitting and self-assembly of the vesicle membranes and by this way how the large coherent structure are formed from smaller specimen.

The main attraction for us to use phase field method is its capability of easily incorporating the complex rheology of microstructured fluids. This is by virtue of its energy-based variational formalism. The conformation of the microstructure is governed by a free energy. This can be added to the mixing energy to form the total free energy of the multi-phase system. Thus, interfacial dynamics and complex rheology are included in a unified theoretical framework. The energetic based phase field formulation can be easily
combined together with other energy formulation to describe more complex phenomenon of vesicle membranes. In Chapter 5, we couple the elastic bending energy together with the energy of fluid field, get the extra stress term caused by the membranes in the momentum equation. Important energy laws are deduced to ensure the well-posedness of the coupled system. More than that, the energy laws also play the key roles in getting the similar asymptotic limit of the phase field function with which we can recover the sharp interface limit of the fluid system (section 5.3) and the extra stress term can be formulated by the geometrical terms such as the mean curvature and Gaussian curvature. The numerical schemes for coupled fluid system are discussed in section 5.4. Also we studied a lot of transformations of vesicle membranes in fluid fields (section 5.6).

Moreover, within the phase field framework, our study here has the potential of opening up a host of exciting new applications of the phase field modeling including the use of the topological quantities in a control setting of the vesicle structures. Based on the classical Gauss-Bonnet formula, we give a serials of formulae for calculating the Euler numbers of surfaces (Chapter 6). It is not only a better indicator of topological changes than the energy functional, but in fact, it gives a quantized jump upon a completion of the topological change (a direct consequence of the Gauss-Bonnet formula) for regular surfaces (section 6.4.1). Furthermore, when the computed surface passes singularity, the new formulae based on the phase field formulation gives a fractional interpolation of the usual Euler number (section 6.2.3). We also verify our formulae in retrieving the topological information in all kinds of case.

Within phase field framework, complex interfaces may be described as a relatively simple phase function. Phase field formulation is a global method allowing topological
changes of the interface. Compare to other numerical methods, phase field method is more unified, global, and relatively easier for implementation. Finally in Chapter 7, we make some concluding remarks and some interesting problems opened for future study.
Chapter 2

Phase Field Model for Equilibrium Vesicle Shapes

In this Chapter, we build the theoretical background of phase field model for equilibrium vesicle shapes.

2.1 Introduction

The framework of our phase field model is started by introducing a phase function \( \phi(x) \), defined on the physical (computational) three dimensional domain \( \Omega \), which is used to label the inside and the outside of the vesicle \( \Gamma \). We visualize that the level set \( \{ x : \phi(x) = 0 \} \) gives the membrane, while \( \{ x : \phi(x) > 0 \} \) represents the inside of the membrane and \( \{ x : \phi(x) \leq 0 \} \) the outside.

More than a general level set function, we consider the function has phases for different areas of the domain \( \Omega \). An idea function \( \phi(x) = \text{tanh} \left( \frac{d(x, \Gamma)}{\sqrt{2} \epsilon} \right) \) makes the inside of \( \Gamma \) almost values at 1 and outside -1. And between two phases, there is a transition layer with width measured by the parameter \( \epsilon \). Based on this phase field function, in section 2.2 of this chapter, using phase field function \( \phi \) we formulate the elastic bending energy to be used in our phase field model and in section 2.3 we further propose our phase field model for equilibrium vesicle shapes. Related to this phase field model, there is a lot of questions need to be answered, such as the existence of energy minimizers, and the verification of the tanh function formulation. In section 2.4, under a very general ansatz,
we calculate the asymptotic limit of our phase field model and prove the consistency of the phase field model to its sharp interface limit. Then in the section 2.5 and section 2.6 we propose the Euler-Lagrange equation and penalty formulation to solve this phase field model. Numerical analysis of the numerical approximation is another important issue. In the last section, we prove several fundamental theorems verifying the convergence of the numerical approximation to the analytic phase field function.

2.2 Phase field formulation

2.2.1 Two lemmas

Before we begin the derivation of our phase field model, we prove two lemmas which will be used widely in this chapter.

**Lemma 2.1.** Suppose that \( \Gamma \) is a smooth surface and \( d(x) \) is the signed distance between \( x \) and \( \Gamma \). Suppose further that \( f \in C^0(\Omega) \) and \( p \in L^1(\mathbb{R}) \) satisfies the bound

\[
\lim_{s \to \pm \infty} \max_{|t| > s} p(t) = 0.
\]

Then

\[
\lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_{\Omega} p(d(x)/\epsilon)f(x) \, dx = \int_{-\infty}^{\infty} p(t) \, dt \int_{\Gamma_0} f(s) \, ds.
\]

**Proof.** Let \( O \) be a neighborhood of \( \Gamma_\epsilon \) within which \( \nabla d \) is Lipschitz. Let \( \eta(t, x) \) be the integral curves of \( \nabla d \) with initial datum \( z \in \Gamma_\epsilon \), i.e.

\[
\dot{\eta}(t, z) = \nabla d(\eta(t, z)).
\]
Note that
\[
\frac{d}{dt}d(\eta(t,z)) = \nabla d(\eta(t,z)) \dot{\eta}(t,z) = |\nabla d(\eta(t,z))|^2 = 1
\]  
(2.4)

and that \(d(\eta(0,z)) = d(z) = 0\). Thus
\[
d(\eta(t,z)) = t,
\]
for all \(z \in \Gamma_{\epsilon}\). Further, let
\[
J(t, z) = \det(\nabla_{t,z} \eta(t,z)).
\]

It is clear from the fact that \(\nabla d(z) = n\), where \(n\) is the unit normal at \(z\), that
\[
J(0, z) = \det(n, z_1, z_2) = 1,
\]

where \(z_1\) and \(z_2\) are an orthonormal pair in the tangent space of \(\Gamma_\epsilon\) at \(z\). Consider thus the change of coordinates \((t, z) \longrightarrow \eta(t, z)\) and let \(U = \eta(\{(-\delta, \delta), \Gamma_\epsilon\}) \subset O\) for sufficiently small but fixed \(\delta\).

\[
\int_U p(\frac{d(x)}{\epsilon}) f(x) \, dx = \int_{-\delta}^{\delta} \int_{\Gamma_\epsilon} p(\frac{d(\eta(t,z))}{\epsilon}) f(\eta(t,z))J(t,z) \, dS(z) \, dt
\]

\[
= \int_{-\delta}^{\delta} p(t/\epsilon) \int_{\Gamma_\epsilon} f(\eta(t,z))J(t,z) \, dS(z) \, dt.
\]

Changing coordinates \(\epsilon s = t\), we find
\[
\int_U p(\frac{d(x)}{\epsilon}) f(x) \, dx = \epsilon \int_{-\delta/\epsilon}^{\delta/\epsilon} p(s) \int_{\Gamma_\epsilon} f(\eta(\epsilon s,z))J(\epsilon s,z) \, dS(z) \, ds.
\]
By continuity and dominated convergence,

\[
\lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_U p\left(d(x)/\epsilon\right) f(x) \, dx = \lim_{\epsilon \to 0} \int_{-\delta/\epsilon}^{\delta/\epsilon} p(s) \int_{\Gamma_\epsilon} f(\eta(\epsilon s, z)) J(\epsilon s, z) \, dS(z) \, ds
\]

\[
= \int_{-\infty}^{\infty} p(s) \int_{\Gamma_0} f(\eta(0, z)) J(0, z) \, dS(z) \, ds
\]

\[
= \int_{-\infty}^{\infty} p(s) \int_{\Gamma_0} f(z) \, dS(z) \, ds.
\]

(2.2) now follows because

\[
\lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_{\{d > \delta\} = U \epsilon} p\left(d(x)/\epsilon\right) f(x) \, dx \leq \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_{|s| > \delta} p(s/\epsilon) \int_{\Omega} |f(x)| \, dx = 0.
\]

**Lemma 2.2.** In addition to Lemma (2.1), assume that \(f \in C^1(\Omega)\) and \(d \in C^2(U)\). For \(P' = p\), let \(P \in L^1(\mathbb{R})\). If (i) \(p\) is odd and or (ii) \(\lim_{s \to \infty} \max_{|t| > \delta} |P(t)| t = 0\), then

\[
\lim_{\epsilon \to 0} \frac{1}{\epsilon^2} \int_{\Omega} p(d(x)/\epsilon) f(x) \, dx < \infty.
\]

**Proof.** We resume exactly as in the proof of Lemma (2.1) to find that

\[
\int_{U} p\left(d(x)/\epsilon\right) f(x) \, dx = \int_{-\delta}^{\delta} p(t/\epsilon) \int_{\Gamma_\epsilon} f(\eta(t, z)) J(t, z) \, dS(z) \, dt.
\]

\[
F_\epsilon(t) = \int_{\Gamma_\epsilon} f(\eta(t, z)) J(t, z) \, dS(z).
\]

\(F_\epsilon(t)\) is continuous in \(\epsilon\) and continuously differentiable for \(t \in (-\delta, \delta)\).
If (i) holds, let $G_\epsilon(t) = (F_\epsilon(t) - F_\epsilon(0))/t$. Then

$$\int_U p(d(x)/\epsilon)f(x)\,dx = \int_{-\delta}^{\delta} p(t/\epsilon)F_\epsilon(t)\,dt$$

$$= \int_{-\delta}^{\delta} p(t/\epsilon)tG_\epsilon(t)\,dt.$$  

Changing coordinates $t = \epsilon s$ and taking absolute values we find

$$\left| \int_U p(d(x)/\epsilon)f(x)\,dx \right| \leq \epsilon^2 \max_{t \in (-\delta,\delta)} G_\epsilon(t) \int_{-\infty}^{\infty} |p(s)s|\,ds.$$  

Dividing by $\epsilon^2$, the remaining terms are finite.

If (ii) holds, changing coordinates $t = \epsilon s$

$$\int_U p(d(x)/\epsilon)f(x)\,dx = \epsilon \int_{-\delta/\epsilon}^{\delta/\epsilon} p(s)F_\epsilon(\epsilon s)\,ds$$

$$= \epsilon P(s)F_\epsilon(\epsilon s)\bigg|_{\delta/\epsilon}^{\delta/\epsilon} - \epsilon^2 \int_{-\delta/\epsilon}^{\delta/\epsilon} P(s)F'_\epsilon(\epsilon s)\,ds.$$  

Dividing both sides by $\epsilon^2$ and taking the limit $\epsilon \to 0$ we find

$$\lim_{\epsilon \to 0} \frac{1}{\epsilon^2} \int_U p(d(x)/\epsilon)f(x)\,dx = \lim_{\epsilon \to 0} \frac{1}{\epsilon} P(s)F_\epsilon(\epsilon s)\big|_{-\delta/\epsilon}^{\delta/\epsilon} - \int_{-\delta/\epsilon}^{\delta/\epsilon} P(s)F'_\epsilon(\epsilon s)\,ds$$

$$= 0 - F'_\epsilon(0) \int_{-\infty}^{\infty} P(s)\,ds$$

$$< \infty.$$  

I
2.2.2 Elastic bending energy

Now we start derive the formula of the elastic bending energy in our phase field model. With the notation at the beginning of this chapter, suppose the vesicle membrane $\Gamma$ is a smooth surface, let us consider a phase field function $\phi(x) = q\left(\frac{d(x)}{\sqrt{2}\epsilon}\right) = \tanh\left(\frac{d(x)}{\sqrt{2}\epsilon}\right)$ defined for all $x \in \Omega$, where $d(x)$ is the signed distance between $x$ and $\Gamma$, positive inside and negative outside; $\epsilon$ is a transition parameter that is taken to be very small.

From $\nabla\phi = q' \frac{1}{\sqrt{2}\epsilon} \nabla d$, $\nabla^2 \phi = q'' \frac{1}{2\epsilon^2} \nabla d \nabla^2 d + q' \frac{1}{\sqrt{2}\epsilon} \nabla^2 d$, $q'(x) = 1 - q^2(x)$ and $q''(x) = -2q(x)(1 - q^2(x))$, we have

\[
\nabla^2 d = \frac{\sqrt{2}\epsilon \nabla^2 \phi}{q'} - \frac{q''}{\sqrt{2}\epsilon q'} \nabla_i \nabla_j d
\]

\[
= \sqrt{2}\epsilon \frac{\nabla^2 \phi}{q'} + \sqrt{2}\epsilon \frac{2q}{1 - q^2} \nabla_i \phi \nabla_j \phi
\]

\[
= \frac{\sqrt{2}\epsilon}{1 - q^2} \left(\nabla^2 \phi + \frac{2q}{1 - q^2} \nabla_i \phi \nabla_j \phi\right)
\]

\[
= \frac{\sqrt{2}\epsilon}{1 - \phi^2} \left(\nabla^2 \phi + \frac{2\phi}{1 - \phi^2} \nabla_i \phi \nabla_j \phi\right). \quad (2.5)
\]

The matrix $\nabla^2 d = \nabla^2 d(x)$, with $d$ being the signed distance to a surface $\Gamma$, always has a zero eigenvalue with $\nabla d$ as the eigenvector. This is due to the fact that $\nabla^2 d$ is symmetric and $|\nabla d| = 1$. On the surface $\Gamma$, the two other eigenvalues are actually the two principle curvatures of $\Gamma$ ($k_1$ and $k_2$ in this case). The the Gaussian curvature $K$ is of course the product of these two eigenvalues while the mean curvature $H$ is given by the mean of the two eigenvalues. Both quantities can in fact be defined and computed on all the level
sets in $\Omega$. Since $|\nabla \phi|^2 = \frac{1}{2\epsilon^2}(1 - \phi^2)^2$, we have an expression for the mean curvature:

$$H = -\frac{1}{2} \text{tr}(\nabla^2 d) = -\frac{\sqrt{2}\epsilon}{2(1 - \phi^2)}(\Delta \phi + \frac{2\phi}{1 - \phi^2}|\nabla \phi|^2)$$

$$= -\frac{\sqrt{2}\epsilon}{2(1 - \phi^2)}(\Delta \phi + \frac{1}{\epsilon^2}\phi(1 - \phi)) .$$

For a given three by three matrix $M$, let $\Lambda(M)$ denote the coefficient of the linear term of the characteristic polynomial of $M$. Thus $\Lambda(M) = \lambda_1(M)\lambda_2(M)$ for a singular matrix $M$ with $\lambda_1$, $\lambda_2$ being the two non-zero eigenvalues of $M$. Then we have the Gaussian curvature

$$K = k_1k_2 = \Lambda(\nabla^2 d(x)) = \frac{2\epsilon^2}{(1 - \phi^2)^2}\Lambda(\nabla^2 \phi + \frac{2\phi}{1 - \phi^2}\nabla_i\phi\nabla_j\phi) . \quad (2.6)$$

With Lemma 2.1, in addition, $\int_{-\infty}^{+\infty} \left(1 - q^2(\frac{x}{\sqrt{2}\epsilon})\right)^2 dx = \frac{4\sqrt{2}\epsilon}{3}$. For the elastic bending energy defined by (1.2), we have

$$\int_\Gamma \frac{k}{2}(H - c_0)^2 ds = \frac{3}{4\sqrt{2}\epsilon} \int_{-\infty}^{+\infty} (1 - q^2(\frac{\tau}{\sqrt{2}\epsilon}))^2 d\tau \int_\Gamma \frac{k}{2}(H - c_0)^2 ds$$

$$\approx \frac{3}{4\sqrt{2}\epsilon} \int_\Omega (1 - \phi^2(x))^2 \frac{k}{2}\left(\frac{\epsilon}{\sqrt{2}(1 - \phi^2)}(\Delta \phi + \frac{1}{\epsilon^2}\phi(1 - \phi^2)) + c_0\right)^2 dx$$

$$= \frac{3k}{8\sqrt{2}\epsilon} \int_\Omega (\epsilon\Delta \phi + (\frac{1}{\epsilon}\phi + c_0\sqrt{2})(1 - \phi^2))^2 dx .$$

So,

$$E(\phi) = \frac{k}{2\epsilon} \int_\Omega \left(\epsilon\Delta \phi + (\frac{1}{\epsilon}\phi + c_0\sqrt{2})(1 - \phi^2)\right)^2 dx \quad (2.7)$$

approaches to the $3/(4\sqrt{2})$ times of the elastic bending energy.
Moreover, because $\phi \approx 1$ inside $\Gamma$ and $-1$ outside $\Gamma$, we know

$$A(\phi) = \int_{\Omega} \phi \, dx \quad (2.8)$$

approaches the volume difference between the inside volume and outside volume. And since

$$\int_{\Gamma} 1 \, ds = \frac{3}{4\sqrt{2}\epsilon} \int_{-\infty}^{+\infty} \left(1 - q^2 \left(\frac{\tau}{\sqrt{2}\epsilon}\right)^2\right)^2 \, d\tau \int_{\Gamma} 1 \, ds$$

$$\approx \frac{3}{4\sqrt{2}\epsilon} \int_{\Omega} (1 - \phi^2)^2 \, dx$$

we know

$$B(\phi) = \int_{\Omega} \frac{1}{2\epsilon} (\phi^2 - 1)^2 \, dx$$

approaches to $2\sqrt{2} \text{area}(\Gamma)/3$, or about 0.9428 times the area of $\Gamma$. Since $|\nabla \phi|^2 = \frac{1}{2\epsilon^2} (1 - \phi^2)^2$, we can rewrite $B(\phi)$ by

$$B(\phi) = \int_{\Omega} \frac{\epsilon}{2} |\nabla \phi|^2 + \frac{1}{4\epsilon} (\phi^2 - 1)^2 \, dx. \quad (2.9)$$

All together, our phase field formulation is to minimize the elastic bending energy $E(\phi)$ under the constraints that $A(\phi)$ and $B(\phi)$ are constants. Since the energy functional is formulated based on the special form $\tanh \left(\frac{d(x)}{\sqrt{2}\epsilon}\right)$ but the minimization problem is over a much bigger function class, to check the consistency, let us verify that in our model, the minimizer $\phi(x)$ is approaching to $\tanh \left(\frac{d(x)}{\sqrt{2}\epsilon}\right)$ for small $\epsilon$. 
2.3 Phase field model

As stated in section 2.2, our phase field model is the variational problem:

\[
\min_{\phi \in L} E(\phi) = \int_{\Omega} \frac{k}{2\epsilon} (\epsilon \Delta \phi + \frac{1}{\epsilon} \phi + c_0 \sqrt{2}) (1 - \phi^2)^2 \, dx
\]

with constraints

\[
A(\phi) = \int_{\Omega} \phi \, dx = \alpha,
\]

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

over the admissible set

\[
L = \{ \phi \in H^2 \mid \phi|_{\partial \Omega} = -1, \nabla \phi \cdot n|_{\partial \Omega} = 0 \}.
\]

Here \(k\) is a constant describing the bending rigidity, \(c_0\) is the spontaneous curvature which can be a constant or variable. Because our original spontaneous curvature \(c_0\) is defined only the surface \(\Gamma\). Here we extend it to the whole domain \(\Omega\) such that at a neighborhood of \(\Gamma\), \(c_0\) keeps to be constant along the integral curves of \(\nabla d\). \(c_0\) has a smooth extension outside the neighborhood. If no otherwise mentioned, we always assume that \(c_0\) is bounded when it is variable. We also define \(C = \sqrt{2}c_0\). Sometimes we also call \(C\) the spontaneous curvature.

First we have the following theorem about the existence of energy minimizer.
Theorem 2.1. (Existence of energy minimizer) Denote $S$ the feasible set of $\phi \in L$ such that $A(\phi) = \alpha$ and $B(\phi) = \beta$. If $S$ is not empty, there is a $\phi^* \in S$ minimizing $E(\phi)$ in $S$.

Proof. As the feasible solution set $S$ is non-empty, we can get a minimizing sequence $\{\phi_n \in S\}_{n=1}^{\infty}$, such that $\lim_{n \to \infty} E(\phi_n) = C^*$, where $C^*$ is the infimum of $E$.

Let $p(\phi) = \frac{1}{\epsilon^2}(\phi^2 - 1)(\phi + C\epsilon)$, we have

$$E(\phi_n) = \frac{k\epsilon}{2} \|\Delta \phi_n - p(\phi_n)\|_{L^2}^2 \geq \frac{k\epsilon}{2} (\|\Delta \phi_n\|_{L^2}^2 - \|p(\phi_n)\|_{L^2}^2)$$

(2.14)

Since $\Omega \in R^3$ and $\partial \Omega \in C^\infty$, we have $\|\phi_n\|_{L^6(\Omega)} \leq C\|\phi_n\|_{H^1(\Omega)}$. And from $B(\phi_n) = \beta$, we know $\phi_n$ is $H^1(\Omega)$ uniformly bounded, thus $\phi_n$ is $L^6(\Omega)$ uniformly bounded. Thus it follows $\|p(\phi_n)\|_{L^2}^2 = \int_{\Omega} (\phi_n^2 - 1)^2(\phi_n + C\epsilon)^2 \, dx$ is uniformly bounded.

From (2.38) and the uniformly bounded $E(\phi_n)$, we have $\Delta \phi_n$ is $L^2(\Omega)$ bounded for all $n$.

Now from the Boundary $H^2$-regularity of $\Delta$ operator, since $\Delta \phi_n$ and $\phi_n$ are uniformly $L^2(\Omega)$ bounded, we have $\phi_n \in H^2(\Omega)$ and uniformly $H^2$ bounded.

As $H^2$ is reflective, there exists a subsequence of $\{\phi_n\}$, denote as $\{\phi_n\}$ again, weakly converging in $H^2$, or $\phi_n \rightharpoonup \phi^*$ in $H^2(\Omega)$. Also, as $\Delta \phi_n$ bounded in $L^2(\Omega)$, passing if necessary to yet another subsequence, we have $\Delta \phi_n \rightharpoonup \Delta \phi^*$ in $L^2(\Omega)$.

Now since $H^2(\Omega) \subset H^1(\Omega) \subset L^4(\Omega)$, thus passing if necessary to yet another subsequence, we have $\phi_n \rightharpoonup \phi^*$ in $H^1$ and $L^4$. Thus

$$\lim_{n \to \infty} A(\phi_n) = \int_{\Omega} \phi^*(x) \, dx = \alpha$$

(2.15)
and

\[
\lim_{n \to \infty} B(\phi_n) = \int_{\Omega} \frac{\varepsilon}{2} |\nabla \phi^*|^2 + \frac{1}{4\varepsilon} (\phi^* - 1)^2 \, dx = \beta .
\] (2.16)

And as \( H^1(\Omega) \subset L^2(\Omega) \), \( \phi_n \to \phi^* \) a.e. in \( \Omega \), thus \( p(\phi_n) \to p(\phi^*) \) a.e. in \( \Omega \).

Fix \( \xi > 0 \), the Egoroff’s Theorem asserts \( p(\phi_n) \to p(\phi^*) \) uniformly on \( \Omega_\xi \) where \( \Omega_\xi \) is a measurable set with \(|\Omega - \Omega_\xi| \leq \xi\). And we have

\[
E(\phi_n) \geq \frac{k\varepsilon}{2} (\|\Delta \phi_n\|^2_{L^2(\Omega_\xi)} - 2 < \Delta \phi_n, p(\phi_n) >_{L^2(\Omega_\xi)} + \|p(\phi_n)\|^2_{L^2(\Omega_\xi)}) .
\] (2.17)

And since \( \Delta \phi_n \) weakly converges to \( \Delta \phi^* \) in \( L^2(\Omega) \), we have

\[
\lim_{n \to \infty} \|\Delta \phi_n\|_{L^2(\Omega_\xi)} \geq \|\Delta \phi^*\|_{L^2(\Omega_\xi)} .
\] (2.18)

With \( p(\phi_n) \to p(\phi^*) \) uniformly on \( \Omega_\xi \), we have

\[
\lim_{n \to \infty} < \Delta \phi_n, p(\phi_n) >_{L^2(\Omega_\xi)} = < \Delta \phi^*, p(\phi^*) >_{L^2(\Omega_\xi)} ;
\] (2.19)

and

\[
\lim_{n \to \infty} \|p(\phi_n)\|_{L^2(\Omega_\xi)} = \|p(\phi^*)\|_{L^2(\Omega_\xi)} .
\] (2.20)

Thus from (2.17), (2.18), (2.19) and (2.20) we have

\[
\lim_{n \to \infty} E(\phi_n) \geq \int_{\Omega_\xi} \|\Delta \phi^* - p(\phi^*)\|^2 \, dx
\] (2.21)
We now let $\xi$ tend to zero, recall the Monotone Convergence Theorem to conclude

$$\lim_{n \to \infty} E(\phi_n) \geq E(\phi^*)$$

Since $\phi^* \in H^2(\Omega)$ and (2.15) and (2.16), $\phi^*$ belongs to the feasible set. Thus $\phi^*$ is the minimizer of $E$, satisfying the constraints. \(\blacksquare\)

Here since $(|\Omega| + \alpha)/2$ describes the volume and $3\sqrt{2}\beta/4$ describes the surface area, similar to the constructive proof in the Appendix of [20], we have the following lemma,

**Lemma 2.3.** If $\frac{|\Omega| + \alpha}{2} > \frac{4\pi}{3} \left( \frac{3\sqrt{2}\beta}{16\pi} \right)^2$, there exist $\delta > 0$, $M > 0$ such that for all $0 < \epsilon < \delta$, there exists $\phi$ with $E(\phi) < M$, $A(\phi) = \alpha$, $B(\phi) = \beta$.

The only difference between this lemma with that in [20] is the spontaneous curvature. And with a bounded spontaneous curvature, the constructive proof can be directly move for this lemma. This lemma gives a sufficient condition such that the feasible set satisfying the constraints is not empty. And we have the following existence theorem. From lemma 2.3, we have

**Corollary 2.1.** If $\frac{|\Omega| + \alpha}{2} > \frac{4\pi}{3} \left( \frac{3\sqrt{2}\beta}{16\pi} \right)^2$, there exist $\delta > 0$, such that for all $0 < \epsilon < \delta$, there is a $\phi^* \in H^2(\Omega)$ minimizing $E(\phi)$ while $A(\phi^*) = \alpha$ and $B(\phi^*) = \beta$.

The condition of $\alpha$ and $\beta$,

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

(2.22)
is very nature and we always assume this condition to make sure there is a surface $\Gamma$ satisfies the volume and surface area constraints, and there is a $\phi^*$ minimize the energy with two constraints.

2.4 Asymptotic limit

Now let’s verify the asymptotic limit of energy minimizer $\phi^*$ is the tanh function used to deduce the phase field formulation in previous subsection under a very general ansatz.

Denote the minimizer of (2.10)-(2.12) by $\phi_\epsilon$. Make the following assumptions on the constrained minimization (2.10)-(2.12);

(A1) $\phi_\epsilon(x) = q(d(x)/\epsilon) + \epsilon h + g$ where $q \in C^2(R)$ and $h \in C^2(\Omega)$, both independent of $\epsilon$, and $\|\nabla^k g\|_{L^\infty} = o(\epsilon)$ for $k = 0, \ldots, 4$.

(A2) $d(x) = d(x, \Gamma_\epsilon)$, where $\{\Gamma_\epsilon\}_{\epsilon \geq 0}$ is a family of uniformly smooth, compact surfaces converging to $\Gamma_0$.

And this ansatz turns out to the following asymptotic limit theorem.

Theorem 2.2. Suppose the variational problem (2.10)-(2.12) has a solution $\phi_\epsilon = q(d/\epsilon) + \epsilon h + g$ satisfying (A1) and (A2). Then $q(t) = \tanh(t/\sqrt{2})$ and $h = 0$. 

Proof. If $\alpha$ and $\beta$ satisfy (2.22), then the minimum energy (2.10) is uniformly bounded by a constant $M$ for sufficiently small $\epsilon$ (Lemma 2.3).

\[
M > E(\varphi) = \int_{\Omega} \frac{1}{\epsilon} \left| q^t \left( \frac{d(x)}{\epsilon} \right) \Delta d(x) + \frac{1}{\epsilon} \left( q^t - (q^2 - 1) q^t \right) - C(q^2 - 1) \right|^2 dx.
\]

\[
= \int_{\Omega} \frac{1}{\epsilon^3} (q'' - q(q^2 - 1))^2 + \frac{1}{\epsilon^2} \Delta d q^t (q'' - q(q^2 - 1)) dx + O \left( \frac{1}{\epsilon} \right). 
\]

Note that in the second term, \( q^t (q'' - q(q^2 - 1)) = \left( \frac{1}{2} q^2 - \frac{1}{4} (q^2 - 1)^2 \right)' \). Integrating against $\Delta d$ and applying the boundary conditions on $q$, we find that the second term is on the order of $O \left( \frac{1}{\epsilon} \right)$. We thus concentrate on the first term. Suppose that \( (q''(t^*) - q(t^*)(q^2(t^*) - 1))^2 > \eta \) for some constant $\eta$ and some $t^* \in \mathbb{R}$. By continuity, there exists a $\delta$ such that \( (q''(t) - q(t)(q^2(t) - 1))^2 > \eta \) for $t \in (t^* - \delta, t^* + \delta)$. Let $U_{\epsilon, \delta} = \{ x \mid d(x)/\epsilon \in (t^* - \delta, t^* + \delta) \}$. Note that $|U_{\epsilon, \delta}| > C\epsilon$ for some constant $C$ depending on $\Gamma$. Then

\[
M > \frac{1}{\epsilon^2} C\eta + O \left( \frac{1}{\epsilon} \right)
\]

for arbitrarily small $\epsilon$. This is a contradiction as $M$ is a uniform constant. Thus, we arrive at the $q'' - q(q^2 - 1) = 0$. Since $\alpha < |\Omega|$, $q$ must have a zero and (2.12) implies that $|q(\pm \infty)| = 1$. It follows that $q(t) = \tanh(t/\sqrt{2})$.

We further examine the next order terms in the energy expansion:

\[
E(\phi) = \int_{\Omega} \frac{1}{\epsilon} (q')^2 (\Delta d + 2c_0) - \frac{2}{\epsilon} q' (\Delta d + 2c_0) (3q^2 - 1) h + \frac{1}{\epsilon} (3q^2 - 1)^2 h^2 dx
\]

As developed above, the first term converges to $\frac{4\sqrt{2}}{3}$ times the spontaneous curvature energy, $\int_{\Gamma} (H - c_0)^2 dS$. Note in the second term that $(q(q^2 - 1))' = (3q^2 - 1)q'$. Hence
an integration may be performed against \((\Delta d + 2c_0)h\) normal to the interface, implying that the second term is bounded as \(\epsilon \to 0\). The third term consequently must satisfy

\[
\lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_{\Omega} (3q^2 - 1)^2 h^2 \, dx = \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_{\Omega} 2h^2 \, dx < \infty.
\]

Since \(h\) is independent of \(\epsilon\), it follows that \(h \equiv 0\).

With the asymptotic limit theorem, we can easy prove the following theorem

**Theorem 2.3.** If the variational problem (2.10)-(2.12) satisfies (A1) and (A2) with the minimizer \(\phi\), then

\[
E(\phi) \longrightarrow \frac{4\sqrt{2}k}{3} \int_{\Gamma_0} (H - c_0)^2 \, ds,
\]

where \(H\) is the mean curvature of the limit interface \(\Gamma_0\), and \(A(\phi)\) approaches the volume difference between the inside volume and outside volume, \(B(\phi)\) approaches to \(2\sqrt{2} \text{area}(\Gamma)/3\) as \(\epsilon \to 0\).

**Proof.** As \(\phi = q(d/\epsilon) + g\) where \(q(t) = \tanh(t/\sqrt{2})\), as calculated in the proof of Theorem 2.2, we have

\[
E(\phi) = \frac{k}{2} \int_{\Omega} \frac{1}{\epsilon}(q')^2(\Delta d + 2c_0)^2 - \frac{2}{\epsilon^2} q'(\Delta d + 2c_0)(3q^2 - 1)g + \frac{1}{\epsilon^3}(3q^2 - 1)^2g^2 \, dx + o(\epsilon)
\]

From lemma(2.1), and \(\Delta d = -2H\) the first term approaches to \((2\sqrt{2}k/3 \int_{\Gamma}(H - c_0)^2 \, ds\).

Since \((q(q^2 - 1))' = (3q^2 - 1)q'\), from lemma (2.2), we know the second term is \(o(\epsilon)\).
And the third term is $o(1/\epsilon)$, thus we have

$$E(\phi) \longrightarrow \frac{4\sqrt{2}k}{3} \int_{\Gamma_0} (H - c_0)^2 \, ds, \text{ as } \epsilon \to 0$$

And it is trivial that $A(\phi)$ approaches the volume difference between the inside volume and outside volume. Applying lemma (2.1) we have $B(\phi)$ approaches to $2\sqrt{2} \text{area}(\Gamma)/3$.

So far we actually proved that our phase field formulation converges to the sharp interface model as $\epsilon \to 0$.

### 2.5 Euler-Lagrange equation

With lagrange multipliers $\lambda_1$ and $\lambda_2$, the constrained variational problem (2.10)-(2.12) can be written as

$$\frac{\delta E}{\delta \phi} + \lambda_1 \frac{\delta A}{\delta \phi} + \lambda_2 \frac{\delta B}{\delta \phi} = 0 \quad (2.23)$$

Denote

$$f(\phi) = \frac{\delta B}{\delta \phi} = -\epsilon \Delta \phi + \frac{1}{\epsilon} (\phi^2 - 1)$$

$$f_c = -\epsilon \Delta \phi + \frac{1}{\epsilon} (\phi^2 - 1)(\phi + C\epsilon) = f(\phi) + C(\phi^2 - 1) \quad (2.24)$$

thus $E = \int_{\Omega} k \frac{f_c^2}{2\epsilon} \, dx$. Here the modified spontaneous curvature is $\sqrt{2}$ times of original spontaneous curvature $c_0$. We also denote

$$g = -\Delta f_c + \frac{1}{\epsilon^2} (3\phi^2 + 2C\epsilon \phi - 1)f_c \quad (2.26)$$
or \( \frac{\delta E}{\delta \phi} = kg \). And (2.27) can be written as

\[
kg + \lambda_1 + \lambda_2 f = 0. \tag{2.27}
\]

And above equations can be rewritten as

\[
\begin{aligned}
\Delta f_c &= \frac{1}{\epsilon^2}(3\phi^2 + 2C\epsilon\phi - 1)f_c + \frac{\lambda_2}{k}(f_c - C(\phi^2 - 1)) + \frac{\lambda_1}{k}, \\
\Delta \phi &= -\frac{1}{\epsilon}(f_c - C(\phi^2 - 1)) + \frac{1}{\epsilon^2}(\phi^2 - 1)\phi
\end{aligned} \tag{2.28}
\]

From theorem 2.1, we know system (2.28) has solution. In the isotropic case with zero spontaneous curvature \( c_0 \), \( f_c = f \). Above system is

\[
\begin{aligned}
\Delta f &= \frac{1}{\epsilon^2}(3\phi^2 - 1)f + \frac{\lambda_2}{k}f + \frac{\lambda_1}{k}, \\
\Delta \phi &= -\frac{1}{\epsilon}f + \frac{1}{\epsilon^2}(\phi^2 - 1)\phi
\end{aligned} \tag{2.29}
\]

**Lemma 2.4.**

\[
\begin{aligned}
\lambda_1 |\Omega| + \lambda_2 c_1 &= \frac{k}{\epsilon^2} \int_{\Omega} f_c(3\phi^2 + 2C\epsilon\phi - 1) \, dx, \\
3\lambda_1 (\alpha + |\Omega|) - \lambda_2 (\beta + 2\beta_2) &= E(\phi) - \frac{2k}{\epsilon^2} \int_{\Omega} f_c(\phi^2 - 1)(\phi + C\epsilon) \, dx.
\end{aligned} \tag{2.30} \tag{2.31}
\]

where \( c_1 = \frac{1}{\epsilon} \int_{\Omega} (\phi^2 - 1)\phi \, dx \), \( \beta_2 = \frac{1}{4\epsilon} \int_{\Omega} (\phi^2 - 1)^2 \, dx \).

**Proof.** (2.30) follows immediately by integrating (2.27) over \( \Omega \). (2.31) follows from the Pohozaev identity by multiply (2.27) by \( x \cdot \nabla \phi \).
First,

\[
\int_{\Omega} kg \nabla \phi \cdot x \, dx = (-\Delta f_c + \frac{1}{\epsilon^2}(3\phi^2 + 2C\epsilon\phi - 1)f_c) \nabla \phi \cdot x \, dx
\]

\[
= k \int_{\Omega} -f_c \Delta (\nabla \phi \cdot x) + \frac{1}{\epsilon^2}(3\phi^2 + 2C\epsilon\phi - 1)f_c \nabla \phi \cdot x \, dx
\]

\[
= k \int_{\Omega} -f_c (\nabla \phi \cdot x + 2\Delta \phi) + \frac{1}{\epsilon^2}(3\phi^2 + 2C\epsilon\phi - 1)f_c \nabla \phi \cdot x \, dx
\]

\[
= k \int_{\Omega} f_c x \cdot (-\nabla \phi + \frac{1}{\epsilon^2}(3\phi^2 + 2C\epsilon\phi - 1)\nabla \phi) - 2f_c \Delta \phi \, dx
\]

\[
= k \int_{\Omega} x \cdot \nabla (\frac{1}{2\epsilon} f_c^2) - 2f_c \Delta \phi \, dx
\]

\[
= k \int_{\Omega} -\nabla \cdot (\frac{1}{2\epsilon} f_c^2) - 2f_c \Delta \phi \, dx
\]

\[
= -3E(\phi) - k \int_{\Omega} 2f_c \Delta \phi \, dx
\]

\[
= E(\phi) - k \int_{\Omega} \frac{2}{\epsilon^2}(\phi^2 - 1)(\phi + C\epsilon)f_c \, dx.
\]

Second,

\[
\int_{\Omega} \lambda_1 \nabla \phi \cdot x \, dx = \lambda_1 (\int_{\Omega} -3\phi \, dx - 3|\Omega|)
\]

\[
= -3\lambda_1 (\alpha + |\Omega|)
\]

Last,

\[
\int_{\Omega} \lambda_2 f \nabla \phi \cdot x \, dx = \lambda_2 \int_{\Omega} -\epsilon \nabla \cdot (\nabla \phi : \nabla \phi) \cdot x + \frac{\epsilon}{2} \nabla(|\nabla \phi|^2) \cdot x + \frac{1}{4\epsilon} \nabla \cdot ((\phi^2 - 1)^2) \cdot x \, dx
\]

\[
= \lambda_2 \int_{\Omega} -\epsilon |\nabla \phi|^2 + 3(\frac{\epsilon}{2} |\nabla \phi|^2 + \frac{1}{4\epsilon} (\phi^2 - 1)^2) \, dx
\]

\[
= \lambda_2 (3\beta - \int_{\Omega} \epsilon |\nabla \phi|^2) \, dx)
\]

\[
= \lambda_2 (\beta + 2\beta_2)
\]
All together we have (2.31). □

**Lemma 2.5.** If (2.10) - (2.12) satisfies (A1) and (A2), then the system

\[
J = \begin{pmatrix}
|\Omega| & c_1 \\
3(\alpha + |\Omega|) & -(\beta + 2\beta_2)
\end{pmatrix}
\]

(2.32)

is invertible, where \(c_1\) and \(\beta_2\) is the same as lemma 2.4

**Proof.**

\[
\det(J) = -|\Omega|(\beta + 2\beta_2) - 3(\alpha - |\Omega|)c_1
\]

Using Lemma 2.2 with \(p = W'(q)\) where \(W(q) = \frac{1}{4}(q^2 - 1)^2\)

\[
c_1 = \frac{1}{\epsilon} \int_{\Omega} W'(\phi) \, dx = \frac{1}{\epsilon} \int_{\Omega} W'(q) + W''(q)g + \frac{1}{2}W'''(q)g^2 \, dx = o(1).
\]

Thus

\[
\det(J) = -|\Omega|(\beta + 2\beta_2) + o(1) \neq 0,
\]

for sufficiently small \(\epsilon\). □

In [20], for zero spontaneous curvature case we proved the uniform boundedness for the Lagrange multipliers for system (2.28) as \(\epsilon \to 0\). We copy it as a lemma here.

**Lemma 2.6.** In zero spontaneous curvature case, if \(\phi_\epsilon\) satisfies (A1) and (A2), then \(\lambda_1\) and \(\lambda_2\) are uniformly bounded in the limit \(\epsilon \to 0\).

With this lemma, we can further prove the uniform boundedness for the Lagrange multipliers in the non-zero spontaneous curvature case.
Theorem 2.4. If $\phi_\epsilon$ satisfies (A1) and (A2), then $\lambda_1$ and $\lambda_2$ are uniformly bounded in the limit $\epsilon \to 0$.

Proof. From Lemma 2.5, we only need to prove the right hand side of (2.30) and (2.31) is uniformly bounded. As $f_c = f + C(\phi^2 - 1)$, we have

$$\frac{k}{\epsilon^2} \int_\Omega f_c (3\phi^2 + 2C\epsilon\phi - 1) \, dx = \frac{k}{\epsilon^2} \int_\Omega f (3\phi^2 - 1) \, dx + \frac{k}{\epsilon^2} \int_\Omega 2C\epsilon\phi f \, dx$$

$$+ \frac{k}{\epsilon^2} \int_\Omega C(\phi^2 - 1)(3\phi^2 + 2C\epsilon\phi - 1) \, dx$$

Since if $C = 0$, from Lemma 2.6, the right hand side is uniformly bounded, i.e.

$$\frac{k}{\epsilon^2} \int_\Omega f (3\phi^2 - 1) \, dx = O(1),$$

we only need to prove when $C \neq 0$, the following identities hold.

$$\frac{1}{\epsilon^2} \int_\Omega (\phi^2 - 1)(3\phi^2 + 2C\epsilon\phi - 1) \, dx = O(1)$$

$$\frac{1}{\epsilon} \int_\Omega \phi f \, dx = O(1)$$

Similarly, we also need to prove the following identities hold for (2.31)

$$\frac{1}{\epsilon^2} \int_\Omega (\phi^2 - 1)^2 (\phi + C\epsilon) \, dx = O(1)$$

$$\frac{1}{\epsilon} \int_\Omega f (\phi^2 - 1) \, dx = O(1)$$

In fact, from Lemma 2.2, we have

$$\frac{1}{\epsilon^2} \int_\Omega q' (3q^2 + 2C\epsilon q - 1) \, dx = O(1).$$
As $\phi^2 - 1 = -\sqrt{2q'} + O(\epsilon^2)$ and $3\phi^2 + 2C\epsilon\phi - 1 = 3q^2 + 2C\epsilon q - 1 + O(\epsilon^2)$, we get (2.33). Similarly, we have (2.35).

Also, as $f = -\epsilon\Delta\phi + \frac{1}{\epsilon}(\phi^2 - 1)\phi = -q'\Delta d + O(\epsilon)$, we can similarly prove (2.34) and (2.36).

2.6 Penalty formulation

Computationally, it is more convenient to use penalty formulation for the two constraints. In stead of the Lagrange multipliers $\lambda_1$ and $\lambda_2$, we can use two penalty constants $M_1, M_2$ to get a modified Elastic bending energy

$$E_M(\phi) = E(\phi) + \frac{1}{2}M_1(A(\phi) - \alpha)^2 + \frac{1}{2}M_2(B(\phi) - \beta)^2.$$  \hfill (2.37)

First we have the following existence theorem.

**THEOREM 2.5.** There exists $\phi_M \in H^2(\Omega)$ such that $E_M(\phi_M) = \inf_{\phi \in H^2} E_M(\phi)$

**Proof.** First we can find a serial $\{\phi_n\}_{n=1}^\infty$ such that $\lim_{n \to \infty} E_M(\phi_n) = \inf_{\phi \in H^2} E_M(\phi)$.

Thus $A(\phi_n), B(\phi_n)$ and $E(\phi_n)$ are uniformly bounded. Similar to the proof of Theorem 2.1. There exists a $\phi_M$ and a subsequence, noted still by $\{\phi_n\}_{n=1}^\infty$ such that $\phi_n \rightharpoonup \phi_M$ in $H^2(\Omega)$ and $E_M(\phi_M) = \lim_{n \to \infty} E_M(\phi_n) = \inf_{\phi \in H^2} E_M(\phi)$. \hfill \boxed{1}

Now we can prove that

**THEOREM 2.6.** The minimum of $E(\phi)$ can be approximated by the minimum of $E_M(\phi)$, or

$$\min_{A(\phi) = \alpha, B(\phi) = \beta} E(\phi) = \lim_{M_1, M_2 \to \infty} \min E_M(\phi)$$
Proof. Suppose $\phi_M$ reaches the minimum of $E_M(\phi)$ and $\phi$ reaches the minimum of $E(\phi)$ with volume and surface area constraints. We only need to prove for every sequence $\phi_M, M_1, M_2 \to \infty$, there exists a subsequence $\phi_{M_n}$ such that

$$\lim_{M_1n, M_2n \to \infty} E_{M_n}(\phi_{M_n}) = \min_{A(\phi) = \alpha, B(\phi) = \beta} E(\phi).$$

For sequence $\phi_M$, it is obvious that $E_M(\phi_M) \leq E_M(\phi) = E(\phi)$. We know that $A(\phi_M), B(\phi_M)$ and $E(\phi_M)$ are uniformly bounded for large $M$. Similar to the proof of Theorem 2.1. There exists a subsequence of $\phi_M$, noted by $\phi_{M_n}$ such that $\phi_{M_n} \to \phi^*$ in $H^2(\Omega)$ and

$$\alpha = \lim_{M_1n, M_2n \to \infty} A(\phi_{M_n}) = A(\phi^*),$$

$$\beta = \lim_{M_1n, M_2n \to \infty} B(\phi_{M_n}) = B(\phi^*),$$

$$E(\phi) \geq \lim_{M_1n, M_2n \to \infty} E(\phi_{M_n}) = E(\phi^*).$$

Thus $\phi^*$ reaches the minimum of $E(\phi)$ with volume and surface area constraints. 

2.7 Numerical approximation

The nonlinear variational problem $\min E_M(\phi)$ is solved via a standard gradient flow approach (see for example [3, 17] and the references cited therein), namely, we consider

$$\phi_t = -\gamma \frac{\delta E_M(\phi)}{\delta \phi}$$
where constant $\gamma$ is a time scale. We can numerically solve this problem under some grid meshes. We need to verify that the phase field function $\phi$ can be approximated by the numerical solutions.

### 2.7.1 Interpolation

First, we can decomposing the domain $\Omega$ by a set of admissible triangulations $T^h$ and for each triangle $K \in T^h$, $\text{diam}(K) \leq h$. And we define the following regular triangular decomposition of domain $\Omega$.

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

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

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

Denote $S^h$ the piecewise linear continuous functions defined on a family of regular triangulation $T^h$. In general, $S^h$ is not belong to $H^2(\Omega)$, and the energy $E$ is not defined in this case. To solve this problem, we can interpret the $\Delta$ operator on $S^h$ in the weak sense.

**Definition 2.2.** $\forall \phi^h \in S^h$, define $\Delta \phi^h$ for an element in $S^h$ such that $\langle \nabla \phi^h, \nabla w^h \rangle = -\langle \Delta \phi^h, w^h \rangle$, $\forall w^h \in S^h$.

It is easy to verify that this definition is well-posed. Also from this definition, we can define the energy $E$ for $\phi^h$.

By this way we can first approximate the phase field function by its interpolation, and we have the following lemma for interpolation solution.
Lemma 2.7. Denote $u^I$ is the interpolation of a function $u \in C^3(\Omega)$ on a family of regular triangulations $T^h$, thus we have $\Delta u^I \rightarrow \Delta u$ in $L^2(\Omega)$ as $h \rightarrow 0$.

Proof. We first prove that $\Delta u^I$ are uniformly bounded. Take $v^I \in S^h$ and $v^I = \Delta u^I$. Thus $\forall w^h \in S^h$, $\langle \nabla u^I, \nabla w^h \rangle = -\langle v^I, w^h \rangle$. Since $u \in C^3(\Omega)$, we have $u^I = u + O(h)$, $\nabla u^I = \nabla u + O(h)$ and $(\Delta u)^I = \Delta u + O(h)$. Thus $\langle v^I, w^h \rangle = -\langle \nabla u, \nabla w^h \rangle + O(h)\|\nabla w^h\|$. Now from the inverse inequality $\|\nabla w^h\| = O(\frac{1}{h})\|w^h\|$ and $(\Delta u)^I = \Delta u + O(h)$, we have $\langle v^I, w^h \rangle = \langle (\Delta u)^I, w^h \rangle + O(1)\|w^h\|$. Taking $w^h = v^I - (\Delta u)^I$, we have $\|v^I - (\Delta u)^I\|^2 = O(1)\|v^I - (\Delta u)^I\|$, or $\|v^I - (\Delta u)^I\| = O(1)$. Since $(\Delta u)^I = \Delta u + O(h)$, we get $\|v^I - \Delta u\| = O(1)$ or $v^I$ is uniformly bounded for all $h > 0$.

Thus given a sequence of $v^I$, denoted by $\{v_n\}_{n=1}^\infty$ with $h \rightarrow 0$, as $v_n$ is uniformly bounded, passing if necessary to a subsequence, we have $v_n \rightarrow v^*$ in $L^2(\Omega)$. Now, for $\phi = v^* - \Delta u \in L^2(\Omega)$, we can have a set of $\phi^h \in S^h(\Omega)$ and $\phi^h \rightarrow \phi$ in $L^2(\Omega)$. And first we have

$$< v^*, \phi > - < v_n, \phi^h > = < v^*, \phi > - < v_n, \phi > + < v_n, \phi - \phi^h >$$

Since $< v_n, \phi > \rightarrow < v^*, \phi >$ and $| < v_n, \phi - \phi^h > | \leq \|v_n\|\|\phi - \phi^h\| \rightarrow 0$, we have $< v_n, \phi^h > \rightarrow < v^*, \phi >$. 

And then

\[
<v_n, \phi^h> = - \langle \nabla u^I, \nabla \phi^h \rangle \\
= - \langle \nabla u, \nabla \phi^h \rangle + O(h)\|\nabla \phi^h\| = \langle \Delta u, \phi^h \rangle + O(h)\|\nabla \phi^h\|
\]

\rightarrow \langle \Delta u, \phi \rangle.

Together, we have \( <v^*, \phi> = \langle \Delta u, \phi \rangle \) or \( \|\phi\| = 0 \). Thus we proved \( v_n \rightarrow \Delta u \).

Then we have

\[
\|v_n\|^2 = - \langle \nabla u^I, \nabla v_n \rangle \\
= - \langle \nabla u, \nabla v_n \rangle + O(h)\|\nabla v_n\| = \langle \Delta u, v_n \rangle + O(h)\|\nabla v_n\|
\]

\rightarrow \langle \Delta u, \Delta u \rangle

Now we can prove that \( v_n \rightarrow \Delta u \) because

\[
\|v_n - \Delta u\|^2 = \|v_n\|^2 - 2 <v_n , \Delta u> + \|\Delta u\|^2 \\
\rightarrow \|\Delta u\|^2 - 2 <\Delta u, \Delta u> + \|\Delta u\|^2 \\
= 0
\]

So for every sequence of \( v^I \), there is a subsequence converts to \( \Delta u \). Then \( v^I \rightarrow \Delta u \)

in \( L^2(\Omega) \) as \( h \rightarrow 0 \).

With this lemma, it is obvious that the following theorem about the approximation of the phase field function by its interpolation.
Theorem 2.7. Denote $\phi^I$ is the interpolation of phase field function $\phi$. If $\phi \in C^3(\Omega)$, we have $A(\phi^I) \to A(\phi)$, $B(\phi^I) \to B(\phi)$, $E(\phi^I) \to E(\phi)$ as the mesh size $h \to 0$.

2.7.2 Numerical approximation

In section 2.6, we know that the minimum of $E(\phi)$ can be approximated by the minimum of $E_M(\phi)$ for $\phi \in H^2(\Omega)$. We can also approximate the minimizer of $E_M(\phi)$ by the numerical minimizers. That is the following theorem.

Theorem 2.8. In $S^h(\Omega)$, there exists a $\phi^h$ minimize the penalized energy $E_M(\phi)$ for fixed penalty coefficients. And if $\phi \in C^3(\Omega)$ reaches the minimum of $E_M$, $E_M(\phi^h) \to E_M(\phi)$ as $h \to 0$.

Proof. First, for a fixed $h$ and fixed penalty coefficients, we have a set of $\phi^h_n$, $n = 1, 2, \ldots$ such that $E_M(\phi^h_n) \to \min E_M(\phi)$ in $S^h$. It is obvious that $\phi^h_n$ is uniformly bounded in $H^1(\Omega)$. Denote $v^h_n = \Delta \phi^h_n$, we have $v^h_n$ is uniformly bounded in $L^2$. Thus there exist a $\phi^h \in H^1(\Omega)$ such that $\phi^h_n \to \phi^h$, passing to a subsequence if necessary. Since $S^h(\Omega)$ is a space with finite dimension. We have $\phi^h \in S^h(\Omega)$ and $\phi^h_n \to \phi^h$. It is obvious that $\phi^h$ minimize $E_M(\phi)$ in $S^h(\Omega)$.

Now, let $h \to 0$, we need to prove that $E_M(\phi^h) \to E_M(\phi)$ if $\phi \in C^3(\Omega)$ reaches the minimum of $E_M$. From Theorem 2.7, It is obvious that $E_M(\phi^h) \leq E_M(\phi^I)$ where $\phi^I$ is the interpolation of $\phi$ in $S^h$. Since $E_M(\phi^I) \to E_M(\phi)$, $E_M(\phi^h)$ is uniformly bounded. Thus $\phi^h$ is uniformly bounded in $H^1(\Omega)$. Denote $v^h = \Delta \phi^h$, we have $v^h$ is uniformly bounded in $L^2$. Thus there exist a $\phi^* \in H^1(\Omega)$ such that $\phi^h \to \phi^*$ in $H^1$, $\phi^h \to \phi^*$ in $L^2$, passing to a subsequence if necessary. Also there exists a $v^* \in L^2(\Omega)$ such that $v^h \to v^*$ in $L^2$, passing to a subsequence if necessary.
Now for any $w \in C^\infty(\Omega)$, there exists $w^h \in S^h(\Omega)$ and $w^h \rightarrow w$ in $H^1$. And we have

$$
< \nabla \phi^h, \nabla w > = < \nabla \phi^h, \nabla w^h > + < \nabla \phi^h, \nabla (w - w^h) >
$$

$$
= - < v^h, w^h > + < \nabla \phi^h, \nabla (w - w^h) >
$$

$$
\rightarrow - < v^*, w >
$$

Also $< \nabla \phi^h, \nabla w > = < \phi^h, \Delta w > \rightarrow < \phi^*, \Delta w > = < \nabla \phi^*, \nabla w >$. We have

$$
< \nabla \phi^*, \nabla w > = - < v^*, w > \text{ for all } w \in C^\infty(\Omega)
$$

or $\Delta \phi^* = v^*$ in distribution sense. From the Boundary $H^2$-regularity of $\Delta$ operator, we have $\phi^* \in H^2(\Omega)$. And $\Delta \phi^h \rightarrow \Delta \phi^*$.

We also have $< \nabla \phi^h, \nabla \phi^h > \rightarrow < \nabla \phi^*, \nabla \phi^* >$ because

$$
< \nabla \phi^h, \nabla \phi^h > = - < v^h, \phi^h > \rightarrow - < v^*, \phi^* > = < \nabla \phi^*, \nabla \phi^* >,
$$

where we used $\phi^h \rightarrow \phi^*$ in $L^2$.

Since $w \in C^\infty(\Omega)$ is dense in $H^1(\Omega)$, $< \nabla \phi^h, \nabla w > \rightarrow - < v^*, w >$ and $< \nabla \phi^*, \nabla w > = - < v^*, w >$ for all $w \in H^1(\Omega)$. Then

$$
< \nabla \phi^h, \nabla \phi^* > \rightarrow - < v^*, \phi^* > = < \nabla \phi^*, \nabla \phi^* >
$$
And we have

\[ \| \nabla \phi^h - \nabla \phi^* \|^2 = \| \nabla \phi^h \|^2 - 2 < \nabla \phi^h, \nabla \phi^* > + \| \nabla \phi^* \|^2 \]

\[ \rightarrow \| \nabla \phi^* \|^2 - 2 < \nabla \phi^*, \nabla \phi^* > + \| \nabla \phi^* \|^2 \]

\[ = 0 \]

Thus \( \nabla \phi^h \rightarrow \nabla \phi^* \) in \( L^2(\Omega) \) or \( \phi^h \rightarrow \phi^* \) in \( H^1(\Omega) \). We have

\[ A(\phi^h) \rightarrow A(\phi^*), \quad B(\phi^h) \rightarrow B(\phi^*) \]

The rest proof is similar to the proof of Theorem 2.1. Let \( p(\phi) = \frac{1}{c^2}(\phi^2 - 1)(\phi + C\epsilon) \), we have

\[ E(\phi^h) = k\epsilon^2 \| \Delta \phi^h - p(\phi^h) \|^2_{L^2} \]

(2.38)

And as \( \phi^h \rightarrow \phi^* \) in \( L^2(\Omega) \), passing if necessary to yet another subsequence, we have \( \phi^h \rightarrow \phi^* \) a.e. in \( \Omega \); and thus \( p(\phi^h) \rightarrow p(\phi^*) \) a.e. in \( \Omega \).

Fix \( \xi > 0 \), the Egoroff’s Theorem asserts \( p(\phi^h) \rightarrow p(\phi^*) \) uniformly on \( \Omega_\xi \) where \( \Omega_\xi \) is a measurable set with \( |\Omega - \Omega_\xi| \leq \xi \). And we have

\[ E(\phi^h) \geq \frac{k\epsilon^2}{2} (\| \Delta \phi^h \|^2_{L^2(\Omega_\xi)} - 2 < \Delta \phi^h, p(\phi^h) >_{L^2(\Omega_\xi)} + \| p(\phi^h) \|^2_{L^2(\Omega_\xi)}) \]  

(2.39)

And since \( \Delta \phi^h \) weakly converges to \( \Delta \phi^* \) in \( L^2(\Omega) \), we have

\[ \lim_{h \rightarrow 0} \| \Delta \phi^h \|^2_{L^2(\Omega_\xi)} \geq \| \Delta \phi^* \|^2_{L^2(\Omega_\xi)}. \]  

(2.40)
With \( p(\phi^h) \rightarrow p(\phi^*) \) uniformly on \( \Omega_\xi \), we have

\[
\lim_{h \to 0} < \Delta \phi^h, p(\phi^h) >_{L^2(\Omega_\xi)} = < \Delta \phi^*, p(\phi^*) >_{L^2(\Omega_\xi)} ;
\] (2.41)

and

\[
\lim_{h \to 0} \| p(\phi^h) \|_{L^2(\Omega_\xi)} = \| p(\phi^*) \|_{L^2(\Omega_\xi)} .
\] (2.42)

Thus from (2.39), (2.40), (2.41) and (2.42) we have

\[
\lim_{h \to 0} E(\phi^h) \geq \int_{\Omega_\xi} |\Delta \phi^* - p(\phi^*)|^2 \, dx
\] (2.43)

We now let \( \xi \) tend to zero, recall the Monotone Convergence Theorem to conclude

\[
\lim_{h \to 0} E(\phi^h) \geq E(\phi^*)
\]

And we further have

\[
\lim_{h \to 0} E_M(\phi^h) \geq E_M(\phi^*).
\]

If \( \phi \in C^3(\Omega) \) reaches the minimum of \( E_M \), from Theorem 2.7, we know \( \lim_{h \to 0} E_M(\phi^I) \geq E_M(\phi^*) \).

Since \( E_M(\phi) \) is the minimum, we know \( E_M(\phi^*) \) reaches the minimum of \( E_M \). Because for every sequence \( \phi^h \), there is a subsequence having limit to the minimum of \( E_M \), we
actually have for every sequence $\phi^h$ which minimizes $E_M$ in $S^h$ with boundary condition,

$$E_M(\phi^h) \to \min E_M(\phi), \text{ as } h \to 0.$$ 

2.8 Conclusion

In this chapter, we build the theory of phase field model for equilibrium vesicle shapes. In section 2.6 we propose the penalty formulation to solve the phase field model. And based on Theorem 2.6, we can approximate the phase field function by solving the penalty formulation using large penalty constants $M_1, M_2$. Further based on Theorem 2.8, we can approximate the penalty solution by numerical solutions. These approximation theorems provide a guideline for our numerical simulations. In the next Chapter, we systematically study the vesicle configurations in the axis-symmetric case by numerical experiments. And furthermore in Chapter 4, we study the non-axisymmetric cases in truly three dimension numerical space.
Chapter 3

Equilibrium Shapes in Axis-symmetrical Case

In this chapter, we study the equilibrium vesicle shapes in the axis-symmetrical case by numerical methods.

3.1 Introduction

In Chapter 2, we build the theory of phase field model for equilibrium vesicle shapes. A major advantage of the phase field formulation is that one does not need to explicitly track the free surface $\Gamma$. For different values of $\alpha$ and $\beta$, different surfaces may be obtained, which may involve topological changes and thus presenting numerical difficulties as pointed out in [5]. On the other hand, efficient numerical techniques within the phase field models for detecting the topological change is given in Chapter 6. For illustration, in subsequent numerical simulations, in this chapter we focus on the three dimensional axis-symmetric case only to reduce the computational efforts involved. The full three dimensional simulations are to be reported in chapter 4.

Theorem 2.6 and Theorem 2.8 in Chapter 2 provide a guideline for our numerical simulations. First in section 3.2, we design the numerical scheme for finding the numerical minimizers efficiently. Then we do some convergence tests to ensure the convergence of our numerical simulations. In section 3.3, we systematically study the bifurcation of
various vesicle configurations. Finally in section 3.4 we study the effect of the spontaneous curvature for both the constant and non-constant cases.

### 3.2 Numerical simulations

#### 3.2.1 Numerical scheme

As stated in the prior chapter, our problem is to minimize the elastic energy $E(\phi)$ in (2.10) for fixed volume ($A(\phi)$ in (2.11) (taking value $\alpha$) and surface area $B(\phi)$ in (2.12) (taking value $\beta$).

This constrained variational problem may be solved by a number of approaches such as the Lagrange Multiplier Method or the method of normalized gradient flow [3]. Here, we adopt the penalty method with penalty coefficients $M_1$ and $M_2$. The problem is then becoming the minimization of $E_M$ defined in (2.37)

Theorem 2.5 argue that minimizers of the energy (2.37) exist. Moreover, Theorem 2.6 states that as the penalty constants $M_1$, $M_2$ approach to infinity, they approach to the minimizer of $E = E(\phi)$ with the given constraints.

As state in section 2.7, the nonlinear variational problem is solved via a standard gradient flow approach:

$$\frac{\partial \phi}{\partial t} = -\frac{\delta E_M(\phi)}{\delta \phi},$$

where $\delta/\delta \phi$ denote the first variation of the functional. For simplicity, we also use the notation $\nabla E(\phi)$ to denote this first variation. Given an initial guess, as $t \to \infty$, the dynamic solutions $\{\phi(t)\}$ converge to a steady state which is a critical point of the energy $E$ [35].
Since we are primarily interested in the minimizers of the energy, only the long time limit of the above gradient flow is important. A backward Euler scheme is employed for the time integration of the above gradient flow to ensure the stability of the time integration and to allow large time steps to be taken for a faster convergence to the steady state. That is:

\[ u^{n+1} - u^n = -\Delta t_n \frac{\delta E(u^{n+1})}{\delta u} = -\Delta t_n \nabla E(u^{n+1}). \]

As in [3, 17], it is easy to verify that the solution of the backward Euler scheme is also the solution of the minimization problem:

\[
\min \tilde{E}^n(u) = \int_\Omega \frac{|u - u^n|^2}{\Delta t_n} \, dx + E(u). \tag{3.1}
\]

Since

\[ E(u^{n+1}) \leq \tilde{E}(u^{n+1}) \leq \tilde{E}(u^n) \leq E(u^n), \]

we see that the backward Euler scheme enjoys the property that the energy is monotonically decreasing in time. Moreover, \( u^n \to \phi \), a critical point of the energy \( E \), as \( n \to \infty \).

To implement the gradient flow approach, a spatial approximation is first established. As the numerical simulations presented in this paper concern mainly on the z-axial symmetrical cases, the three dimensional problem is thus simplified to a two dimensional one. The computational domain is taken to be a subset of the half plane in the x-z plane. The cross section of the vesicle in this half plane \( (x > 0) \) is computed and
the vesicle is obtained by rotating the two dimensional shape on the x-z plane around the
z-axis. Thus effectively, we may relate $x$ with the radial distance to the z-axis. Without
loss of generality, we let the cross section of the vesicle be located inside the domain
$[0, r] \times [0, a]$ on the x-z plane. The energy functional 3.1 is then discretized on a spatial
$m \times n$ mesh in the domain $[0, r] \times [0, a]$ in the $x - z$ plane using standard difference
approximations, which leads to a discrete gradient flow. The particular form of the
discretization is given in the section 3.2.2.

We note that, in our computation domain, the cross section of the vesicle surface
$\Gamma$ of interest becomes a one dimensional curve, which can be parameterized by a single
variable. Though a reduction to an ordinary differential-integral equation is possible,
such a formulation generally works well only when the curve does not undergo any
topological changes. The phase field approach developed here can handle such changes
with ease and it can be used for the full three dimensional computation as well, including
the anisotropic cases.

The solution of the Euler scheme for the discrete gradient flow at each step satisfies
a nonlinear system of equations and it is solved by the Newton’s Method. The resulting
systems of linear equations at each Newton iteration are solved using a version of the
PCG method for sparse matrices with an SSOR preconditioner. Newton’s method is
generally locally convergent. For a small enough time step, the new solution is very close
to the solution at the previous time step, and the Newton’s iteration converges quickly
to a critical point of $\tilde{E}$. However, small $\Delta t_n$ implies that many time integration steps
have to be taken in order to converge to the steady state. In our algorithm, we adjust
the value of $\Delta t_n$ so that the Newton’s method always converges in 3 to 5 steps. This
allows efficient computation at each time step. At the same time, it leaves room for a
large step size when the solution is not varying very fast in time, and thus leads to a
speedy convergence to the steady state. In section 3.2.2, we give detailed descriptions of
the algorithm.

3.2.2 Discretization and algorithms

Here, we provide more detailed descriptions of the discrete energy and the nu-
umerical algorithm.

We use a uniform $m \times n$ mesh with $h$ being the mesh parameter so that $r = mh,$
and $a = nh.$ The differential operators is replaced by the standard finite difference
operators defined on the given mesh.

**Discrete energy**  Recall that the energy functional has the form:

$$
E = \int_{\Omega} \frac{k}{2} |\Delta \phi - \frac{1}{\epsilon^2}(\phi^2 - 1)(\phi + \epsilon \sqrt{2}c_0)|^2 \, dx + \frac{M_1}{2} \left( \int_{\Omega} \phi(x) \, dx - \alpha \right)^2 \\
+ \frac{M_2}{2} \left( \int_{\Omega} \left[ \frac{\epsilon}{2} |\nabla \phi|^2 + \frac{1}{4\epsilon}(\phi^2 - 1)^2 \right] \, dx - \beta \right)^2. 
$$

(3.2)

To discretize the energy functional (3.2), we use the following quadrature:

$$
\int_{\Omega} f(x) \, dx \approx I_h(f) = \frac{2}{9} \pi h^3 \sum_{i=1}^{m} \sum_{j=0}^{n} i \omega_1(i) \omega_2(j) f_{i,j} 
$$

(3.3)
for any function \( f \) defined on \( \Omega \), where \( f_{i,j} \) is the value of \( f \) at the grid point \((ih,jh)\) in the \( m \times n \) mesh, and weight functions \( \omega_1 \) and \( \omega_2 \) are defined as following:

\[
\omega_1(i) = \begin{cases} 
1 & \text{if } i = 0 \text{ or } m \\
2 & \text{if } i \text{ is even and } i \neq m \\
4 & \text{otherwise}
\end{cases}, \quad (3.4)
\]

and

\[
\omega_2(j) = \begin{cases} 
1 & \text{if } j = 0 \text{ or } n \\
2 & \text{if } j \text{ is even and } j \neq n \\
4 & \text{otherwise}
\end{cases}. \quad (3.5)
\]

Now, let us turn to the discretization of the terms \( \Delta \phi \) and \( |\nabla \phi|^2 \). Since

\[
\Delta \phi(r,z) = \frac{\partial^2 \phi}{\partial r^2} + \frac{\partial^2 \phi}{\partial z^2} + \frac{1}{r} \frac{\partial \phi}{\partial r}, \quad \text{and} \quad |\nabla \phi(r,z)|^2 = \left(\frac{\partial \phi}{\partial r}\right)^2 + \left(\frac{\partial \phi}{\partial z}\right)^2, \quad (3.6)
\]

we take their discrete forms as follows:

\[
(\Delta_h \phi)_{i,j} = \frac{\phi_{i+1,j} + \phi_{i-1,j} + \phi_{i+1,j-1} + \phi_{i+1,j+1} - 4\phi_{i,j}}{h^2} + \frac{\phi_{i+1,j} - \phi_{i-1,j}}{2ih^2}, \quad (3.7)
\]

\[
|\nabla_h \phi|_{i,j}^2 = \frac{(\phi_{i,j+1} - \phi_{i,j-1})^2 + (\phi_{i+1,j} - \phi_{i-1,j})^2}{4h^2}, \quad (3.8)
\]

The discrete boundary conditions are \( \phi_{m+1,i} = -1 \) and \( \phi_{j,-1} = \phi_{j,n+1} = -1 \) for \( i = 0,1,...,m \) and \( j = 0,1,...,n \). Here, we also set \( \phi_{0,j} = \phi_{1,j} \) for all \( j \) at the \( z \)-axis. The boundary conditions are applied to the formula (3.7) and (3.8) at the boundary. In our
numerical simulation, as a comparison, we also implemented a cell centered difference approach in the \(x\) (or \(r\)) direction, that is, the grid points in \(x\) are at the points \(\{(i + 1/2)h\}_{i=0}^{n-1}\). We then introduce a ghost point at \(-h/2\) and impose the boundary condition \(\phi(-h/2, z_j) = \phi(h/2, z_j)\) for all \(j\). In such a discretization, grids points avoid the \(z\)-axis. Numerical experiments indicate that the two discretization approaches yield effectively the same results.

Combine (3.2), (3.3), (3.7) and (3.8), we can get the discrete form of the energy, which we denote by \(E_h\). The existence of minimizers for \(E_h\) is established in section 2.8 for any given mesh. The convergence of the discrete minimizers to minimizers of the continuous problem is also established in section 2.8 as the mesh parameters goes to zero, at least for any fixed parameter \(\epsilon\). The limiting behavior for small \(\epsilon\) and small mesh parameter \(h\) is a delicate issue that will be studied more carefully in our future works. For convenience, we let \(\nabla E_h\) denote the gradient vector of \(E_h\) and \(\Delta E_h\) denote the Hessian matrix of \(E_h\).

**Gradient flow algorithm** Clearly, a critical point of the energy \(E_h\) correspond to a grid function at which all components of \(\nabla E_h\) vanish. For a more efficient implementation, we adopt a strategy to dynamically constrain some values of the grid function during the solution process. In particular, at grid points that correspond to small gradient components, changes of the grid function make insignificant contribution to the variation in energy, thus, no update of the grid function values at those grid points is performed. As the grids points correspond to large gradient components often are located near the interface, such a strategy naturally leads to a fast algorithm that allow
the computation being more focused in the vicinity of the phase boundary (in the same spirit of the fast level set methods [46]). The details are given in the following.

Given $\alpha$, $\beta$, $\epsilon$, and penalty parameters $M_1$, $M_2$.

1. Initialize $u_{old} = u_0$ to match with an initial shape and take an initial small time step $\Delta t$.

2. Compute $\nabla E_h(u_0)$, put constraints on the components $\{u_i\}$ of $u_0$ that correspond to grid points with small $\{\frac{\partial E_h}{\partial u_i}\}$ and their adjacent points.

3. Compute using Newton’s Method to get a new solution $u_1 = u_0 - (\Delta E(u_0) + 2I/(\Delta t))^{-1}(\nabla E_h(u_0) + 2(u_0 - u_{old})/(\Delta t))$ where the updates only take place for unconstrained components.

4. Continue Newton’s iteration with

$$u_{k+1} = u_k - (\Delta E(u_k) + 2I/(\Delta t))^{-1}(\nabla E_h(u_k) + 2(u_k - u_{old})/(\Delta t))$$

for unconstrained components and for $k = 1, 2, ...$ until the norm $\|\nabla E_h(u_k) + 2(u_k - u_{old})/(\Delta t)\|$ is smaller than some given tolerance. Denote the solution as $u_{new}$. If the number of Newton steps in this loop is larger than 5, stop.

5. If the number of iteration in step 4 is larger than 5, half $\Delta t$, return to step 3 to repeat Newton’s method; If the iteration number is less than 3, double $\Delta t$.

6. Compute $\|\nabla E(u_{new})\|$, if small enough, exit. Otherwise set $u_{old} = u_0 = u_{new}$ and go to step 2.
As noted before, the linear systems in steps 3 and 4 are solved using the PCG method for sparse matrices with an SSOR preconditioner. Our numerical experiments indicate that the above algorithm is very stable and robust.

3.2.3 Convergence tests

For a particular phase field simulation, the quality of the numerical result is affected by the choice of computational domain, the transition thickness parameter (or the effective width of the diffusive interface) $\epsilon$, the number of grid points, and the choices of other parameters used in the simulation. Based on the experience, we generally take a domain significantly larger than the region enclosed by the membrane to be computed. The parameter $\epsilon$ is taken to be just a couple of percentage points of the domain size to ensure a relatively sharp interfacial region. The mesh size is normally taken to be several times smaller than $\epsilon$ to ensure adequate spatial resolution. To ascertain the accuracy and robustness of our numerical algorithms and the parameter selections, we here present results of some numerical tests on the convergence and performance of our method. All of these convergence tests are done with zero spontaneous curvature.

The first example is for the same set of parameters ($\epsilon$, $Vol$ and $Area$) in the same domain of size 2 by 2, but with different grids of the size $100 \times 100$ and $200 \times 200$ respectively. We choose $\epsilon = 0.03$, $Vol = 1.1000$ and $Area = 6.9474$ and the penalty parameters $M_1 = M_2 = 10^5$.

The density plots of two numerical approximations of $\phi$ are shown in Figure 3.1. Little difference between the solutions is visible. Moreover, the computation of the energy
$W$ gives energy valued at 71.8767 and 73.4440 respectively. The 2% energy difference is mostly due to the integration errors under different grids.

![Density plots of $\phi$ with 100x100 and 200x200 grids](image)

**Fig. 3.1.** Density plots of $\phi$ with 100x100 and 200x200 grids

The convergence is also evident when different domain sizes are used (so long they are large enough to contain the vesicle). We compute the problem using two different grids, a $100 \times 150$ grid and a $40 \times 375$ grid, but with same mesh parameter ($h = 0.02$). This effectively leads to two different domains of sizes $2 \times 3$ and $0.8 \times 7.5$ (see the results in Figure 3.2). The same parameters as in the previous run (depicted in Figure 3.1) are used, except with the area $Area = 6.3640$. The energy is 60.6037 for the $100 \times 150$ grid and 61.2120 for the $40 \times 375$ grid. The small error indicates that the result is insensitive to the change of the computation domain.

We also investigate the dependence on the penalty parameters $M_1$ and $M_2$. For the case of $200 \times 200$ grid and the set of parameters being the same as in Figure 3.2, we list the values of the corresponding Lagrange multipliers $\lambda_i$ ($i = 1, 2$) in Table 3.1. For minimizing the energy $E$ given in (2.10) with constraints $A(\phi) = \alpha$ and $B(\phi) = \beta$ (for
area and volume), the multipliers are defined as constants satisfying

$$\lambda_1 \nabla A + \lambda_2 \nabla B + \nabla E = 0$$

at the minimum. Here, $\nabla$ again refers to first variations of the respective functionals.

With the penalty formulation, the relations between the multipliers and the penalty constants are given by

$$\lambda_i = \lim_{M_1, M_2 \to \infty} \lambda_i(M_1, M_2), \quad \text{for} \quad i = 1, 2$$

with $\lambda_1(M_1, M_2) = M_1 (A(\phi) - \alpha)$, $\lambda_2(M_1, M_2) = M_2 (B(\phi) - \beta)$.

We can see that for the ever increasing penalty coefficients $M_1, M_2$, the multipliers converge to two constants. This confirms that our solutions indeed are the constrained minimizers of the energy functional.

The final example is designed to test the dependence on the parameter $\epsilon$ which measures the interface thickness. As it is well known that, the grid size has to be smaller than the thickness of the transition layer in order to resolve the interface, we thus take
Table 3.1. Convergence of the multipliers

<table>
<thead>
<tr>
<th>$M_1 = M_2$</th>
<th>1</th>
<th>2</th>
<th>4</th>
<th>8</th>
<th>16</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda_1 (\times 10^{-2})$</td>
<td>4.0428</td>
<td>3.6964</td>
<td>3.5577</td>
<td>3.4951</td>
<td>3.4669</td>
</tr>
<tr>
<td>$\lambda_2 (\times 10^{-3})$</td>
<td>-1.0198</td>
<td>-0.9224</td>
<td>-0.8832</td>
<td>-0.8655</td>
<td>-0.8576</td>
</tr>
<tr>
<td>$M_1 = M_2$</td>
<td>32</td>
<td>64</td>
<td>128</td>
<td>256</td>
<td>512</td>
</tr>
<tr>
<td>$\lambda_1 (\times 10^{-2})$</td>
<td>3.4526</td>
<td>3.4424</td>
<td>3.4401</td>
<td>3.4372</td>
<td>3.4376</td>
</tr>
<tr>
<td>$\lambda_2 (\times 10^{-3})$</td>
<td>-0.8535</td>
<td>-0.8506</td>
<td>-0.8495</td>
<td>-0.8491</td>
<td>-0.8492</td>
</tr>
</tbody>
</table>

the 100 $\times$ 200 grid, with $Area = 5.8867$ and $Vol = 1.1000$, for $\epsilon$ being 0.02 and 0.015. The difference in the numerical solutions is very small, as shown in Figure 3.3 and the corresponding energy values 73.6980 and 72.7080 are very close to each other.

To summarize, the above numerical tests indicate that the simulation of the phase field model can indeed give convergence numerical solutions. Moreover, as our above experimental results indicate, the choices of various parameter values used in the simulations are capable of ensuring the convergence of the numerical scheme and ensuring the validity of the simulation results when we probe the energy landscape and predict the vesicle shapes.

3.3 Simulation results with zero spontaneous curvature

We now present computational results that illustrate the various vesicle structures and the energy landscape without spontaneous curvature. Through out this section, the spontaneous curvature is fixed to be zero. Also as we know, $\alpha$ not the truly the volume of the vesicle and $\beta$ is not truly the surface area. One should not confused by these notations.
For the numerical simulations, through a re-scaling, we may take a fixed volume value by fixing $\alpha$ and vary the surface area by fixing $\beta$. In all the simulations, we take the volume enclosed by the vesicle to be 1.1000 (the particular value has no physical significance as it is due to a inadvertently chosen scaling in the simulations). For a perfect sphere, it corresponds to the radius being 0.6404 with the surface area being 5.1536.

For different values of surface area with a given volume that is enclosed by the surface, the different basic shapes (density plots of $\phi$) obtained in the simulation are shown in Figure 3.4. The sharp contrast of the change of color outlines the vesicle boundary. Here, rather than using sophisticated physiological or biological terminologies, we try to use some more common objects to name the various shapes judging from their shape resemblance (viewed in the three dimensional space). For a better visual effect, we give some three dimensional views in Figure 3.5. Though the shapes computed having the same volume, they have different aspect ratios that make them difficult to be displayed in pictures with the same scale. For this reason, the plots in the Figures 3.4 and 3.5 do not share the same scale and the some vesicle shapes may appear larger than others.
Fig. 3.4. The basic configurations: ball, pancake, dimpled-disc, gourd, longan, twin-bubble, round-pot, cherry, pitomba, bangle, torus and shell.
Naturally, some of the shapes in Figure 3.4 are very similar to each other and are not necessarily topologically different from each other. In biological terms, the pancake or dimpled-disc shape may be referred as a discocyte while the round-pot, cherry or pitomba shape are classified as a stomatocyte (mouth). These shapes have been experimentally observed. Other non-axisymmetric vesicle shapes exist as well but they are not discussed here.

Fig. 3.5. 3D views of the twin-bubble, dimpled disc, round-pot and torus

Figure 3.6 shows the overall energy landscape and the hysteresis of the solution branches. The numerical values of the energy in all figures in this section are those of $E(\phi)$ in (2.10). In the energy plots, the vertical axis corresponds to the energy and the values of the area $\beta$ are represented by the horizontal axis. The various solution branches are computed through the path following approach. When a particular solution branch loses its stability when we probe the parameter values, the numerical solution may jump
to a different branch, we record the values of the parameters at which such jumps take place. As we are solving a nonlinear problem, hysteresis phenomena are expected, that is, when the parameter goes up and down, the solution may follow different paths.

We now give detailed explanation to each of the curves in Figure 3.6. The arrows along the curves in the later energy pictures indicate the directions of the change of the area value. The reference to the color scheme may be ignored if monochrome display or printout is used.

We begin by examining the red line redrawn in Figure 3.7 (left), which is the deformation of the torus shape. The curve can be extended infinitely on both ends. The shape is stable, in the sense that if we start from the configuration on the curve, it stays on the curve when the surface area changes. There is also a vertical asymptotic limit at the left end. When the area is less than such a critical value, the shape changes and it becomes the shape of a longan (an outer sphere containing a small spherical core, this name is used to distinguish from the solution branch representing the shell shape). In Figure 3.8, we give an example to illustrate the changing of the shape.

The blue line redrawn in Figure 3.7 (right) consists of three different deformations. When the area is small (< 5.0117), the vesicle shape looks like a ball. However, the surface area in this case is too small to keep up with the volume. In reality, there is simply no solution, i.e., no corresponding geometric shape. In the phase field formulation, the solution exists due to an extension of the interface width. From the value 5.0117 to 6.9792, the vesicle changes the shape from a spherical ball to a pancake. After the value increase to 7.0004, the shape of the vesicle makes a jump to a torus (and the energy actually drops). Figure 3.9 shows such a transformation.
The green solid line, redrawn in Figure 3.10, is for the deformation of gourd shape. It is stable in both directions (with area either increasing or decreasing) in the sense that small perturbations do not drive the solution onto other branches. This green solid line coincides with the blue dash line, which appears in Figure 3.7 (right), below value 5.0117 (when they all become spherical ball), see Figure 3.11 for an illustration.

When the area is between 5.0117 to 5.1018, the energy value of the pancake is lower than the gourd. It then surpasses the later after the value 5.1018, see Figure 3.12. If we start at a ball and increase the area, it goes to a pancake and then to a torus when the area becomes large. Both solution curves, however, are stable individually (checked by the numerical simulations with the addition of small perturbations).

The Green line in Figure 3.13 indicates that the twin-bubble shape in Figure 3.4 jumps to the gourd shape when the area decreases. However, this process is not reversible: when the area of a gourd increases (Figure 3.14), it keeps on being a gourd as in Figure 3.10 (the Green line). When the area of a twin-bubble increases, it changes to a round-pot (cherry) shape and then to a shell shape. However, the energy is almost the same (even with possible small jumps) (Figure 3.15).

The dotted black line in Figure 3.16 indicates the deformation of a shell shape when the area decreases. It first leads to a bangle (with no obvious energy jump), then to a torus (with energy jump at $\beta = 6.6027$), then a longan (energy jump at around $\beta = 5.2768$) and finally to a spherical ball (energy jump at around $\beta = 5.0647$) (Figure 3.17). It overlaps with part of the red line in Figure 3.7 (left). Corresponding to each piece of the energy curve (in between the jumps), the curve is reversible, that is, the shapes can change back and forth between the jumps.
The dotted cyan curve in Figure 3.18 indicates the change of the shape of longan to a pancake (or a discocyte, a dimpled-disc), and then a torus when the area increases, as in Figure 3.19 illustrated. The energy shows (small) jumps whenever there is a topological change of the configuration.

Finally, the dotted red curve in Figure 3.20 indicates the change of the shape of cherry to a round-pot then to a pancake when the area increases, as in Figure 3.21 illustrated. The jump to the pancake shape occurs at the same value of surface area as the jump from the longan shape to the pancake depicted in the figure 3.19. Before the jump, the energy stays very close to that of the black dotted line in Figure 3.16 and is only slightly larger. One may view the two close solution branches as one with the symmetry (in the $z$ variable) and one that loses the symmetry.

Based on the above results, we see that the application of the phase field approach to the computation of $z$-axial symmetric vesicle lead to various interesting configurations that of different shapes. In Figure 3.22, we summarize the transformations between the different shapes, the arrows point to directions with increasing areas along the solution paths. Some of the configurations, to our knowledge, are obtained for the first time using the numerical simulation.

Clearly, due to the $z$-axial symmetry imposed on the solutions, we may not be able to reach from one particular configurations to all other configurations with the continuation in the area parameter. Further investigation with full three dimensional simulations is needed in order to give a complete description of the solution manifold. Nevertheless, the simulation results presented here again demonstrate the effectiveness of the phase field approach in tracking surfaces of varying topologies.
Fig. 3.6. Global energy landscape and hysteresis loops

Fig. 3.7. The change of energy for a torus shape (left) and for a spherical ball to a pancake, a dimpled-disc then to a torus (right).
Fig. 3.8. Deformation of torus with areas at: 7.4246, 6.8943, 5.8336, 5.3457, and 5.1972

Fig. 3.9. Deformation of a ball to pancakes, a dimpled-disc and then to a torus with the area valued at: 5.0275, 5.3457, 5.8336, 6.3640, 6.9791 and 7.0004

Fig. 3.10. The change of energy for the gourd shape
Fig. 3.11. Both the pancake and the gourd shrink to the same ball when the area is small.

Fig. 3.12. The energy of the pancake surpasses that of the gourd.

Fig. 3.13. The change of energy for a twin-bubble to a gourd and a shell.
Fig. 3.14. The deformation of a twin-bubble to a gourd with areas 5.8867 and 5.8761

Fig. 3.15. The deformation of a twin-bubble to a round-pot and then a shell with a fixed volume and areas of: 5.8867, 6.6928, 6.7140, 7.7322, 7.9656 and 10.6278
Fig. 3.16. Deformation of a shell shape with decreasing area

Fig. 3.17. Deformation of a shell to a bangle, a torus, a longan and finally a ball with the area valued at: 9.5459, 6.6291, 6.0988, 5.3457, 5.1972 and 5.0381

Fig. 3.18. The change of energy from longan to a pancake, and a torus.
Fig. 3.19. The deformation of a longan to a pancake and then to a torus when the volume fixed and the area valued at: 5.0912, 5.4624, 6.4170, 6.4435 and 7.0004

Fig. 3.20. The change of energy from a cherry to a round-pot, then a pancake

Fig. 3.21. The deformation of a cherry to a round-pot and then a jump to a pancake when the volume fixed and the area valued at: 7.9656, 6.4594, 6.4382
Fig. 3.22. A pictorial illustration of solution paths through various configurations.
3.4 Effect of spontaneous curvature

In the formula (1.1) of the elastic bending energy, $c_0$ is the spontaneous curvature that describes the asymmetry effect of the membrane or its environment. The consideration on the non-zero $c_0$ case here allows us to make further investigation on the membrane asymmetry effect through numerical simulations. For other numerical simulations on the effect of the spontaneous curvature, one may consult [5, 47, 53]. The spontaneous curvature $c_0$ can be a constant, it can also be variable. We first give some examples of simulation results with a constant spontaneous curvature. And then the effect of a non-constant spontaneous curvature is discussed.

3.4.1 Surfaces corresponding to constant spontaneous curvatures

As only axis-symmetric shapes are under considerations, except noted otherwise, most of the vesicles of our numerical experiments are shown by their cross-sections in the $r$-$z$ plane. The 3-d vesicles are obtained by rotating these two dimensional shapes around the $z$-axis. To create a three dimensional impression, figure 3.23 shows the cross-section views and the 3-d cutting views of two vesicle shapes obtained in the later examples. A $45^\circ$ cut is made in all 3-d views to reveal the interior of the vesicle.

Numerical convergence studies have been performed to assure the validity of the solutions. Indeed, the numerical results presented in this section correspond to simulations using different computational grids. Such different choices are explicitly stated for each simulation as the differences are necessary for maintaining the accuracy of the
Fig. 3.23. Visual illustrations of the cross-section views and full 3-d views of two vesicle shapes.

simulations. We also studied the effect of the parameter $\epsilon$, and we only present results for values of $\epsilon$ that appear to trustily characterize the sharp interface limits.

Figure 3.24 shows the deformation of a gourd shape corresponding to different values of the spontaneous curvature: $C = 0.0, 1.6, 2.0$ and $3.0$ ($C$ is in fact $\sqrt{2}$ times of the spontaneous curvature $c_0$ by our scaling). The grid used for producing this figure is a $150 \times 100$ grid where the mesh size $h = 0.02$ and $\epsilon = 0.03$ are. The two constants $\alpha = 1.10$ and $\text{beta} = 12.00$ are fixed for these shapes. We note similar solution branches produced in [5] do not allow the topological changes where the numerical experiments stopped when a thin neck forms between two components. With the phase field formulation, we are able to handle the topological events easily.

A close examination of the shapes in figure 3.24 leads to a conclusion that a larger value of spontaneous curvature tends to make the vesicle shapes approaching to surfaces with constant mean curvature such as sphere. As a single constant mean curvature surface is not always compatible with the volume and surface constraints, topological transformations thus take place and the gourd finally splits into several smaller spheres for large enough values of the spontaneous curvature. In the last picture, one of the two
bubbles is in fact almost a perfect sphere. In the next section, there are more examples for the nucleation of these kinds of smaller spheres of different radii if the spontaneous curvature is not a constant.

To further illustrate the spontaneous curvature effect, Figure 3.25 shows the deformation of the last shape in Figure 3.24 where spontaneous curvature and volume are fixed while the surface area is varying. With the surface area increasing, the ellipsoid splits into two small spheres which finally grow up to the same size with the old sphere. The grid for this figure is changed to $200 \times 50$ ($h = 0.02$), while other parameters are kept the same: $\epsilon = 0.03$, $\alpha = 1.10$.

Figure 3.26 shows the deformation of a bangle with different spontaneous curvature effect. The grid used in this figure is $200 \times 100$ with $h = 0.01$ while other parameters are chosen as $\epsilon = 0.02$, $\alpha = 1.10$ and $\beta = 14.00$. When $C$ changes from 0.0 to 0.4, there is only a minor change taking place to make the shape more sphere like. And when $C$ changes from 0.4 to 0.8, there is a more dramatic deformation and the shape changes from a bangle to a torus. After that, when $C$ increases from 0.8 to 2.8, no obvious change of the shape seems to occur. The simulation result indicates that the torus is a very
Fig. 3.25. Deformation from the last shape of Figure 3.24 by increasing the surface area ($\beta = 12.00, 12.40, 12.60, 13.40$ from left to right) with the same $C = 4.0$.

stable shape for large spontaneous curvatures. Besides the torus, in our experiments, the sphere and the ellipsoid are also very stable for large values of the spontaneous curvature.

Figure 3.27 shows the deformation of a dimpled-disk with different spontaneous curvatures. Again, the grid used for this figure is $100 \times 100$ with $h = 0.02$, while other parameters are given by $\epsilon = 0.03$, $\alpha = 1.10$ and $\beta = 13.00$. When $C$ changes from $0.0$ to $2.0$, and then later to $8.0$, the dimples start to get swelled.

Figure 3.28 shows another example of the topological changes of the surface. This corresponds to a deformation from a longan to an ellipsoid with different spontaneous curvatures. The grid used in this figure is $200 \times 100$ with $h = 0.01$, $\epsilon = 0.02$, $\alpha = 1.10$ and $\beta = 10.00$. For $C$ in between $0.0$ and $1.0$, there is no obvious change, but when $C$ goes from $1.0$ to $2.0$, the smaller sphere vanishes.

### 3.4.2 Non-constant spontaneous curvature cases

In the energy formula 2.10, we can allow the spontaneous curvature to vary in space to model the spatial inhomogeneity. We limit our consideration to the case where the spontaneous curvature is always bounded in order to make sure that the phase field function goes to a limiting profile (like the tanh function) as $\epsilon \to 0$. We note that much of
Fig. 3.26. Deformation from a bangle to a torus with different spontaneous curvatures. $C = 0.0, 0.4, 0.8$ and $2.8$ from left to right.

choices of the non-constant spontaneous curvatures are artificial but they are motivated by practical considerations, experimental results and other theoretical studies.

The numerical algorithms used to simulate the non-constant spontaneous curvature cases largely remain the same but the actual implementation is slightly more involved as the variational form of the energy may change during the solution process.

Our first numerical example is shown in figure 3.29, where we take the spontaneous curvature as

$$C = c \begin{cases} 
(1 + 2z) & \text{for} \ 0 \leq z < 2.8 \\
1 & \text{for} \ z \geq 2.8 
\end{cases}$$

This curvature only depends on the domain, not the surface itself. The grid for this figure is $150 \times 100$, $h = 0.02$, $\epsilon = 0.03$, $\alpha = 1.10$ and $\beta = 12.00$.

In figure 3.29, with $c$ increasing, the gourd splits into more and more smaller spheres. When $c$ is small, the spheres are likely to stay at positions where the spontaneous curvatures are large so that they lead to a smaller energy, as shown from the second to the fifth graphs. Since the spontaneous curvature is linearly increasing with respect to the $z$-axis, one can see the top spheres are trying to stay as high as possible which is why
we choose $C = c$ for $z \geq 2.8$. Otherwise, the spheres would move quickly up to the top of the domain. When $c$ is big enough so that the spontaneous curvature is larger than the curvatures of the spheres, things start to reverse as the spheres are likely to stay at the position with a smaller curvature, as shown in the final graph.

Figure 3.30 shows the energy and the Euler number graph of the shapes shown in Figure 3.29. The Euler numbers can be computed from the phase field models using the Gauss-Bonnet formula:

$$\int_{\Gamma} K \, ds = 2\pi \chi$$

where $K$ is the Gaussian curvature and the Euler number is $\chi/2$. For the axis-symmetric shapes, we can calculate the Gaussian curvature in terms of the phase field function $f$, and thus the Euler number can be calculated by the following general formula:

$$\frac{\chi}{2} = \int \int \frac{\partial_y f \left( \partial_r^2 \phi (\partial_z \phi)^2 + \partial_z^2 \phi (\partial_r \phi)^2 - 2 \partial_r \phi \partial_z \phi \partial_r^2 \phi \right)}{4((\partial_r \phi)^2 + (\partial_z \phi)^2)^{\frac{3}{2}}} \, dr \, dz. \quad (3.9)$$

where the integration is taken on the $r$-$z$ plane $\Omega$. 

Fig. 3.27. Deformation of a dimpled-disk with different spontaneous curvatures. $C = 0.0, 2.0, 8.0$ from left to right.
Fig. 3.28. Deformation from a longan to an ellipsoid with different spontaneous curvatures. $C = 0.0, 1.0, 2.0$ from left to right.

By taking $\phi = \tanh\left(\frac{d(x)}{\sqrt{2}\epsilon}\right) + O(\epsilon^2)$, we can further simplify (6.25) into

$$\chi = \frac{35\epsilon}{32\sqrt{2}} \int \int \partial_r \phi \left(1 - \phi^2\right) \left((1 - \phi^2) \Delta \phi + 2 \phi |\nabla \phi|^2\right) dr dz + O(\epsilon). \quad (3.10)$$

where the operators $\nabla$ and $\Delta$ are taken in the $r$-$z$ plane. One can refer to Chapter 6 for details of above formulae (6.25) and (3.10).

With the spontaneous curvature increasing, the energy first decreases and then increases with its minimum reached at $c = 0.6$. The right graph shows the Euler number of the shapes, which increase step by step from 1 to 2 then to 3 while the shape splits from one sphere into two and three spheres. The position when the energy reaches its minimum is a critical point. Beyond such a point, the shape splits into three spheres and the spheres are going to stay at positions with smaller values of the spontaneous curvature.

In general, the spontaneous curvature depends on the vesicle shape itself. Thus, in the next experiment, we consider the case where the spontaneous curvature depends on the direction of the normal vector to the surface. In this case, the energy functional
Fig. 3.29. Deformation from a gourd to several ellipse spheres with different non-constant spontaneous curvatures.

is given by

$$E(\varphi) = \int_{\Omega} \frac{1}{\epsilon} \left( \epsilon \Delta \varphi + \frac{1}{\epsilon} \varphi(1 - \varphi^2_0) + C(1 - \varphi^2)(4\epsilon^2 \varphi^2_z - 1) \right)^2 dx.$$ 

Since the phase field boundary is measured by $\sqrt{2}\epsilon$, the spontaneous curvature is in fact $c_0 = C(4\epsilon^2 \varphi^2_z - 1)/\sqrt{2}$, which is $C/\sqrt{2}$ when the normal vector is parallel to the z-axis, and it changes to $-C/\sqrt{2}$ when the normal vector is perpendicular to the z-axis.

Figure 3.31 shows the deformation of a torus corresponding to this non-constant spontaneous curvature. The grid for this figure is $200 \times 100$, $h = 0.01$, $\epsilon = 0.02$, $\alpha = 1.10$ and $\beta = 12.00$. Based on results of previous simulations, we know that the torus is very stable with a constant spontaneous curvature. If the spontaneous curvature is non-constant, it may deform into many exotic shapes. In the first row, the spontaneous curvature is positive at both the top and the bottom of the torus while it is negative at the position where the normal vector is perpendicular to the z-axis. In the second
row, the spontaneous curvature changes in the reverse direction of the first row. And the resulting behavior is very different, indicating the existence of hysteresis.

Our final experiment shows how the \textit{singular} change in spontaneous curvature affects the vesicle shapes, that is, the spontaneous curvature effect exists only at a point or a tiny part of the surface which often happens when a large molecule sticks onto a bio-membrane. Figure 3.32 shows the case where $C$ is a non-zero constant only on the surface where the points are close to the axis ($r < 0.1$). The surface bulks gradually when the spontaneous curvature increases at the top and bottom. This experiment successfully explained that lots of the cells and virus may grow bulges on their surface, and this could be from the large spontaneous curvature effects at those bulges. The grid for this figure is $200 \times 100$ with $h = 0.01$, and the parameters are $\epsilon = 0.02$, $\alpha = 0.30$ and $\beta = 4.20$. 

Fig. 3.30. The energy (left) and the Euler number (right) graphs of the shapes shown in Figure 3.29
Fig. 3.31. Deformation of a torus with different non-constant spontaneous curvatures $c_0 = C(4\epsilon^2 \varphi_z^2 - 1)/\sqrt{2}$. From left to right $C = 0.0, 5.0, 10.0, 15.0$ in the upper row and $C = 0.0, -5.0, -10.0, -15.0$ in the bottom row.

3.5 Conclusion

In this chapter, we study the static deformation of a vesicle membrane under the elastic bending energy, with prescribed bulk volume and surface area. In the case of zero spontaneous curvature, we discover several axial symmetric configurations using numerical simulations. The energetic bifurcation landscape is also examined in detail.

We also studied the effect of the spontaneous curvature. We made some analysis on how the constant spontaneous curvature affect the vesicle membrane shapes. Also, some examples of the non-constant spontaneous curvatures were also provided. The experiments provide convincing evidence on the fact that our phase field approach can effectively incorporate the spontaneous curvature effect and can handle topological changes in the deformation of membrane shapes.
The application of the phase field formulation gives us the advantage of avoiding keeping track the free interfaces. Moreover, this approach fits in existing methods developed to study the interaction of these configurations and the external applied fields, the specific species inside and surrounding the vesicle, and other surface energies (due to anisotropy). More extensive three dimensional simulations and more detailed analysis will be carried out in Chapter 4.
Chapter 4

Simulation in Three Dimensional Non-symmetrical case

4.1 Introduction

As in our previous Chapter 2, we introduce a phase function $\phi(x)$, defined on the physical (computational) domain $\Omega$, which is used to label the inside and the outside of the vesicle $\Gamma$. We visualize that the level set $\{x : \phi(x) = 0\}$ gives the membrane, while $\{x : \phi(x) > 0\}$ represents the inside of the membrane and $\{x : \phi(x) \leq 0\}$ the outside. Since this function is defined on the Eulerian reference coordinates, we do not need to follow the motion of the specific level set. While we derive the corresponding interface motion through the dynamics of this phase function $\phi$.

In this chapter, we study the minimizing problem (2.10) under the constraints of the modified volume (2.11) the modified area (2.12). These energy functionals are defined as the bulk integrals on the whole domain, rather than the surface integrals as those in (1.3) and (1.1). In Theorem 2.2, we prove that under some general ansatz (A1) and (A2),

$$\phi(x) = \tanh\left(\frac{d(x)}{\sqrt{2}\epsilon}\right) + O(\epsilon^2),$$  \hspace{1cm} (4.1)

we see that $\phi$ is approaching to the Heaviside function with 1 inside of the interface and $-1$ outside. $\Gamma$ still coincides with the zero level set of $\phi$. Moreover (4.1) indicates that
the parameter $\epsilon$ is effectively the thickness of the transition region between $\{\phi = 1\}$ and $\{\phi = -1\}$.

When we substitute the limiting profile of $\phi$ in (2.10), Theorem 2.3 tells us that this energy $E(\phi)$ will approach to the same energy as in (1.3) as $\epsilon$ approaches zero. Moreover, $A(\phi)$ goes to the difference of inside volume and outside volume and $B(\phi)$ is approaching to $2\sqrt{2} \text{area}(\Gamma)/3$, or about 0.94 times the area of $\Gamma$.

Hence we manage to transform the original problem of minimizing the bending surface energy with the prescribed surface area and bulk volume constraints into the one of finding the function $\phi = \phi(x)$ on the whole domain that minimizes the energy $E = E(\phi)$ with the constraints of prescribed values for $A$ and $B$.

Recall that in Chapter 3, we do a serial of numerical experiments in the axis-symmetrical case where we use Newton’s method for each time step. Because that is in fact a 2d problem, it does not cost too much in solving the linear system required by Newton’s method and we can optimize the time step size based on the convergence speed of Newton’s method. In this chapter, we solve this problem in truly three dimensional case. We can use the same method, but the cost in Newton’s method will increase a lot. And more than the penalty method, we also try to use the Euler Lagrange equation for solving this problem in three dimensional case.

In section 4.2, we present the phase field formulation, applying the Lagrange multipliers for the two constraints. It is slightly different approach of the penalty constrains method used in the Chapter 3. The purpose is to testing the difference and connection of these two methods. Finite different method and spectral method can all be used for
this phase field model. However, spectral method have much more advantages in implementation and accuracy for this problem. In section 4.3, we discussed the Forward Euler scheme for this problem based on the spectral method. The method for adjust the volume and surface area constrains and the time step adjustment are also discussed in this section. In section 4.4, we first show some convergence test for our method, then we made a lot of interesting experiments to show a beautiful truly 3-d vesicles world. Besides the 3-d axis-symmetrical shapes, we also show some non-axis-symmetrical vesicles. More examples are designed to illustrate how the spontaneous curvature works on a vesicle surface. Finally, we give some experiments showing the emerging and splitting of the vesicle membranes. We made some conclusion remarks and present the direction of our future work in the final section of the Chapter.

4.2 Time dependent Euler Lagrange equation

For a dynamical deformation, we look at the following gradient flow (fastest decent) equation:

$$\phi_t = -\gamma \frac{\delta E}{\delta \phi} + \lambda_1 \frac{\delta A}{\delta \phi} - \lambda_2 \frac{\delta B}{\delta \phi},$$

where the right hand side is the Euler-Lagrange equation of the modified problem. The two scalar parameter $\lambda_1$ and $\lambda_2$ are the Lagrangian multiplier for the two constraints.

For simplicity, we will take $k = 1$ and using the notation defined in (2.24), (2.25) and (2.26), we arrive at the following equation:

$$\phi_t = -\gamma g + \lambda_1 + \lambda_2 f.$$  \hspace{1cm} (4.2)
In order to derive the explicit expression of the Lagrangian multipliers $\lambda_1$ and $\lambda_2$, we start by taking the integration of the equation (4.2). Since the volume, hence the integral of $\phi$ is a constant, we have

$$\lambda_1|\Omega| + \lambda_2 \int_{\Omega} f \, dx = \gamma \int_{\Omega} g \, dx \quad (4.3)$$

Next, we take the time derivative of fixed $B(\phi)$:

$$\int_{\Omega} \epsilon \nabla \phi \cdot \nabla \phi_t + \frac{1}{\epsilon} (\phi^2 - 1) \phi \phi_t \, dx = 0$$

or equivalently,

$$\int_{\Omega} f \phi_t \, dx = 0. \quad (4.4)$$

Substitute this equation (4.2) into the equation (4.4), we have

$$\lambda_1 \int_{\Omega} f \, dx + \lambda_2 \int_{\Omega} f^2 \, dx = \gamma \int_{\Omega} fg \, dx \quad (4.5)$$

Collecting (4.2), (4.3) and (4.5) we arrive at the following closed system:

$$\begin{cases}
\frac{\partial \phi}{\partial t} + \gamma g - \lambda_1 - \lambda_2 f = 0, \\
\lambda_1|\Omega| + \lambda_2 \int_{\Omega} f \, dx - \gamma \int_{\Omega} g \, dx = 0, \\
\lambda_1 \int_{\Omega} f \, dx + \lambda_2 \int_{\Omega} f^2 \, dx - \gamma \int_{\Omega} fg \, dx = 0
\end{cases} \quad (4.6)$$

The above system, equipped with the initial values $u(x,0) = u_0(x)$, $d(x,0) = d_0(x)$ and periodic boundary condition will be used to simulate the full 3-dimension deformation
and configuration of the membranes. Here $f$ and $g$ are defined as those in (2.24) and (2.26).

Although a Dirichlet boundary condition $\phi|_{\partial \Omega} = -1$ is a more nature and physical condition, the periodic boundary condition holds when the interface $\epsilon$ is sufficient small compared with the overall physical domain $\Omega$. For a more practical reason, periodic boundary condition makes it easier to apply the Fourier transform in our numerical scheme which works much better than the general finite difference scheme.

In the case of $k = 1$, since we have

$$E(\phi)_t = \int_{\Omega} \frac{\delta E}{\delta \phi} \phi_t \, dx = \int_{\Omega} g(-\gamma g + \lambda_1 + \lambda_2 f) \, dx.$$  

Substitute the equation (4.6), we immediately derive the following energy dissipation law of the above system:

$$W_t = -\frac{1}{\gamma} \int_{\Omega} (\gamma g - \lambda_1 - \lambda_2 f)^2 \, dx. \quad (4.7)$$

We want to remark that in the problems that only the volume is conserved and the area is allow to change, we can modify the original equation (4.6) by putting $\lambda_2 = 0$ and ignore the last equation.

4.3 Numerical scheme

We use forward Euler to solve (4.6).

$$\frac{\phi_{n+1} - \phi_n}{\Delta t} = -\gamma g_n + \lambda_1(\phi_n) + \lambda_2(\phi_n)f_n$$
where \( \lambda_1 \) and \( \lambda_2 \) are functions of \( \phi \) and they are decided by the second and the third equations of (4.6).

Because of the energy law, forward Euler scheme can make sure the decreasing of the energy with sufficient small time step \( \Delta t \).

The following two subsections gives some remarks on the adjustment of the Lagrange coefficients \( \lambda_1, \lambda_2 \) and the technique used in time steps.

### 4.3.1 Lagrange coefficients adjustment

The two lagrange coefficients can be used to adjust the volume and surface area. We need to adjust the volume and surface area due to several reasons. We may preset the values but the initial shape of the vesicle may not totally satisfy the prescribed volume and surface area. Some experiments study the shape transformation of the vesicles by changing its volume or surface area. Also, although the theory value of the Lagrange coefficients \( \lambda_1, \lambda_2 \) help strictly preserving the \( A(\phi) \) and \( B(\phi) \) to be constants, due to the truncation errors in numerical experiments \( A(\phi) \) and \( B(\phi) \) are not strictly preserved and they may have slight shifts from their originally values with time going on. One technique we used here is to adjust \( \lambda_1 \) and \( \lambda_2 \) to adjust \( A(\phi) \) and \( B(\phi) \).

Now, suppose \( A_{fix} \) and \( B_{fix} \) is our desired volume and surface area respectively. And current volume \( A_n = A_{fix} + \Delta A_n \), and surface area \( B_n = B_{fix} + \Delta B_n \). We choose two positive constants \( c_1 = c_2 \leq 0.5 \) and let

\[
\frac{d}{dt}A(\phi) = -c_1 \frac{\Delta A_n}{\Delta t}
\]
and
\[ \frac{d}{dt} B(\phi) = -c_2 \frac{\Delta B_n}{\Delta t} \]

By this way, from formula (4.2), we get a repaired formula of (4.3) as
\[ \lambda_1 |\Omega| + \lambda_2 \int_{\Omega} f \, dx = \gamma \int_{\Omega} g \, dx - c_1 \frac{\Delta A_n}{\Delta t}; \quad (4.8) \]

Meanwhile, we get a repaired formula of (4.5) as
\[ \lambda_1 \int_{\Omega} f \, dx + \lambda_2 \int_{\Omega} f^2 \, dx = \gamma \int_{\Omega} f g \, dx + c_2 \frac{\Delta B_n}{\Delta t}; \quad (4.9) \]

From equations (4.8) and (4.9) we can got the adjusted \( \lambda_1 \) and \( \lambda_2 \) to make sure the volume and surface of the vesicle are strictly preserved.

The two constant \( c_1 \) and \( c_2 \) cannot be choose to be 1. If so, the adjustment of the Lagrange coefficients maybe too much, which makes the values of \( A(\phi) \) and \( B(\phi) \) vibrant and it is easy to get blow up.

In some experiments, the initial volume \( A_0 \) and surface area \( B_0 \) are much different with the preset value \( A_{fix} \) and \( B_{fix} \), which may results very large adjustments and the system is also easy to get blow up. To void this case, we need divide this experiment into several steps. For each step, we preset different values. And those preset values come from positions close to \( A_0 \) and \( B_0 \) gradually to \( A_{fix} \) and \( B_{fix} \).

Another remark is that the energy law does not strictly hold when adjust the two Lagrange coefficients, the energy function \( W(\phi) \) may be not keep strictly decreasing. One may do not care the energy law until the values of volume and surface area are close
enough to the preset values, or keeping a small time step until the energy is sensitive to adjustments. To stop the adjustment one can just simply stop the adjustment by setting \( c_1 = c_2 = 0 \).

### 4.3.2 Time step adjustment

Our time step adjustment is based on the energy law. The numerical simulation begins with a larger time step and the energy decreases very fast. As stated in previous subsection, stop the Lagrange coefficients adjustment when you need do the energy control for the time step adjustment.

The energy may not decrease for a large time step when the energy is close to a local minimum. We just simply half the time step in this case. we will continue to half it until the energy decrease. The energy law which holds in discrete case ensure its decreasing at time step small enough.

Besides the halving of the time steps, one can also try to double the time step every 10 steps.

In our numerical simulation, we think the energy reaches its local minimum when \( \| \gamma g - \lambda_1 - \lambda_2 f \|_{L_2} < 1e - 4 \) or the time step \( \Delta t < 1e - 13 \). We also would like to point out that although the time step is adjustable most of the case in our numerical experiments it belongs to the interval from \( 1e - 6 \) to \( 1e - 7 \). And when the energy reaches its minimum, the time step size decreases very quickly below \( 1e - 13 \).
4.3.3 Parallel Implementations

Parallel implementation can be done on both distributed memory systems via MPI and shared memory systems via OPENMP. In both cases, we need divide the z-axis into several groups, and each processor process the one group of them. Because the 2-D DFFTs the $x - y$ plans has no connection, it is very easy to parallel them. The difficulties exist in the case for the parallel implementation for DFFTs on z-axis. For MPI programming, we need interchange data between processors to reconstruct the data structure along the $x - y$ plans instead of the original z-axis. After finished the parallel DFFTs on z-axis, we need interchange data between processors to recover the original data distribution. It is relatively easier For OPENMP programming in this case as it uses implicit communication between processors. And we share the memory of the three dimensional array data of the phase field function. One may need add some extra space into the x-dimension because increasing the array size can help avoiding the false sharing which decrease the performance of OPENMP dramatically.

One may also use the freeware package of FFTW which provides the interfaces for parallel implementation via MPI and OPENMP. In our numerical experiments, we apply OPENMP for a shared memory system which contains 16 processors. Using the method mentioned in prior paragraph, we implement the parallel code only using the serial interface of FFTW for 1-d and 2-d DFFTs. And we get very scalable performance.
4.4 Numerical simulation

Some parameters are fixed throughout this section: $\gamma = 3.0$, the domain is the box $[-\pi, \pi]^3$ except specially indicated.

4.4.1 Initial phase field selection

Most of our numerical simulations do not have any prescribed volume and surface area. The vesicle just starts from an initial shape. In this way, we set the $A_{fix}$ and $B_{fix}$ to be $A_0$ and $B_0$. However, if the initial phase field function $\phi_0(x) \neq \tanh \left( \frac{d(x)}{\sqrt{2}\epsilon} \right)$, the initial volume and initial surface area calculated from formula (2.11) and (2.12) are very inaccurate. If starting from this kinds of initial $\phi_0$, the process may preserve two unreasonable values of the volume and the surface area. However, we can easily get a better phase field function if we let the program running for a while from that not good initial phase field function without preserving the volume and surface area. Here we only need the first equation in (4.6). By this way, the energy decreases very quickly and very soon the phase field function $\phi_0(x)$ will behaviors like $\tanh \left( \frac{d(x)}{\sqrt{2}\epsilon} \right)$. By our experience, once the energy decreases no more than one fifth of it in a time period of $1.0e - 4$, we think the $\phi_0$ is good enough to be used as an initial phase field function.

Figure 4.1 shows an example of how we get an initial phase field function. The domain is the box $[-\pi, \pi]^3$ with grid size $64 \times 64 \times 64$ and $\epsilon = 0.1736$. The vesicle is an ellipse sphere, axis-symmetric with the x, y, z axes. The top graph of figure 4.1 shows the energy curve which decreases very quickly. At the beginning, the phase field function is shown in the first graph of the second row, which is the cross-section of the x-z plan of
the phase field. Once the energy decreases no more than one fifth of it in a time period of $1.0e - 4$, we get our a good initial phase field shown in the second graph of the bottom row. The last graph is its 3-d views, one of the view has a $45^\circ$ cut along the z-axis to show the inside structure of the surface.

The last two graphs of the figure 4.1 show the computed surface and volume curves. Although the real surface of the ellipse sphere almost does not change, its value calculated by the surface formula (2.12) changes a lot from 66.38 to 45.61 in figure 4.1. And it is already good enough to use 45.61 as the vesicle’s fixed surface area.

4.4.2 Convergence verification

For a particular phase field simulation, the quality of the numerical result is affected by the choice of computational domain, the transition thickness parameter (or the effective width of the diffusive interface) $\epsilon$, the number of grid points, and the choices of other parameters used in the simulation. In this 3-d phase field simulation via FFTD, we take the domain fixed at the box $[-\pi, \pi]^3$. All of other domains can be scaled into this box. By this way, we should choose the initial membrane shapes being enclosed into this box. The parameter $\epsilon$ is taken to be just a couple of percentage points of the domain size to ensure a relatively sharp interfacial region. The mesh size is normally taken to be several times smaller than $\epsilon$ to ensure adequate spatial resolution. To ascertain the accuracy and robustness of our numerical algorithms and the parameter selections, we here present results of some numerical tests on the convergence and performance of our method.
The first example is for the same set of parameters ($\epsilon = 0.2454$, and same initial $\phi_0$ in the same domain) except the different grid sizes $40 \times 40 \times 40$ and $64 \times 64 \times 64$ respectively.

The final 3-d shape is shown in the top figure 4.2. This is a shape with the same cross-section of x-y plan. To compare in detail, the second row gives the density plots of the cross-sections. The first graph is the cross-section of the initial $\phi_0$. With time going on, the same initial $\phi_0$ makes the shapes in two different mesh size keep at the almost same volume (-120.12 and -120.03) and surface area (90.61 and 90.57). The second graph and the third graph are the final results for grid $40 \times 40 \times 40$ and $64 \times 64 \times 64$ respectively. Moreover, their final energy valued at 45.23 ($t = 0.1864$) and 45.17 ($t = 0.1634$) respectively. The last row of the figure 4.2 shows the energy plots. The energy decreases almost to the same values for two different grid size. The energy is keeping decreasing slower and slower. After the energy decreasing speed slower than a number, we stop the calculation.

The second experiment is designed to test the dependence of the parameter $\epsilon$ which measure the thickness of the layer thickness. In this experiment, the shape is the same as the above experiment with $64 \times 64 \times 64$ grid but decrease the $\epsilon$ from 0.2464 to 0.1736.

The two shapes are almost the same except the boundary layer width. And the corresponding final energy values 43.26 ($t = 0.2050$) and 45.17 ($t = 0.1634$) are very close to each other.

The convergence can also be proved by the two Lagrange multipliers $\lambda_1$ and $\lambda_2$. Figure 4.4 shows the their plots. The first graph is for $40 \times 40 \times 40$ grid with
\( \epsilon = 0.2464 \); the second graph is for 64 \( \times \) 64 \( \times \) 64 grid with \( \epsilon = 0.2464 \); the last graph is for 64 \( \times \) 64 \( \times \) 64 grid with \( \epsilon = 0.1736 \). The two Lagrange multipliers converge very fast for all these three conditions. And the converged values \( \lambda_1 = -1.31, -1.31, -1.23 \) and \( \lambda_2 = -1.84, -1.87, -2.07 \) are also very closed to each other.

Another experiment is designed to test the convergence due to different time step sizes. In this experiment, Forward Euler scheme is applied to three vesicles starting from the same initial shape with different time step sizes, \( 2.5 \times 10^{-7} \), \( 1.25 \times 10^{-7} \) and \( 6 \times 10^{-8} \). There is no coefficient adjustment in this process. Due to the time discretization, the volume and surface area may slightly change.

The initial shape shown in the first tow of Figure (4.5) is a non axisymmetric torus got after the initial shape adjustment from an artificially designed torus. All there vesicles are running for a time period till \( t = 0.215 \). The values of energy are dropped from \( 49.119952 \) to \( 39.179532 \), \( 39.179536 \), \( 39.179542 \) respectively. The difference between them is less than \( 10^{-5} \) while the running steps are \( 8.6 \times 10^5 \), \( 1.72 \times 10^6 \) and \( 3.58 \times 10^6 \) respectively. Compare to the decreasing energy values, the volume and surface area values are preserved excellently. All the volume values are strictly preserved at \(-194.486373\), never changed. The surface area values changed from \( 46.068421 \) to \( 46.068457 \), \( 46.068439 \) and \( 46.068430 \) respectively. The changing of the surface area value is below \( 3.0 \times 10^{-5} \).

As the errors are so small, we can say that the final results are independent with the time step sizes while strictly preserving the values of volume and surface area. The shapes at time \( t = 0.215 \) and energy plots for three vesicles are exactly the same. The second row in Figure (4.5) shows the final vesicle shape and its cross section, the bottom picture gives the energy plot.
To summarize, the above numerical tests indicate that the simulation of the phase field model can indeed give convergence numerical solutions. Moreover, as our above experimental results indicate, the choices of various parameter values used in the simulations are capable of ensuring the convergence of the numerical scheme and ensuring the validity of the simulation results when we predict the vesicle shapes.

4.4.3 3-D numerical experiments

In this section, we will first compare some results with those we got in the axisymmetric condition. Then we will give some interesting true 3-d non-symmetric vesicle shapes. All of these experiments are given either for zero spontaneous curvature case or non-zero spontaneous curvature case.

4.4.3.1 Axis-symmetric cases

In this section we compare some results in axis-symmetric cases. We can confirm the existence of most shapes we got in 3d axis-symmetric cases can exists in freely 3-d condition.

Figure 4.6 shows a pancake shape and gourd shape vesicles got in freely 3-d condition.

In this experiment, the pancake is transformed from a ellipse shape which is a ellipse in $x - z$ plan and disc in $x - y$ plan. The flatter the ellipse is, the more pinch the final pancake will have. And for a flat enough initial ellipse shape, the final pancake will pinch off to a torus. This transformation is shown in Figure 4.7
Another experiment is shown in Figure 4.8. It begins with a pot-like shape, with initial volume $-207.48$ and surface area 52.04 shown in the upper picture. By preserving the initial volume and surface area, it finally transforms to be a skull, shown in the left bottom picture; with a smaller preset surface area 45.06 and 48.30, it will transform to be a round pot like shapes, shown in the right bottom pictures. This experiment is done with no spontaneous curvature.

4.4.3.2 Symmetric torus and non-symmetric torus

In our experiments, we find most non-symmetric shapes will finally comes to be a symmetric shapes in equilibrium state. For example, a nonsymmetric torus starts as an initial shape shown in the first graph in Figure 4.9 will finally comes to be a symmetric torus shown in the third graph in Figure 4.9. In this experiment, the volume always keeps at value $-211.43$, and the surface area keeps at 41.59.

However, Figure 4.10 shows another example that nonsymmetric torus in equilibrium state does exist. The bottom row shows that the radius of the two circles are much different, and the radius of the hole at the center of the torus is very small which makes this torus has no room to change to a symmetric torus, because a symmetric torus has a smaller hole than a non-symmetric torus which is shown in Figure 4.9.

4.4.3.3 Non-zero spontaneous curvature cases

In this section, we gives some examples to show how spontaneous curvature works on the shapes of a vesicle.
The gourd vesicle in Figure 4.6 is got with no spontaneous curvature. If give the initial shape a spontaneous curvature valued at 3.00, the gourd shape will finally spit into 3 smaller sphere like vesicles. This transformation is shown in Figure 4.11.

Figure 4.12 shows how the spontaneous curvature on some points effects the shapes of a surface. The upper row shows the transformation of a disk. With a spontaneous curvature on its top and bottom, the surface at these two points bulks up. The bottom row shows the results of the transformation of a sphere with spontaneous curvature at eight directions. We note that the initial shapes are ellipse, so that there is room for the surface to grow up.

4.4.3.4 Constraint self-assembly

The self-assembly in the mixture of different species are determined by the competition of the phobic and philic interaction between them. This competition can be reflected in the presence of the corresponding terms (sometimes implicitly) in the phase field formulation.

However, the final configuration can also be affected by the geometric or chemical configuration of the real molecules. Worm like micellar fluids (see [18, 2] and their references) can be a good example. A micelle is formed when a variety of molecules such as soaps, shampoos and detergents) are added to water. The molecule may be a fatty acid, phospholipids, or other similar molecules. The molecule has a strongly polar end and a non-polar hydrocarbon chain end. When this type of molecule is added to water, the non-polar hydrophobic tails of the molecules clump into the center of the concentration. The polar, hydrophilic head of the molecule will be associated with the
water molecules on the outside of the micelle. The geometric shape and the size of the micelle are determined by the combination of the philic/phobic competition and the size of the molecule.

There are many such examples [18]. In the diblock polymers, the overall molecule sizes (length) are fixed [29]. This is also true in the case of the lipid membrane [48] and the surfactant monolayers. The lipid size (hence the membrane thickness) is fixed. The extra constraint will dramatically change the phase separation process and overall properties of the mixtures.

In view of these considerations, we want to present the prototype example that will show the transition from the presence of small drops to the presence of filaments and then to the membrane sheet, all with the fixed (constraint) length (the radius in the sphere and the filament, the thickness of the membrane). In practice, we impose such constraint by adding the constraint between the different quantities, such as volume to area.

Here we gives some examples to show how several small vesicles merger together.

In the left group pictures in Figure 4.13 three spheres merge into a torus. In the beginning, the three same sized spheres are arranged as a triangle, and they are closed to each other. Although sphere is an equilibrium state for a vesicle, merging together can result a smaller elastic bending energy. They first touch together; then they merged to a triangle like torus; finally this triangle like torus deformed to a round normal torus. In this experiment, the volume always keeps at value $-222.51$, the surface area keeps at 31.94, and $\epsilon = 2h = 0.1964$. 
The right five pictures in Figure 4.13 shows six spheres merge into a cylinder. In fact, as period boundary condition applied, you may consider these pictures show numerous spheres merges into a cylinder by extend the pictures periodically up and down. Please noticed that in the beginning those spheres are not aligned in a straight line and the final result is a straight cylinder. In this experiment, the volume always keeps at value $-232.18$, the surface area keeps at $22.34$, and $\epsilon = 2h = 0.1964$.

When we change the boundary condition, we achieve the formation of the membrane.

Figure 4.14 starts from eight spheres whose initial positions are symmetric with respect to the center of the domain. Although they are not in a plan, they merge together and gradually form a round disk. In this experiment, the volume always keeps at value $-235.82$, the surface area keeps at $26.90$, and $\epsilon = 1.25h = 0.1227$.

Figure 4.15 starts from nine spheres aligned on a plan. Because we use period boundary condition, one can think that numerous spheres are aligned regularly on a plan. As they are close to each other, they merge together while preserving the total volume (-185.70) and surface area (83.68). Because the surface area is larger than the area of two flat surfaces $(2(2\phi)^2 \approx 78.96)$, the surface can not be flat. It finally grows some pumps with holes on it. In the bottom line of Figure 4.15, we move the pump to the center of the image and give its cut view which shows a very special topological structure. In this experiment, the $\epsilon = 1.768h = 0.1736$. We get the same structure from some perturbation experiments by changing the $\epsilon$ from $1.768h$ to $1.5h$ and changing the surface area from 83.68 to 87.00, which shows that this special structure is
The Euler number we calculated by the method introduced in the following section 4.4.4 is 8.10.

### 4.4.4 Euler number

The Euler number is used to detect any topological change in this process [21]. Let the $3 \times 3$ matrix

$$M(x) = \frac{1}{2\sqrt{\pi(a - b)|\nabla \phi|}} \left( \nabla^2 \phi - \frac{\nabla|\nabla \phi|^2 \cdot \nabla \phi}{2|\nabla \phi|^4} \nabla_i \phi \nabla_j \phi \right), \quad (4.10)$$

where we choose $a = 0.5$ and $b = -0.5$; and let $F$ denote the coefficient of the linear term of the characteristic polynomial of $M$. If $M = (m_{ij}); i, j = 1, 2, 3$, then

$$F = m_{11}m_{22} + m_{11}m_{33} + m_{22}m_{33} - m^2_{12} - m^2_{13} - m^2_{23}$$

The Euler number is calculated by

$$\frac{\chi}{2} = \int_{b \leq \phi(x) \leq a} F(x) \, dx. \quad (4.11)$$

Here we give an example on how to use formula (4.11) to detect the topological change. In the top two row pictures of Figure 4.16, a set of five sphere-like vesicles are randomly arranged closely to each other. As time going on, those vesicles merge together one by one and finally come to be a torus. The change of the Euler number in this experiment is shown in bottom picture of Figure 4.16. It shows that the Euler number decreases from 5 to 0 step by step. One can also observe some fractional Euler numbers.
before the completion of each merge. It shows the deduction of the self-intersections of the membrane. The final shape in the second row is not a vesicles already reaches its equilibrium state. This experiment is to show how we detect the topological changes using the technique introduced in Chapter 6.

4.5 Conclusion

In this chapter, we present our numerical scheme in studying the deformation of a three dimensional vesicle membrane under the elastic bending energy, with prescribed bulk volume and surface area. Different with the numerical methods using in Chapter 3, we employ a phase field formulation with the Lagrange multipliers for the constrains in the preserving the volume and surface area, as well as the geometric constraints for the molecule sizes. In the implementation, we use a Forward Euler scheme and its effects are discussed. We present several interesting experiments are given to illustrate the transformation of the vesicle shapes. The results verified our earlier attempts for the axial-symmetric configurations, as well as the new cases for the presence of the spontaneous curvatures. Finally, the examples were tested to capture the geometric-constraint self-assembly and configurations.

The three dimensional numerical simulations build us a basis for more extensive simulation of vesicle membranes within fluid fields. In the next chapter, we couple the phase field transformation with the fluid dynamics.
Fig. 4.1. Initial phase field selection: Energy graph (top); starting phase field (left most at the second row); finally selected phase field (second at the second row) and its 3d view (last two graphs of the second row); the surface and the volume curves are shown in the bottom row.
Fig. 4.2. Different grid size compare: The 3-d view is at the top. The second row shows the cross-section of x-y plan of the initial phase field $\phi_0$, the final phase field of grid $40 \times 40 \times 40$ and $64 \times 64 \times 64$ respectively. The last row shows the energy plots of these two different grids respectively.
Fig. 4.3. Different $\epsilon$ size compare for the same grid size $64 \times 64 \times 64$. The first row shows the cross-section of x-y plan of the shapes with two different layer width. The second row shows the energy plots. In both rows, the left graph is for the $\epsilon = 0.1736$ and the right graph is for $\epsilon = 0.2464$.

Fig. 4.4. Lagrange multipliers $\lambda_1$ and $\lambda_2$ plots for different grid sizes and different $\epsilon$ values.
Fig. 4.5. Test convergence for different time steps. First row is the initial vesicle and its cross section; second row is the vesicle at time $t = 0.215$ and its cross section; energy plot is the bottom picture.

Fig. 4.6. A pancake shape (up) and a gourd shape (bottom) vesicles are got in freely 3-d condition. The left graphs are their initial shapes.
Fig. 4.7. A flat ellipse shape vesicle pinch off to a torus.

Fig. 4.8. Top left picture is the start vesicle. With a larger preset surface area, it will transform to a skull, shown in the top right picture; with a smaller preset surface area, it will transform to be a round pot like shape, shown in the bottom pictures (the left picture has a surface area 45.6 and the right one is 48.30).
Fig. 4.9. A nonsymmetric torus coming to be a symmetric torus.

Fig. 4.10. An example of nonsymmetric torus. Top: the starting shape (left) and the final nonsymmetric shape (right); Bottom: the cross sections in x-z plan of the two shapes in the first row.
Fig. 4.11. A gourd split into three same sized sphere like vesicles with spontaneous curvature 3.00.

Fig. 4.12. Spontaneous curvature on some points bulks the surface. Left, the initial shapes. Right the equilibrium shapes.
Fig. 4.13. In the left group, from up to bottom, three spheres merge into a torus. The six spheres in the right group merge into a cylinder.

Fig. 4.14. Eight spheres merge into a disk. In the beginning, those eight spheres are not in a plan but they are symmetric with respect to the center of the domain.
Fig. 4.15. Nine spheres merge into a membrane with pump and holes. Bottom: the final shape and its cut view after moving the pump to the center of the image.
Fig. 4.16. The Euler number comes from 5 to 0 step by step as the five vesicles in the first two rows merge together one by one.
Chapter 5

Fluid Coupled System

5.1 Introduction

From Chapter 2 to Chapter 4, we build the theory for studying the equilibrium vesicle shapes within the phase field framework by minimizing the elastic bending energy with fixed volume and surface area constraints. Most of time, vesicles are small tenuous objects fluctuating in fluid fields, such as the blood cells. In this chapter, we present the theory of fluid coupled system and its numerical simulations. Our phase field model based on an energetic formulation. This is an important advantage makes us capable to easily incorporate with other energy form to deduce models describing some complex phenomena of vesicle membranes.

In section 5.2, we couple the elastic bending energy together with the energy of fluid field. And by the variation of the elastic bending energy, we set up the fluid momentum equation. Within the fluid fields, the constraints still hold. For the two constrains, we can still use the penalty formulation or the Euler Lagrange formulation. In the coupled system, if we ignore the effect of the fluids, we will recover the systems for calculating the equilibrium vesicle shapes used in Chapter 3 and Chapter 4.

And the vesicle membrane is transported due to the fluid. On the other hand, the vesicle membrane will give a stress to the fluids. In general, this stress only happens on the surface. Within the framework of phase field formulation, it is easy to formulate
the extra stress term. An important issue here is to verify the consistency of the extra stress term in our phase field model to that in the sharp interface model. This is given in section 5.3.

The numerical schemes for the phase field transformation and the fluid Navier-Stokes equation are discussed in section 5.4. Energy laws play the key role in design the scheme for phase field transformation. Finally in section 5.6, we give a lot of transformations of vesicle membranes in fluid fields to verify our methods.

5.2 Fluid coupled systems

To simulate the movement and transformation of vesicles in fluid fields, we need to couple the motion of the fluids together with the transformation of the phase field function. For the fluid system part, we can use the impressible Navier Stokes equation; for the shape transformation, we can use either Allen-Cahn or Cahn-Hilliar dynamics.

5.2.1 Penalty formulation

The phase field formulation is to minimize the elastic bending energy \( E(\phi) \) defined in (2.10) with the value of \( A(\phi) \) in (2.11) fixed to be \( \alpha \) and \( B(\phi) \) in (2.12) fixed to be \( \beta \). As illustrated in Chapter 3 and Chapter 4, we can use either penalty formulation or the Euler Lagrange formulation for the two constraints. In stead of the Lagrange multipliers, first we use two penalty constants \( M_1, M_2 \) to get a modified Elastic bending energy

\[
E_M(\phi) = E(\phi) + \frac{1}{2} M_1 (A(\phi) - \alpha)^2 + \frac{1}{2} M_2 (B(\phi) - \beta)^2.
\] (5.1)
For the equilibrium system, Theorem 2.6 tells that as the penalty constants $M_1$, $M_2$ approach to infinity, the dynamic of $E_M(\phi)$ approaches to the dynamic of $E(\phi)$ with the given constraints. We start form the penalty constrained energy $E_M(\phi)$ to deduce the Allen-Cahn equation for phase transformation:

$$
\phi_t = -\gamma \frac{\delta E_M(\phi)}{\delta \phi} = -\gamma \left( \frac{\delta E(\phi)}{\delta \phi} + M_1 \left( A(\phi) - \alpha \right) \frac{\delta A(\phi)}{\delta \phi} + M_2 \left( B(\phi) - \beta \right) \frac{\delta B(\phi)}{\delta \phi} \right)
$$

where $\gamma > 0$ is a constant describing a time scale. Using the notation defined in (2.24), (2.25) and (2.26), we have

$$
E = \int_\Omega \frac{k}{2c} \phi^2 dx, \quad \frac{\delta E}{\delta \phi} = kg \quad \text{and further}
$$

$$
\phi_t = -\gamma (kg + M_1 (A - \alpha) + M_2 f (B - \beta)).
$$

Adding the transport of fluid fields $u$, we have

$$
\phi_t + (u \cdot \nabla) \phi = -\gamma (kg + M_1 (A - \alpha) + M_2 f (B - \beta)). \quad (5.2)
$$

Now, let’s turn to the N-S equation. Here we consider the incompressible fluids. We need deduce an extra stress caused by the vesicle membrane in the momentum equation follows from a variation of the domain.

Let $x(s) : \Omega \times [0, \infty) \rightarrow \Omega$ be a diffeomorphism with

$$
x(0) = \text{id}, \ x'(0) = y, \ \nabla x(0) = I, \ \text{and} \ \nabla x = F.
$$
Consider the variation of $\phi$ by transforming its argument with $x(s)$, i.e. let $\tilde{\phi}(s, X) = \phi(x(s, X))$, or $\phi(s, x) = \tilde{\phi}(X(s, x))$ where $X$ and $x$ are the original and transformed coordinates respectively. And $X'(0) = -y$. Denote by $\delta$ the operator $\frac{d}{ds}|_{s=0}$. Then a few applications of the chain-rule will give

\[
\delta \phi = -\nabla_i \tilde{\phi} y_i = -\nabla_i \phi y_i,
\]
\[
\delta \nabla_i \phi = -\nabla_i \nabla_k \phi y_k - \nabla_j \phi \nabla_i y_j,
\]
\[
\delta \Delta \phi = -\nabla_l \Delta \phi y_l - 2\nabla_i \nabla_j \phi \nabla_i y_j - \nabla_j \phi \Delta y_j.
\]

Since

\[
\frac{\delta E_M}{\delta \phi} = kg + M_1(A - \alpha) + M_2 f(B - \beta)
\]

So finally

\[
\delta E_M(\phi) = \int_{\Omega} \frac{\delta E_M}{\delta \phi} \delta \phi \, dx = \int_{\Omega} \left( -kg + M_1(A - \alpha) + M_2 f(B - \beta) \right) \nabla \phi \cdot y \, dx
\]

Thus the momentum equation for fluid is

\[
u_t + u \cdot \nabla u + \nabla p - \nu \Delta u - (kg + M_1(A - \alpha) + M_2 f(B - \beta)) \nabla \phi = 0 \quad (5.3)
\]

Notice that the term $M_1(A - \alpha) \nabla \phi$ can be combined with pressure term, thus the momentum equation can also be written as

\[
u_t + u \cdot \nabla u + \nabla p - \nu \Delta u - (kg + M_2 f(B - \beta)) \nabla \phi = 0 \quad (5.4)
\]
Collecting (5.2) together with (5.3), we have the 3-d bubble equations in Newtonian fluid here

\[
\begin{align*}
\frac{\partial u}{\partial t} + (u \cdot \nabla) u - \nu \Delta u + \nabla p - (kg + M_1(A - \alpha) + M_2 f(B - \beta)) \nabla \phi &= 0, \\
\phi_t + (u \cdot \nabla) \phi + \gamma (kg + M_1(A - \alpha) + M_2 f(B - \beta)) &= 0 \\
\nabla \cdot u &= 0,
\end{align*}
\]

(5.5)

with the initial values \( u(x, 0) = u_0(x), \phi(x, 0) = \phi_0(x) \) and periodic or Dirichlet boundary conditions. Here \( k \) is the bending rigidity, \( f \) is defined in (2.24) and \( g \) is defined in (2.26).

For the problem only preserving the volume, it is easy to modify the equation of (5.5) by setting \( M_2 = 0 \).

Now we can deduce the energy law for this system. From the first equation of (5.5), we have

\[
\frac{d}{dt} \int_{\Omega} \frac{1}{2} |u|^2 \, dx = -\int_{\Omega} \nu |\nabla u|^2 \, dx + \int_{\Omega} (kg + M_1(A - \alpha) + M_2 f(B - \beta)) u \cdot \nabla \phi \, dx
\]

From the second equation of (5.5), we have

\[
\frac{d}{dt} E_M(\phi) = \int_{\Omega} \frac{\delta E_M}{\delta \phi} \phi_t \, dx = -\gamma \int_{\Omega} (kg + M_1(A - \alpha) + M_2 f(B - \beta))^2 \, dx
\]

\[
-\int_{\Omega} \frac{\delta E_M}{\delta \phi} \nabla \phi \, dx
\]

Add the above two equations together, we have the following basic energy law

\[
\frac{d}{dt} \left( \int_{\Omega} \frac{1}{2} |u|^2 \, dx + E_M(\phi) \right) = -\int_{\Omega} \nu |\nabla u|^2 + \gamma (kg + M_1(A - \alpha) + M_2 f(B - \beta))^2 \, dx . \quad (5.6)
\]
5.2.2 Euler Lagrange formulation

Instead of using the penalty coefficients $M_1$ and $M_2$, we can directly use the two Lagrange multipliers $\lambda_1$ and $\lambda_2$ to model this system. Now,

$$\phi_t + (u \cdot \nabla)\phi = -\gamma\left(\frac{\delta E}{\delta \phi} + \lambda_1 \frac{\delta A}{\delta \phi} + \lambda_2 \frac{\delta B}{\delta \phi}\right) = -\gamma(kg + \lambda_1 + \lambda_2 f). \quad (5.7)$$

From $A(\phi)_t = B(\phi)_t = 0$, we have

$$\lambda_1 |\Omega| + \lambda_2 \int_\Omega f \, dx + k \int_\Omega g \, dx = 0 \quad (5.8)$$

and

$$\lambda_1 \int_\Omega f_c \, dx + \lambda_2 \int_\Omega f_c f \, dx + k \int_\Omega f_c g \, dx + \frac{1}{\gamma} \int_\Omega f_c (u \cdot \nabla)\phi \, dx = 0. \quad (5.9)$$

where $f_c$ is defined in (2.25). Similar to the penalty constraints, the extra stress caused by a vesicle membrane is

$$\left(\frac{\delta E}{\delta \phi} + \lambda_1 \frac{\delta A}{\delta \phi} + \lambda_2 \frac{\delta B}{\delta \phi}\right) \nabla \phi = (kg + \lambda_1 + \lambda_2 f) \nabla \phi$$

and the momentum equation is

$$u_t + u \cdot \nabla u + \nabla p = \nu \Delta u + (kg + \lambda_1 + \lambda_2 f) \nabla \phi. \quad (5.10)$$
Collecting (5.7), (5.8), (5.9), together with (5.10), we have the 3-d bubble equations in Newtonian fluid here

\[
\begin{align*}
\frac{\partial u}{\partial t} + (u \cdot \nabla) u - \nu \Delta u + \nabla p - (kg + \lambda_1 + \lambda_2 f) \nabla \phi &= 0, \\
\nabla \cdot u &= 0, \\
\frac{\partial \phi}{\partial t} + (u \cdot \nabla) \phi + \gamma (kg + \lambda_1 + \lambda_2 f) &= 0, \\
\lambda_1 |\Omega| + \lambda_2 \int_{\Omega} f \, dx + \int_{\Omega} g \, dx &= 0, \\
\lambda_1 \int_{\Omega} f_c \, dx + \lambda_2 \int_{\Omega} f_c f \, dx + k \int_{\Omega} f_c g \, dx + \frac{1}{\gamma} \int_{\Omega} f_c (u \cdot \nabla) \phi \, dx &= 0
\end{align*}
\]

(5.11)

Comparing systems (5.5) and (5.11), we see

\[
\lambda_1 \approx M_1 (A(\phi) - \alpha), \quad \lambda_2 \approx M_2 (B(\phi) - \beta).
\]

(5.12)

The energy law for (5.11) is the same

\[
\frac{d}{dt} \left( \int_{\Omega} \frac{1}{2} |u|^2 \, dx + E(\phi) \right) = - \int_{\Omega} \nu |\nabla u|^2 + \gamma (kg + \lambda_1 + \lambda_2 f)^2 \, dx.
\]

(5.13)

### 5.2.3 Equilibrium systems

By setting the fluid velocity to be zero, we can get the corresponding two systems for equilibrium systems, one with penalty constants, another one with Lagrange multipliers. And we get the equilibrium state as $t \to \infty$. The one with penalty constants is

\[
\phi_t = -\gamma (kg + M_1 (A - \alpha) + M_2 f (B - \beta));
\]

(5.14)
with energy law

$$\frac{d}{dt}E_M(\phi) = -\int_\Omega \gamma(kg + M_1(A - \alpha) + M_2 f(B - \beta))^2 \, dx.$$  \hfill (5.15)

The one with Lagrange multipliers is

$$\left\{ \begin{aligned}
\frac{\partial \phi}{\partial t} + \gamma(kg + \lambda_1 + \lambda_2 f) &= 0, \\
\lambda_1 |\Omega| + \lambda_2 \int_\Omega f \, dx + \int_\Omega g \, dx &= 0, \\
\lambda_1 \int_\Omega f_c \, dx + \lambda_2 \int_\Omega f_c f \, dx + k \int_\Omega f_c g \, dx &= 0
\end{aligned} \right.$$  \hfill (5.16)

with energy law

$$\frac{d}{dt}E(\phi) = -\int_\Omega \gamma(kg + \lambda_1 + \lambda_2 f)^2 \, dx.$$  \hfill (5.17)

5.3 Asymptotic limits

In section 2.4, we get the asymptotic limit in Theorem 2.2 rigorously for equilibrium system under ansatz (A1) and (A2).

In fluid coupled system, we have the energy laws (5.6) and (5.13) to ensure the elastic bending energy $E(\phi)$ is uniformly bounded. And we have the following theorem
about asymptotic limit under a similar ansatz:

\[(B1) \quad \phi_\epsilon(x, t) = q(d(x, \Gamma_\epsilon(t))/\epsilon, t) + \epsilon h(x, t) + g(x, t) \text{ where } q(\cdot, t) \in C^2(\mathbb{R}) \]

and \( h(\cdot, t) \in C^2(\Omega) \), both independent of \( \epsilon \), and \( \|\nabla^k g(\cdot, t)\|_{L^\infty} = o(\epsilon) \)
for \( k = 0, \ldots, 4 \).

\[(B2) \quad \text{For fixed } t, \{\Gamma_\epsilon(t)\}_{\epsilon \geq 0} \text{ is a family of uniformly smooth, compact} \]

surfaces converging to \( \Gamma_0(t) \).

**Theorem 5.1.** Suppose the fluid coupled system (5.5) or (5.11) has a solution \( \phi_\epsilon(x, t) = q(d(x, \Gamma_\epsilon(t))/\epsilon, t) + \epsilon h(x, t) + g(x, t) \) satisfying (B1) and (B2). Then \( q(\cdot) = \tanh(\cdot/\sqrt{2}) \)
and \( h = 0 \)

**Proof.** From lemma 2.3, at time \( t = 0 \), the energy \( E(\phi_\epsilon) \) is uniformly bounded for all \( \epsilon \) small enough. By Energy law (5.6) or (5.13), at any time \( t \), \( E(\phi_\epsilon) \) is uniformly bounded for all \( \epsilon \) small enough. The rest of proof is similar to the proof of Theorem 2.2 for fixed time \( t \).

Under a more restrictive assumption than (B1):

\[(B1a) \quad \phi_\epsilon(x, t) = q(d(x, \Gamma_\epsilon(t))/\epsilon, t) + \epsilon h(x, t) \text{ where } q(\cdot, t) \in C^2(\mathbb{R}) \]

and \( h(\cdot, t) \in C^2(\Omega) \), both independent of \( \epsilon \).

We have the following corollary.
Corollary 5.1. If the solution of the fluid coupled system (5.5) or (5.11) satisfies (B1a) and (B2), then \( \phi(x, t) = q(d(x, \Gamma(t))/\epsilon) \) where \( q(\cdot) = \tanh(\cdot/\sqrt{2}) \).

With this corollary, we have the following lemma.

Lemma 5.1. If the fluid coupled system (5.5) or (5.11) satisfies (B1a) and (B2) with solution \( \phi \), then

\[
\begin{align*}
 f &= -\epsilon \Delta \phi + \frac{1}{\epsilon} (\phi^2 - 1) \phi = -q' \Delta d \\
 f_c &= f + C(\phi^2 - 1) = -q' \Delta d + C(q^2 - 1) \\
 g &= -\Delta f_c + \frac{1}{\epsilon^2} (3\phi^2 + 2C\epsilon \phi - 1) f_c \\
 &= -\Delta f + \frac{1}{\epsilon^2} (3\phi^2 - 1) f - \Delta(C(\phi^2 - 1)) + \frac{2C}{\epsilon} \phi f_c + \frac{C}{\epsilon^2} (3\phi^2 - 1)(\phi^2 - 1) \\
 &= q' \Delta^2 d + \frac{1}{\epsilon} q''((\Delta d)^2 + 2\nabla d \nabla \Delta d) - \frac{2}{\epsilon} Cqq' \Delta d + \frac{2}{\epsilon} C^2 q(q^2 - 1) \\
 &\quad - (q^2 - 1) \Delta C - \frac{4}{\epsilon} qq' \nabla C \nabla d.
\end{align*}
\]

We can also take

\[
g_0 = q' \Delta^2 d + \frac{1}{\epsilon} q''((\Delta d)^2 + 2\nabla d \nabla \Delta d) \tag{5.18}
\]

which is \( g \) when the spontaneous curvature is zero. Now we denote \( V_{\text{div}} \) is the subspace of \( V = (H_0^1(\Omega))^3 \) of divergence-free functions. Now, we consider the splitting of the
gradient operator into its normal \((\bar{n}(\bar{n} \cdot \nabla))\) and surface \((\nabla_{\Gamma})\) components;

\[
\nabla_{\Gamma} = \nabla - \bar{n}(\bar{n} \cdot \nabla),
\]

\[
\Delta_{\Gamma} = \nabla_{\Gamma} \cdot \nabla_{\Gamma} = \Delta + 2H\bar{n} \cdot \nabla - \bar{n}\bar{n} : \nabla^2.
\] (5.20)

The reader should also note that \(n_i \nabla_i n_k = n_i \nabla_k n_i = 0\) because \(n = -\nabla d\), \(|n| = 1\). Some useful identities are

\[
\Delta d = -2H,
\] (5.21)

\[
H^2 - K = \frac{1}{2} (\nabla^2 d : \nabla^2 d) - \frac{1}{4} (\Delta d)^2.
\] (5.22)

and the following lemma.

**Lemma 5.2.**

\[
\Delta_{\Gamma} H = -\frac{1}{2} (\Delta^2 d - \nabla \cdot (\nabla d \nabla d \cdot \nabla \Delta d)).
\] (5.23)

*Proof.* Using identities (5.21) and (5.20),

\[
\Delta^2 d = -2\Delta H = -2\Delta_{\Gamma} H - 4Hn_k \nabla^k H + 2n_i n_k \nabla^i \nabla^k H
\]

\[
= -2\Delta_{\Gamma} H + 2\nabla^i n_i n_k \nabla^k H + 2n_i n_k \nabla^i \nabla^k H
\]

\[
= -2\Delta_{\Gamma} H + 2\nabla^i (n_i n_k \nabla^k H)
\]

\[
= -2\Delta_{\Gamma} H + \nabla \cdot (\nabla d \nabla d \cdot \nabla \Delta d).
\]

The following is a geometric lemma.
Lemma 5.3. Let $\Gamma$ be a compact surface embedding in $\mathbb{R}^3$, $\phi$ is a function defined on $\mathbb{R}^3$, and vector $v$ is defined in $\mathbb{R}^3$ and decomposed by $v = v_\Gamma + v_n\vec{n}$ where $v_\Gamma$ is the tangential vector and $v_n$ is the normal component. We have the following surface integration by parts,

$$\int_\Gamma \phi \nabla v_\Gamma \, dS + \int_\Gamma \nabla \phi \cdot v_\Gamma \, dS = 0 \quad (5.24)$$

Proof. Taking a parallel surface $\Gamma_d$ with a uniform distance $d$ to $\Gamma$. And denote the space between $\Gamma_d$ and $\Gamma$ by $\Omega_d$. We have the following equation

$$\int_{\Omega_d} \phi \nabla \cdot v \, dx = -\int_{\Omega_d} \nabla \phi \cdot v \, dx + \int_{\Gamma_d} \phi v_n \, dS - \int_{\Gamma} \phi v_n \, dS$$

Divide by $d$ and take limit as $d \to 0$ we have

$$\int_\Gamma \phi \nabla \cdot v \, dS + \int_\Gamma \nabla \phi \cdot v \, dS = \lim_{d \to 0} \frac{1}{d} \left( \int_{\Gamma_d} \phi v_n \, dS - \int_{\Gamma} \phi v_n \, dS \right)$$

As

$$\lim_{d \to 0} \frac{1}{d} \left( \int_{\Gamma_d} \phi v_n \, dS - \int_{\Gamma} \phi v_n \, dS \right) = \int_{\Gamma_d} \frac{\partial}{\partial n} (\phi v_n) \, dS + \int_{\Gamma} -2H \phi v_n \, dS$$

we have

$$\int_\Gamma \phi (\nabla \cdot v - \frac{\partial}{\partial n} v_n + 2H v_n) \, dS + \int_{\Gamma} \nabla \phi \cdot v - \frac{\partial \phi}{\partial n} v_n \, dS = 0$$

or

$$\int_\Gamma \phi \nabla v_\Gamma \, dS + \int_\Gamma \nabla \phi \cdot v_\Gamma \, dS = 0$$
With these identities we have the following theorem.

**Theorem 5.2.** Suppose $v \in V_{\text{div}}$, and the solution of the fluid coupled system (5.5) or (5.11) satisfies (B1a) and (B2), we have

$$\lim_{\epsilon \to 0} \int_{\Omega} g_0 \nabla \phi \cdot v \, dx = \frac{4\sqrt{2}}{3} \int_{\Gamma} \left( -\Delta_{\Gamma} H v_N + \nabla_{\Gamma}(H^2 - K) \cdot v_{\Gamma} \right) \, dS, \quad (5.25)$$

$$= -\frac{4\sqrt{2}}{3} \int_{\Gamma} (\Delta_{\Gamma} H + 2H(H^2 - K))v_N - (H^2 - K)\nabla_N v_N \, dS \quad (5.26)$$

where the scalar $v_N$ is the normal component of $v$ and the vector $v_{\Gamma}$ is the projection of $v$ onto surface $\Gamma$.

**Proof.** First we have

$$2H^2 - K = \frac{1}{2}(\nabla^2 d : \nabla^2 d) = \frac{1}{2}(\nabla \cdot (\nabla^2 d\nabla d) - \nabla \Delta d \cdot \nabla d) = \nabla H \cdot \nabla d. \quad (5.27)$$

Taking $\Theta = \Delta^2 d\nabla d - \Delta d\nabla \Delta d - \nabla^2 d\nabla \Delta d - \nabla^2 \Delta d\nabla d$, we have

$$\int_{\Omega} g_0 \nabla \phi \cdot v \, dx = \int_{\Omega} \frac{1}{\epsilon} (q')^2 \Delta^2 d(\nabla d \cdot v) + \frac{1}{2\epsilon} \nabla(q')^2 \cdot v((\Delta d)^2 + 2\nabla d\nabla \Delta d) \, dx$$

$$= \frac{1}{\epsilon} \int_{\Omega} (q')^2 \left( \Delta^2 d\nabla d - \Delta d\nabla \Delta d - \nabla^2 d\nabla \Delta d - \nabla^2 \Delta d\nabla d \right) \cdot v \, dx$$

$$= \frac{1}{\epsilon} \int_{\Omega} (q')^2 (\Theta \cdot v) \, dx.$$
where for the second equal sign, we used the integration by parts and the fact that 
\( \nabla \cdot v = 0 \). We can calculate the normal direction component of \( \Theta \) by

\[
\Theta_N = \Theta \cdot \nabla d = \Delta^2 d - \Delta d \nabla \Delta d \cdot \nabla d - \nabla d \nabla^2 d \nabla \Delta d - \nabla d \nabla^2 d \nabla d \\
= \Delta^2 d - \nabla \cdot (\nabla d \nabla d \cdot \nabla \Delta d) \\
= -2\Delta \Gamma H
\]

Also as

\[
\Theta = -2\Delta H \vec{n} - 4H \nabla H - \nabla (\nabla d \cdot \nabla \Delta d) \\
= -2\Delta H \vec{n} - 4H \nabla H + 2\nabla (\nabla H \cdot \nabla d) \\
= -2\Delta H \vec{n} - 4H \nabla H + 2\nabla (2H^2 - K) \\
= -2\Delta H \vec{n} + 2\nabla (H^2 - K)
\]

Thus the projection of \( \Theta \) on surface \( \Gamma \)

\[
\Theta_\Gamma = 2\nabla_\Gamma (H^2 - K)
\]

Since \( \int_{-\infty}^{\infty} (q'(x))^2 \, dx = \frac{2\sqrt{2}}{3} \),

\[
\lim_{\epsilon \to 0} \int_{\Omega} g_0 \nabla \phi \cdot v \, dx = \frac{4\sqrt{2}}{3} \int_{\Gamma} \Theta \cdot v \, dS = \frac{4\sqrt{2}}{3} \int_{\Gamma} ( -\Delta_\Gamma H v_N + \nabla_\Gamma (H^2 - K) \cdot v_\Gamma ) \, dS.
\]

And because

\[
0 = \nabla \cdot v = \nabla_\Gamma \cdot v_\Gamma + \nabla_N v_N - 2H v_N
\]
we have
\[ \nabla_{\Gamma} \cdot v_{\Gamma} - 2Hv_{N} = -\nabla_{N}v_{N} \]

Thus from Lemma 5.3 we have

\[
\lim_{\epsilon \to 0} \int_{\Omega} g_{0} \nabla \phi \cdot v \, dx = -\frac{4\sqrt{2}}{3} \int_{\Gamma} (\Delta_{\Gamma} H v_{N} + (H^2 - K) \nabla_{\Gamma} \cdot v_{\Gamma}) \, dS
\]

\[
= \frac{4\sqrt{2}}{3} \int_{\Gamma} (\Delta_{\Gamma} H + 2H(H^2 - K))v_{N} + (H^2 - K)(\nabla_{\Gamma} \cdot v_{\Gamma} - 2Hv_{N}) \, dS
\]

\[
= \frac{4\sqrt{2}}{3} \int_{\Gamma} (\Delta_{\Gamma} H + 2H(H^2 - K))v_{N} - (H^2 - K)\nabla_{N}v_{N} \, dS
\]

For non-zero spontaneous curvature, we can further have

**Theorem 5.3.** Suppose constant spontaneous curvature \(c_0\) and \(v \in V_{\text{div}}\), and the solution of the fluid coupled system (5.5) or (5.11) satisfies (B1a) and (B2), we have

\[
\lim_{\epsilon \to 0} \int_{\Omega} f \nabla \phi \cdot v \, dx = \frac{4\sqrt{2}}{3} \int_{\Gamma} H v_{N} \, dS
\]

(5.29)

and

\[
\lim_{\epsilon \to 0} \int_{\Omega} f \nabla \phi \cdot v \, dx = \frac{4\sqrt{2}}{3} \int_{\Gamma} H v_{N} \, dS
\]

(5.28)

where the scalar \(v_{N}\) is the normal component of \(v\) and the vector \(v_{\Gamma}\) is the projection of \(v\) onto surface \(\Gamma\).
Proof. With constant spontaneous curvature,

\[ g = g_0 - \frac{2}{\epsilon} Cqq' \Delta d + \frac{2}{\epsilon} C^2 q(q^2 - 1) \]

Since \( q' = (1 - q^2)/\sqrt{2} \), first,

\[
\lim_{\epsilon \to 0} \int_{\Omega} -\frac{2}{\epsilon} Cqq' \Delta d \nabla \phi \cdot v \, dx = \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_{\Omega} 2\sqrt{2} C (q - q^3) H' \frac{q'}{\epsilon} (\nabla d \cdot v) \, dx
\]

\[
= \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_{\Omega} 2\sqrt{2} CH \nabla \left( -\frac{1}{4} + \frac{1}{2} q^2 - \frac{1}{4} q^4 \right) \cdot v \, dx
\]

\[
= - \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_{\Omega} 2\sqrt{2} C \left( -\frac{1}{4} + \frac{1}{2} q^2 - \frac{1}{4} q^4 \right) \nabla H \cdot v \, dx
\]

\[
= \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_{\Omega} \frac{\sqrt{2}}{2} C (q^4 - 2q^2 + 1) \nabla H \cdot v \, dx
\]

\[
= \frac{4}{3} C \int_{\Gamma} (2H^2 - K) v_N + \nabla \Gamma H \cdot v_{\Gamma} dS.
\]

\[
= \frac{4\sqrt{2}}{3} c_0 \int_{\Gamma} (2H^2 - K) v_N + \nabla \Gamma H \cdot v_{\Gamma} dS.
\]

And

\[
\lim_{\epsilon \to 0} \int_{\Omega} \frac{2}{\epsilon} C^2 q(q^2 - 1) \nabla \phi \cdot v \, dx = \lim_{\epsilon \to 0} \int_{\Omega} \frac{2}{\epsilon} C^2 \nabla \left( \frac{1}{4} q^4 - \frac{1}{2} q^2 \right) \cdot v \, dx
\]

\[
= 0
\]
All together, we have

\[ \lim_{\epsilon \to 0} \int_{\Omega} g \nabla \phi \cdot v \, dx = 4 \sqrt{2} \int_{\Gamma} \left( -\Delta_{\Gamma} H + c_0(2H^2 - K) \right) v_N + \nabla_{\Gamma}(H(H + c_0) - K) \cdot v_{\Gamma} \, dS \]

\[ = \frac{4\sqrt{2}}{3} \int_{\Gamma} \left( -\Delta_{\Gamma} H + c_0(2H^2 - K) \right) v_N - (H(H + c_0) - K) \nabla_{\Gamma} \cdot v_{\Gamma} \, dS \]

\[ = \frac{4\sqrt{2}}{3} \int_{\Gamma} \left( -\Delta_{\Gamma} H + c_0(2H^2 - K) \right) v_N - (H(H + c_0) - K)(2Hv_N - \nabla_N v_N) \, dS \]

\[ = -\frac{4\sqrt{2}}{3} \int_{\Gamma} \left( \Delta_{\Gamma} H + 2H(H^2 - K) + c_0K \right) v_N + (H(H + c_0) - K) \nabla_N v_N \, dS \]

Now, for function \( f = -q'\Delta d \), we have

\[ \lim_{\epsilon \to 0} \int_{\Omega} f \nabla \phi \cdot v \, dx = \lim_{\epsilon \to 0} \int_{\Omega} -q'\Delta d \nabla \phi \cdot v \, dx = \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_{\Omega} 2q' H v_N \, dx = \frac{4\sqrt{2}}{3} \int_{\Gamma} H v_N \, dS. \]

With above theorem, we can recover the stress in the sharp interface limit now.

**Theorem 5.4.** Suppose the solution of the fluid coupled system (5.5) or (5.11) satisfies (B1a) and (B2) with constant spontaneous curvature \( c_0 \). The sharp interface limit of the stress on the surface is

\[ \text{[Stress]}_{\Gamma} = \frac{4\sqrt{2}}{3} \left( -\Delta_{\Gamma} H + c_0(2H^2 - K) + \lambda_2 H \bar{n} + \nabla_{\Gamma}(H(H + c_0) - K) \right) \]
Proof. Suppose $v \in V_{\text{div}}$, we can take the weak form of the N-S equation on the whole domain as

$$
< u_t, v >_{\Omega} + < (u \cdot \nabla)u, v >_{\Omega} + \nu < \nabla u, \nabla v >_{\Omega} - < p, \nabla v >_{\Omega} 
+ < \text{[Stress]}_v, v >_{\partial \Omega} = < (k + \lambda_2 f) \nabla \phi, v >_{\Omega}
$$

Taking $\epsilon \to 0$, dividing the domain into two parts, the inside and outside of $\Gamma$, denoted by $\Omega_i$ and $\Omega_o$, for the N-S equation on both area, we have

$$
< u_t, v >_{\Omega_i} + < (u \cdot \nabla)u, v >_{\Omega_i} + \nu < \nabla u, \nabla v >_{\Omega_i} + < p, \nabla v >_{\Omega_i} 
+ < \text{[Stress]}_{\Gamma}, v >_{\Gamma} + < \text{[Stress]}_v, v >_{\partial \Omega \cap \partial \Omega_i} = 0
$$

$$
< u_t, v >_{\Omega_o} + < (u \cdot \nabla)u, v >_{\Omega_o} + \nu < \nabla u, \nabla v >_{\Omega_o} + < p, \nabla v >_{\Omega_o} 
+ < \text{[Stress]}_{\Gamma}, v >_{\Gamma} + < \text{[Stress]}_v, v >_{\partial \Omega \cap \partial \Omega_o} = 0
$$

All together, we have

$$
< \text{[Stress]}_{\Gamma}, v >_{\Gamma} = \lim_{\epsilon \to 0} < (k + \lambda_2 f) \nabla \phi, v >_{\Omega}
$$

Thus from Theorem 5.4, we have

$$
\text{[Stress]}_{\Gamma} = \frac{4\sqrt{2}}{3} \left( (-\Delta_{\Gamma}H + c_0(2H^2 - K) + \lambda_2 H)\hat{n} + \nabla_{\Gamma}(H(H + c_0) - K) \right)
$$
And among the extra stress term, setting $\lambda_2$ to be zero, we get the part caused only due to the elastic bending energy is term.

**Corollary 5.2.** Suppose the solution of the fluid coupled system (5.5) or (5.11) satisfies (B1a) and (B2) with constant spontaneous curvature $c_0$. The sharp interface limit of the stress caused due to the elastic bending energy on the surface is

$$[\text{Stress}]_{\Gamma} = \frac{4\sqrt{2}}{3} ((-\Delta_{\Gamma} H + c_0 (2H^2 - K))\mathbf{n} + \nabla_{\Gamma} (H(H + c_0) - K))$$

**Remark 5.1.** If in the proof of this theorem, we only consider the test function $v \in V_{\text{div}}$ with $\nabla_N v_N = 0$, using the second equation in formula 5.28, we can further get the stress term by

$$[\text{Stress}]_{\Gamma} = \frac{4\sqrt{2}}{3} ((-\Delta_{\Gamma} H - 2H^2 - K) - c_0 K)\mathbf{n}.$$  

And thus for the equilibrium system, the curvature of the surface must satisfies that

$$\Delta_{\Gamma} H + 2H(H^2 - K) + c_0 K = 0 \quad (5.30)$$

which is exact the generalized form of Euler-Lagrangian equation of Willmore’s problem (1.4).

### 5.4 Numerical scheme

We use forward Euler to solve $\phi$ in (5.5).

$$\frac{\phi_{n+1} - \phi_n}{\Delta t} = -(u_n \cdot \nabla)\phi_n - \gamma (g_n + M_1 (A(\phi_n) - \alpha)) + M_2 (B(\phi_n) - \beta) f_n$$
which can be split into two equations:

\[
\frac{\phi_{n+1}' - \phi_n}{\Delta t} = -\gamma (g_n + M_1 (A(\phi_n) - \alpha) + M_2 (B(\phi_n) - \beta) f_n) \tag{5.31}
\]

and

\[
\frac{\phi_{n+1} - \phi_n'}{\Delta t} = -(u_n \cdot \nabla) \phi_n \tag{5.32}
\]

Since \(\frac{\phi_{n+1}' - \phi_n}{\Delta t} = -\gamma \frac{\delta E_M(\phi_n)}{\delta \phi}\), we can always choose \(\Delta t\) small enough to ensure that \(E_M(\phi_{n+1}') < E_M(\phi_n)\), where the energy \(E_M(\phi)\) is defined by (5.1).

After solve \(\phi_{n+1}\), we solve \(u_{n+1}\) by using a second order implicit time discretization of the viscous term, with the pressure and convective terms treated explicitly. This scheme is proved to be stable under the standard CFL condition [32].

Let \(F = \eta (g + M_1 (A - \alpha) + M_2 f (B - \beta)) \nabla \phi\), the fluid part of system (5.5) is equivalent to the following pressure Poisson equation formulation:

\[
\begin{align*}
\frac{\partial u}{\partial t} + (u \cdot \nabla) u + \nabla p &= \nu \Delta u + F, \\
\Delta p &= -\nabla \cdot (u \cdot \nabla u + \nabla \cdot F), \\
\frac{\partial p}{\partial n}|_\Gamma &= -n \cdot (\nu (\nabla \times \nabla \times u) + F)|_\Gamma, \\
u|_\Gamma &= 0
\end{align*}
\tag{5.33}
\]
We first apply the Crank-Nicholson to the viscous term and Adams-Bashforth discretization for both the convection pressure terms, a second order semi-implicit time discretization of the first equation of (5.33) is given by

\[
\frac{u_{n+1} - u_n}{\Delta t} + \frac{3}{2}(u_n \cdot \nabla u_n + \nabla p_n) - \frac{1}{2}(u_{n-1} \cdot \nabla u_{n-1} + \nabla p_{n-1}) = \frac{\nu}{2} \Delta (u_{n+1} + u_n) + \frac{F_{n+1} + F_n}{2}.
\]

(5.34)

The pressure term is then solved by

\[
\Delta p_{n+1} = -\nabla \cdot (u_{n+1} \cdot \nabla u_{n+1} + \nabla \cdot F_{n+1})
\]

(5.35)

\[
\frac{\partial p_{n+1}}{\partial n}\big|_\Gamma = -\mathbf{n} \cdot (\nu (\nabla \times \nabla \times u_{n+1}) + F_{n+1})\big|_\Gamma
\]

(5.36)

The time step of \(u\) is chosen to satisfy the usual CFL condition

\[
\|u\|_\infty \frac{\Delta t}{\Delta x} = \text{CFL} \leq 1
\]

The time steps of \(u\) and \(\phi\) may be different. In general, the CFL condition is easy to be satisfied with a relatively larger time step of \(u\) which is fixed in the whole process. The time step of \(\phi\) is dynamically adjusted to ensure that \(E(\phi'_{n+1}) < E(\phi_n)\).

We indicate that in our numerical experiments, the time step of \(u\) is in general 10 more times of that of \(\phi\). In another words, we run one step solving \(u\) after 10 more steps of solving \(\phi\). Thus the demand for the performance of solving \(u\) is not so strictly as that of solving \(\phi\). We use spectral method for solving \(\phi\) while using spectral and Finite Difference methods solving \(u\).
5.5 Implementation

In our numerical simulation, we assume period boundary condition in \( \Omega = [-\pi, \pi]^3 \) for \( \phi \) in three directions and \( u \) only in \( z \) direction, homogeneous boundary condition for \( u \) in \( x \) and \( y \) directions. Thus we can apply 3-d DFFT to \( \phi \) and 1-d DFFT to \( u \) in \( z \).

By applying the DFFT in \( z \)-direction to the variables, letting \( \Omega_z \) to be the \( x - y \) section cut from \( \Omega \) as \( z \)-axis valued at \( z \), \( \Gamma_z = \partial \Omega_z \) and \( N_n = u_n \cdot \nabla u_n + \nabla p_n \) we have formula (5.34) to be

\[
\frac{\hat{u}_{n+1} - \hat{u}_n}{\Delta t} + \frac{3}{2} \hat{N}_n - \frac{1}{2} \hat{N}_{n-1} = \nu \left( \Delta \hat{u}_{n+1} + \hat{u}_n \right) - z \frac{2}{2} \left( \hat{u}_{n+1} + \hat{u}_n \right) + \frac{\hat{F}_{n+1} + \hat{F}_n}{2}.
\]

or

\[
\left( \frac{2}{\nu \Delta t} + z^2 \right) \hat{u}_{n+1} - \Delta \hat{u}_{n+1} = \left( \frac{2}{\nu \Delta t} - z^2 \right) \hat{u}_n + \Delta \hat{u}_n + \frac{1}{\nu} \left( -3 \hat{N}_n + \hat{N}_{n-1} + \hat{F}_{n+1} + \hat{F}_n \right)
\]

(5.37)

in \( \Omega_z \) with homogeneous boundary condition on \( \Gamma_z \) for every \( z \).

The pressure term is then solved by

\[
z^2 - \Delta \hat{p}_{n+1} = \mathcal{F}(\nabla \cdot (u_{n+1} \cdot \nabla u_{n+1} + \nabla \cdot F_{n+1}))
\]

(5.38)

in \( \Omega_z \) with Newmann boundary condition

\[
\left. \frac{\partial \hat{p}_{n+1}}{\partial n} \right|_{\Gamma_z} = -n \cdot \mathcal{F}(\nu (\nabla \times \nabla \times u_{n+1} + F_{n+1})) \left|_{\Gamma_z} \right.
\]

where \( \mathcal{F} \) is DFFT in \( z \) dirction.
Solving (5.37) and (5.38) in $\Omega_z$ need solve two Helmholtz equations

$$\xi U - \Delta U = G$$

(5.39)

in $\Omega_z$ with homogeneous or Newmann boundary condition. Because we use uniform grid mesh for DFFT of $\phi$ in $\Omega$, we can not use other spectral method such as Chebyshev spectral method to solve (5.39) as it need Chebyshev collocation. Here we use Finite Difference with the matrix-diagonalization procedure for this problem. Thus the domain is spanned by $(N+1) \times (N+1) \times N$ grid points. The DFFT of $\phi$ is made at $N \times N \times N$ grid points by cutting two sides of $\Omega$ where the value of $\phi$ can be recovered by period boundary condition. Each $\Omega_z$ is distributed uniform $(N+1) \times (N+1)$ grid points.

Let $D_N$ denote a $(N+1) \times (N+1)$ Finite differentiation matrix which can be any $k$-diagonal matrix where $k \geq 3$ is an odd number, the larger $k$ is, the more accuracy got. In our implementation, $k = 9$. $U$ is also another $(N+1) \times (N+1)$ matrix, and

$$U_x \approx UD_N^T, \quad U_y \approx D_N U, \quad \Delta U \approx D_N^2 U + U(D_N^2)^T$$

Let $\tilde{U} = U(2:N,2:N)$ and the analogous definitions for $\tilde{G}$ and $\tilde{D}_N^2$. For homogeneous boundary condition, (5.39) reads

$$\xi \tilde{U} - (\tilde{D}_N^2 \tilde{U} + \tilde{U}(\tilde{D}_N^2)^T) = \tilde{G}. \quad (5.40)$$

Suppose $\tilde{D}_N^2$ is diagonalizable hence $\tilde{D}_N^2 = L\Lambda L^{-1}$, where $\Lambda$ is the diagonalization of the eigenvalues $\lambda_i$ of $\tilde{D}_N^2$ which can be complex numbers. Let $\hat{U} = L^{-1}\tilde{U}(L^T)^{-1}$ and
\[ \hat{G} = L^{-1} \hat{G}(L^T)^{-1} \], (5.40) is equivalent to

\[ \xi \hat{U} - (\Lambda \hat{U} + \hat{U} \Lambda) = \hat{G}. \]  

(5.41)

Solving \( \hat{U} \) by

\[ \hat{U}_{ij} = \frac{\hat{U}_{ij}}{\xi - (\lambda_i + \lambda_j)}, \]

we can recover \( \hat{U} = LU L^T \) and the boundary values of \( U \) set to be zero.

We can use similar procedure to solve equation (5.40) with Newmann boundary condition. Please refer [32] for the details.

Finally, we need do IDFFT in z-direction to transform \( \hat{u} \) and \( \hat{p} \) back to \( u \) and \( p \) after solving \( \hat{u} \) and \( \hat{p} \) in all \( \Omega_z \) for every \( z \).

No matter for the 3d DFFT for \( \phi \) in \( \Omega \) or solving (5.39) for every \( \Omega_z \), we can always divide the jobs into independent smaller jobs with different \( z \) and distribute them into different processors running paralleled. The consideration of parallel implementation is similar to that in solving the truly 3d equilibrium vesicle shapes. One can refer 4.3.3 for details.

5.6 Numerical simulation

The domain in our numerical simulation are fixed is the box \([-\pi, \pi]^3\) except specially indicated. The initial phase field selection is the same as that in section 4.4.1.
5.6.1 Convergence verification

For the phase field simulation of vesicles in fluid fields, the quality of the numerical result is affected by the choice of computational domain, the transition thickness parameter (or the effective width of the diffusive interface) $\epsilon$, the number of grid points, and the choices of other parameters used in the simulation such as the initial velocities, the viscosity of fluid. Similar to the 3-d phase field simulation for equilibrium vesicle shapes in Chapter 4, we take the domain fixed at the box $[-\pi, \pi]^3$. All of other domains can be scaled into this box. By this way, we should choose the initial membrane shapes being enclosed into this box. The parameter $\epsilon$ is taken to be just a couple of percentage points of the domain size to ensure a relatively sharp interfacial region. The mesh size is normally taken to be several times smaller than $\epsilon$ to ensure adequate spatial resolution. To ascertain the accuracy and robustness of our numerical algorithms and the parameter selections, we here present results of some numerical tests on the convergence and performance of our method.

Fig. 5.1. Left: shape transformation of a disk being flushed upward; Right: Lagrange multipliers plot.
We use penalty formulation in vesicle transformation study, so first, I show you a convergence test for penalty constants $M_1$ and $M_2$ in Figure 5.1. Starting from a disk with fluid going upward, the vesicle has a shape transformation. We repeat this experiment in three times with different penalty constants $M_1 = M_2 = 1000, 10000, 100000$ respectively. The left picture shows the plot of Lagrange multipliers $\lambda_1 = M_1(A(\phi) - \alpha)$, $\lambda_2 = M_1(B(\phi) - \beta)$. In this picture, we can identify two curves each of them actually composed by three different curves corresponding to different values of $M_1$ and $M_2$. The perfect coincident of those curves illustrates the convergence of Lagrange multipliers.

Second, we test for different values of $\epsilon$. Two similar tests are performed with same parameters ($k = 3, \gamma = 1, \nu = 1, M_1 = M_2 = 10000$, grid sizes is $65 \times 65 \times 64$) except the values of $\epsilon$, one is $2h$ another one is $1.77h$. They even have the same initial shapes as showed in Figure 5.2. From this figure, we can also know that their shapes at time 0.04 are almost the same. and the total system energy behaviors coincide.

Third, we test for different values of the grid meshes. Two similar tests are performed with same parameters ($epsilon = 0.1964, k = 3, \gamma = 1, \nu = 1, M_1 = M_2 = 10000$) except the grid meshes, one is $65 \times 65 \times 64$ another one is $81 \times 81 \times 80$. They even have the same initial shapes as showed in Figure 5.3. From this figure, we can also know that their shapes at time 0.035 are almost the same. and the total system energy behaviors coincide very well. And compare with previous test, we can also know that the different values of $\epsilon$ has more effect on the experiment than that of different grid meshes.

The last convergence test is for different time step sizes. Although we can adjust the time step sizes in our experiments, in order to estimate the effect of different time step sizes, we make this experiment for two similar tests with different fixed time step
sizes. Their parameters are the same ($\epsilon = 1.77h = 0.1736$, $k = 3$, $\gamma = 1$, $\nu = 1$, $M_1 = M_2 = 10000$ and grid mesh $65 \times 65 \times 64$) except time step sizes. For phase field transformation time step size, one is $3e-7$ another one is $5e-7$. For fluid field dynamics time step size, one is $1e-5$ another one is $5e-6$. They have the same initial shapes as showed in Figure 5.4. From this figure, we can also know that their shapes at time 0.037 are almost the same. and the total system energy behaviors coincide very well.

5.6.2 3-D numerical experiments

Our first experiment is to check the effect of different values of Reynald’s number $Re$. In our systems, the viscosity $\nu = 1/Re$. We know the larger viscosity, the quick the total energy decreases. Here we perform two similar tests with different values of $Re$, one is 1.0 another one is 0.1. All the other parameters are the same: $\epsilon = 2h = 0.1964$, $k = 3$, $\gamma = 1.0$, $M_1 = M_2 = 1e5$ and grid mesh $65 \times 65 \times 64$. They have the same initial shapes as showed in Figure 5.5. However, due to different values of Reynald’s number, the energy decreases with different speeds. From this figure, we can also know that their shapes at time 0.043 are totally different.

The second example illustrates how the energy transform between vesicle and fluid. Figure 5.6 shows a shape transformation of a disk within a fluid field whose starting velocity is zero. Because the the starting disk is not a energy minimizer, it deforms to a dimpled disk. In this process, some of its elastic bending energy transforms to fluid energy. And the fluid may cause the disk dimples too much and in this process some fluid energy transforms to elastic bending energy, and so forth. However, their total energy is always monotone decreasing due to the energy law.
Figure 5.7 further illustrates the transformations of vesicles in fluid fields. The top row shows how a small ball below a torus is flushed upward and finally merges together with the torus. In this experiment, $\epsilon = 2h = 0.196$, $\gamma = 1.0$, $Re = 1.0$, $M_1 = M_2 = 1e5$ and grid mesh $65 \times 65 \times 64$. When the ball flushed close to the torus, they merge together and reach a lower energy state. Here we would like to point out that the bending rigidity $k = 1000$. This large number explains why the final shape is not flushed into a torus again.

The bottom of Figure 5.7 shows how two gourd shape vesicles skew with fluid going upward very fast in the middle of them. In this experiment, each gourd shapes reaches its energy minimum. Same as above experiment, the elastic bending rigidity is very high ($k = 5000$) thus these gourd shapes stay at a very stable state. With fluid flushing upward, the pressure are not uniform at different hight positions, which results the skew of the two gourd shapes. This is a three dimensional non-symmetrical experiment with parameters: $\epsilon = 2h = 0.196$, $\gamma = 1.0$, $Re = 1.0$, $M_1 = M_2 = 1e4$ and grid mesh $65 \times 65 \times 64$

### 5.6.3 Detecting topological changes

Topological changes are naturally handled in our phase field model. In Chapter 6, we deduced a serials of formulae to calculate the Euler number of vesicle membranes. We may also detect the topological events by calculating the Euler number.

In Figure 5.8 there is an ellipsoid being flushed into a torus. From the plot of Euler number, we see there is a topology change and the Euler number jump from 1 to 0. And at the time around 0.03, the Euler number are fractional, which means there
is singularity of the surface. Actually, the third graph (time = 0.031) in the first row shows this singularity. The formula of the Euler number is described in Theorem (6.1). And we used the parameter auto-selection algorithm introduced in section 6.2.4.

5.7 Conclusion

In this section, we study the vesicle transformation in fluid fields. We successfully coupled the phase field formulation with fluid dynamics. Two kinds of systems, using either the Euler Lagrange multiplier or the penalty coefficients, are developed. And we get the energy for both systems. Similar to Chapter 2, we study the systems’ asymptotic limit and recover the sharp interface limit for both the system and the extra stress caused due to membrane. The numerical schemes for coupled fluid systems are carefully discussed. And finally we perform lots of convergence test for different parameters to ensure the convergence of the system.

With the present of the fluid field, the vesicle can have very complex shape transformations and even topological changes. Using the formulae deduced in the Chapter 6, we can successfully detect the topological changes in numerical simulations. And in the next chapter, we present this technique in detail.
Fig. 5.2. Top: initial shape is the left one, another two are the shapes at time 0.04 with $\epsilon = 2h, 1.77h$ respectively; bottom: the total energy plots.
Fig. 5.3. Top: initial shape is the left one, another two are the shapes at time 0.035 with grid $81 \times 81 \times 80$ and $65 \times 65 \times 64$ respectively; bottom: the total energy plots.
Fig. 5.4. Top: initial shape is the left one, another two are the shapes at time 0.037 with different time step sizes; bottom: the total energy plots.
Fig. 5.5. Top: initial shape is the left one, another two are the shapes at time 0.043 with different values of Reynald’s number; bottom: the total energy plots.

Fig. 5.6. Top: shape transformation of a disk within a fluid field with starting zero velocity; Bottom: Energy plot from left to right, vesicle membrane elastic bending energy, fluid field energy, total energy.
Fig. 5.7. Vesicle transformations in fluid fields. (Top: A small ball below a torus being flushed upward finally merges together with the torus; Bottom: with fluid going upward very fast in the middle of two gourds shape vesicles, they finally skew symmetrically.)
Fig. 5.8. Vesicle transformations in fluid fields with topology change. (Top: an ellipsoid being flushed into a torus, from left to right, the times of shape are $0, 0.005, 0.031, 0.060$ respectively; Bottom: the plot of the euler number.)
Chapter 6

Topological Information

6.1 Introduction

As the numerical simulations shown in previous chapters, the phase field approach is usually combined with energetic variational formulations that lead to a diffuse-interface modeled by a mixing energy. It allows topological changes of the interface to take place naturally [38, 42, 49]. Such a feature gives it many advantages in the numerical simulations of the interface variation and the interfacial motion (cf. [10]).

In this chapter, we continue the study of the phase field model but from a different, and perhaps also very novel, point of view. We are motivated by the fact that in many engineering and biological applications such as the modelling of blood cells in vascular systems, topological information of the vesicle membranes are of critical value. Thus, how to detect and control the topological change of the interface in the phase field modelling and numerical simulation becomes an important issue. Partly due to the nature of the phase field method (and all other level set methods) in their standard formulation, there is no mechanism preventing the topological change of the membranes or other interfaces. In fact, some of the topological changes are due purely to the formulations, instead of the underlined physics. To our knowledge, there has not been any discussion in the literature on how to recover relevant topological information from the phase field simulations, nor to address further control mechanisms.
The general phase field model is based on the introduction of a phase function (or order parameter) $\phi = \phi(x)$, defined on the physical (computational) domain $\Omega$ that encloses $\Gamma$. The function $\phi$ is used to label the inside and the outside of the vesicle $\Gamma$: the level set $\{x : \phi(x) = 0\}$ gives the membrane, while $\{x : \phi(x) > 0\}$ represents the interior of the membrane and $\{x : \phi(x) < 0\}$ the exterior. A transition thickness parameter is also chosen to characterize the typical length scale of the transition layer (or the thickness of the regularized, diffuse-interface). For time dependent problems, it is natural to allow $\phi = \phi(x,t)$. The objective of our study here is to propose some robust and efficient methods for retrieving or recovering interesting topological information within the phase field framework. In particular, we will develop some robust formulae for computing the Euler number for the modeled interface based on order parameter $\phi$.

We expect that our study here has the potential of opening up a host of exciting new applications of the phase field modeling including the use of the topological quantities in a control setting. Our numerical simulation indicates that the generalized Euler number ($\chi/2$ in 3-D and $\chi$ in 2-D) is not only a better indicator of topological changes than the energy functional we had been using in our previous chapter 3, but in fact, it gives a quantized jump upon a completion of the topological change (a direct consequence of the Gauss-Bonnet formula) for regular surfaces. Moreover, when the computed surface passes singularity, the new formula for $\chi$ based on the phase field formulation gives a fractional interpolation of the usual Euler number.

The study of the Euler number (in terms of $\chi$), (or the Euler-Poincaré index number $\eta$) may serve as a guidance in the study of other topological quantities within the phase field framework. The ideas proposed in this chapter may be equally applicable
to other simulations methods for free boundary and interface problems such as the level set methods. Our work here is also likely to shed light on the study of many geometrical modeling problems where providing topological information or controlling topological changes may be highly desirable.

The rest of the chapter is organized as follows: in section 6.2, we briefly recall the phase field model and we discuss a formulation of the Euler number (in terms of $\chi$) within the phase field framework that can be used to recover some topological information. We present a set of formulae in various 3-D and 2-D cases. We also discuss the Euler-Poincaré index number $\eta$ when the surfaces involve singularities. In section 6.4, we illustrate the method of computing the quantity $\chi$ in two applications and demonstrate the effectiveness and the robustness of the our formulation. Finally, some concluding remarks are given in section 6.5.

6.2 The Euler Number

Given an oriented (regular) compact (i.e., without boundary) surface $\Gamma$, the well-known Gauss-Bonnet formula states that

$$\int_{\Gamma} K \ ds = 2\pi \chi,$$

where $K = k_1 k_2$ is the Gaussian curvature of the surface in $R^3$, $ds$ is the area element and $\chi$ in 3-D ($\chi$ in 2-D) is the Euler number [15]. The number $\chi$ is a commonly used topological quantity. For some frequently encountered surfaces, we have $\chi = 2$ for a sphere, $\chi = 0$ for a torus and $\chi = -2$ for a torus with 2 holes. For 2-D curves, $K$ is
the curvature and $\chi = 1$ for a circle. To be convenient, in this chapter we call $\frac{\chi}{2}$ as the Euler number in 3-D cases and $\chi$ in 2-D cases.

In this section, it is our goal to find a suitable expression of the Euler number $\frac{\chi}{2}$ in 3-D (or $\chi$ in 2-D) when the surface is implicitly defined by a phase field formulation. We first give the general formula of the Euler number under a general phase field definition for both two and three dimensional spaces. Then we give some simplified formulae under some specific ansatz assumptions corresponding to our applications. For simplicity, we focus on the static case only when deriving the formulae. In the time dependent case, since we are mostly interested in the topological information of a spatially distributed interface at a fixed time stance, the generalizations to time dependent problems are obvious.

### 6.2.1 The three dimensional case

Let $\Gamma$ be a smooth oriented compact surface in a domain $\Omega$ in $\mathbb{R}^3$, we note that $\Gamma$ is allowed to have multiple disconnected pieces. Let $p$ be a monotone increasing function defined from $\mathbb{R}$ to $\mathbb{R}$ with $p(0) = 0$. For each function $p$, we take a phase field function $\phi = \phi(x)$ of $\Omega$ as $\phi(x) = p(d(x))$ where the signed distance function $d(x) = \text{dist}(x, \Gamma)$ is defined to be positive inside $\Omega$ and negative outside $\Omega$. The level sets of $\phi$ are denoted by $\Gamma_\mu = \{x \in \Omega | \phi(x) = \mu\}$. In particular, we have $\Gamma = \Gamma_0$. We also define $\Omega(a, b) = \{x \in \Omega | b < \phi(x) < a\}$, which forms a banded (layered) neighborhood around the surface for $b < 0 < a$. 
Theorem 6.1. Using the notations above, for any monotone increasing function $p$, there exists $b < 0 < a$, such that the following matrix $M$, where

$$M(x)_{ij} = \frac{1}{2\sqrt{\pi(a-b)|\nabla \phi|}}(\nabla_i \nabla_j \phi - \frac{\nabla |\nabla \phi|^2}{2|\nabla \phi|^4} \nabla \phi \nabla_i \phi \nabla_j \phi),$$  (6.2)

is a singular matrix for $\forall x \in \Omega(a,b)$ in the sense that it always has a zero eigenvalue, and the Euler number of $\Gamma$

$$\frac{\chi}{2} = \int_{\Omega(a,b)} F(x) \, dx$$  (6.3)

where $F$ is the coefficient of the linear term of the characteristic polynomial of $M$.

Proof. Since $\phi$ depends only on the distance $d$, and $p$ is monotone increasing, there exists real numbers $a$ and $b$, with $b < 0 < a$, sufficiently close to 0, such that $\Gamma_\mu$ are close to the parallel translations of $\Gamma$ in the normal direction for all $b \leq \mu \leq a$, and all $\Gamma_\mu$ have the same topology as $\Gamma$.

Direct computation shows

$$\nabla_i \nabla_j d = \nabla_i \nabla_j p - \frac{p''}{p'} \nabla_i d \nabla_j d = \frac{1}{p} [\nabla_i \nabla_j \phi - \frac{p''}{p'} \nabla_i d \nabla_j d].$$

The matrix $\nabla^2 d = \nabla^2 d(x)$, with $d$ being the signed distance to a surface $\Gamma$, always has a zero eigenvalue with $\nabla d$ as the eigenvector. This is due to the fact that $\nabla^2 d$ is symmetric and $|\nabla d| = 1$. On the surface $\Gamma$, the two other eigenvalues are actually the two principle curvatures of $\Gamma$ ($k_1$ and $k_2$ in this case). The Gaussian curvature $K$ is of course the product of these two eigenvalues while the mean curvature $H$ is given by the mean of the two eigenvalues. Both quantities can in fact be defined and computed on
all the level sets in $\Omega(a, b)$. For instance, the Gaussian curvature $K$ can be conveniently computed from the sum of the three principal $2 \times 2$ minors of $\nabla^2 d$ (see section (6.2.6) for an example in the cylindrically symmetric case).

Define $\Lambda(M) = \lambda_1(M)\lambda_2(M) = \Lambda(\nabla^2 d(x))$ for a singular matrix $M$ with $\lambda_1, \lambda_2$ being the two non-zero eigenvalues of $M$. Then, assuming that $k_1, k_2$ remain constant along the normal directions in $\Omega'$, we have

$$\frac{\chi}{2} = \frac{1}{4\pi} \int_{\Gamma} k_1(x)k_2(x) \, ds$$

$$= \frac{1}{4\pi (a-b)} \int_{p^{-1}(a)}^{p^{-1}(b)} p'(\tau) d\tau \int_{\Gamma} k_1(x)k_2(x) \, ds$$

$$= \frac{1}{4\pi (a-b)} \int_{\Omega(a,b)} p'(d(x))k_1(x)k_2(x) \, dx$$

$$= \frac{1}{4\pi (a-b)} \int_{\Omega(a,b)} p'(d(x))\Lambda(\nabla^2 d(x)) \, dx$$

$$= \frac{1}{4\pi (a-b)} \int_{\Omega(a,b)} \frac{1}{p'(d(x))} \Lambda(\nabla^2 \phi - p'' \nabla_i d \nabla_j d) \, dx . \quad (6.4)$$

Now, since $p$ is monotone increasing, we have $p'(d(x)) = |\nabla \phi(x)|$ and

$$p''(d(x)) = \nabla |\nabla \phi| \cdot \frac{\nabla \phi}{|\nabla \phi|}(x) = \frac{\nabla |\nabla \phi|^2 \cdot \nabla \phi}{2|\nabla \phi|^2}(x) .$$

Hence we get the general formula for the Euler-number in the three dimensional case:

$$\frac{\chi}{2} = \frac{1}{4\pi (a-b)} \int_{\Omega(a,b)} \frac{1}{|\nabla \phi|} \Lambda(\nabla_i \nabla_j \phi - \frac{\nabla |\nabla \phi|^2}{2|\nabla \phi|^4} \nabla_i \phi \nabla_j \phi) \, dx \quad \text{(6.6)}$$

$$= \frac{1}{4\pi (a-b)} \int_{\Omega(a,b)} \frac{1}{|\nabla \phi|} \Lambda(M(x)) \, dx .$$
From the notation of $M$ and $F$, we know $M(x)$ is singular for $\forall x \in \Omega(a, b)$ in the sense that it always has a zero eigenvalue, and equation (6.3) holds.

The formula (6.3) forms the basis for our efforts to recover topological information, in particular the Euler number.

### 6.2.2 The two dimensional case

**Theorem 6.2.** If $\Omega \in \mathbb{R}^2$, with the same notation as in the Theorem (6.1), for any monotone increasing function $p$, there exists $b < 0 < a$, such that

$$
\chi = \frac{1}{2\pi(a-b)} \int_{\Omega(a,b)} -\Delta \phi + \frac{\nabla|\nabla \phi|^2 \cdot \nabla \phi}{2|\nabla \phi|^2} dx .
$$

**Proof.** Using the same argument as above, it can be derived as follows:

$$
\chi = \frac{1}{2\pi} \int_{\Gamma} K(x) \, ds
$$

$$
= \frac{1}{2\pi(a-b)} \int_{\Omega(a,b)} p'(d(x))K(x) \, dx
$$

$$
= \frac{1}{2\pi(a-b)} \int_{\Omega(a,b)} -\Delta \phi + p''(d(x)) \, dx
$$

$$
= \frac{1}{2\pi(a-b)} \int_{\Omega(a,b)} -\Delta \phi + \frac{\nabla|\nabla \phi|^2 \cdot \nabla \phi}{2|\nabla \phi|^2} dx .
$$

\[\text{I}\]
6.2.3 Cases involving singularities on the interfaces

Both theorems 6.1 and 6.2 require $\Gamma$ being a smooth oriented compact surface. However, in realistic physical applications, we always encounter the singular cases where either the curves or the surfaces intersect or have some sharp angles or cones. Figure 6.1 illustrate several simple singular cases in 2-D while Figure 6.2 shows two singular shapes in 3-D.

![Fig. 6.1. Singular cases in 2-D.](image)

With the possible occurrence of the singularities, we will employ the general Gauss-Bonnet formula. In the 2-D case, suppose the curves are piecewise smooth with $n$ vertices (sharp corners) and the inner angles for each vertices are $\{\alpha_i, i = 1, ..., n\}$. The Gauss-Bonnet formula reads like

$$2\pi \eta = \int_{\Gamma} K \, ds + \sum_{i=1}^{n} (\pi - \alpha_i) = 2\pi \chi + \sum_{i=1}^{n} (\pi - \alpha_i)$$

where $\eta$, the Euler-Poincaré index number, is the topological integer, the genus of the surface [15].
We give illustrations, in Figure 6.1 and Figure 6.3, of the values of $\chi$ defined by $2\pi \chi = \int_\Gamma K \, ds$ in the singular cases. For the configurations such as the third picture in Figure 6.1, $2\pi \eta = \int_\Gamma K \, ds + 2(\pi - \alpha)$. In particular, for the cases in Figure 6.3, $\alpha = \pi, 0, \frac{\pi}{2}$ for the cases a, b and c respectively. And in all of these cases, the Euler-Poincaré index number $\eta$ is always 2, represents the number of bubbles.

On the other hand, the value of $\chi$ can be used to detect the change of topology even with the presence of the singular cases. Again, using the example in Figure 6.3, the Euler numbers $\chi$ are 2, 1, and 1.5 respectively, with the singularity being signaled by the fractional value. We want to point out that in the first case, the Euler number $\chi$ is still equal to the Euler-Poincaré index number $\eta$ even with the singularity.

When we consider the definition of $\chi$ for the 3-D singular cases, we may also get a fractional Euler number when singularity appears. For example, for the configuration in the first picture of the figure 6.2, suppose the angle of the tangent cone is $\alpha$, the Euler number can be derived from the following explicit analytic formula by calculating the
Fig. 6.3. Singular cases in 2-D. The inner intersect angles are $\pi$, 0, $\pi/2$ for cases a, b and c respectively.

ratio between the spherical cap cut by the $\alpha$-cone and the total area of the sphere:

$$\frac{\chi}{2} = \frac{1}{4\pi} \int_{\Gamma} K \, ds = 1 - \frac{1}{4\pi} (2\pi(1 - \sin \alpha)) = \frac{1}{2} + \sin \alpha.$$ (6.9)

Finally, we discuss the validity of formulae (6.3) and (6.7) in singular cases. Figure 6.4 shows that $\Gamma_\mu$ seem to have different (visual) topology as $\Gamma$ for some $b < \mu < a$.

However, in reference to the Figure (6.4), because each $\Gamma_\mu$ has singular vertices with angle either $\alpha$ or $\beta = \pi - \alpha$, the Euler number $\xi$ for every $\Gamma_\mu$ are the same as that of $\Gamma_0$. Thus Theorem 6.1 and Theorem 6.2 still hold for this singular case where the Euler number is a fractional number.

One will encounter a crucial issue, the *singular complement*, in the numerical simulations of the interfaces involving singularities. This is crucial in calculating the fractional Euler number correctly. To clarify this phenomenon, let us examine Figure (6.5)

Because of the *elbow* associated with $\Gamma_a$, $\Gamma_a$ has a different Euler number from $\Gamma_0$. This phenomenon, hereafter being referred as the *singularity compensation*, do
occur in all numerical experiments involving interfacial singularities due to the numerical smoothing of the surfaces. This appears to be bringing difficulties into the application of Theorem 6.1 and Theorem 6.2. However, noticing that the *elbow* has very large curvature, if a method can be designed to filter out such an *elbow*, the Euler number calculated for the remaining $\Gamma_a$ would remain the same as $\Gamma_0$. Such a technique will be introduced and developed later in section 6.3.

### 6.2.4 Stability and parameters auto-selection

Although the proofs of the Theorem 6.1 and Theorem 6.2 are given under the condition that for every $b < \mu < a$, $\Gamma_\mu$ has the same topology as $\Gamma_0$, to correctly identify the Euler number, one can relax such a condition to requiring the Euler number of $\Gamma_\mu$ being the same of that of $\Gamma_0$. By the analysis of section (6.2.3), it is desirable that the parameters $a$ and $b$ are chosen to be quite different from 0. Figure (6.6) gives an illustration of such a case.
Fig. 6.5. By getting rid of the singular complement, $\Gamma_0$, $\Gamma_a$ and $\Gamma_b$ have the same Euler number.

The advantage of choosing $a$ and $b$ some distance away from 0 is to ensure that $\Omega(a, b)$ contains plenty grid points, which in turn makes the integration for the Euler number more accurate and stable.

However, in general, it is not true that all the neighboring curves or surfaces always share the same Euler number. In Figure (6.7) $\Gamma_0$ and $\Gamma_b$ clearly have different Euler numbers. The largest $b$ can only be selected where the two circles of $\Gamma_b$ are tangent to each other. How to choose the value of $b$ in such situations becomes a very relevant issue in our computation of the Euler numbers.

On the other hand, in the Figure (6.7), we may notice that $\Gamma_a$ always has the same Euler number as $\Gamma_0$ and $a$ can be very different from 0. Thus the selection of $a$ and $b$ may be problem dependent. In some cases, we can select the integration area to be either $\Omega(0, a)$ or $\Omega(b, 0)$ in order to get the correct Euler number.

Denote the Euler number as $E(b, a)$ corresponding to the integration region $\Omega(a, b)$, in order to see the impact of $a$ and $b$, we employ the following algorithm in our numerical simulations:
Algorithm: parameter auto-selection for $a$. Given a phase field function $\phi$ defined on region $\Omega$, select $a$ relatively far away from 0 (for instance, $a = 1$). Select a tolerance number $\nu$ (for instance, $\nu = 0.1$) and a small step $h$ (we can use, as an example, $h = a/50$).

- Step 1: If $|E(0,a) - E(0,a/2)| < \nu$, exit; else set $a = a - h$.

- Step 2: If $a < h$ exit with $a = 0$; else loop back to the step 1.

The above algorithm is used to select the best $a$. A similar algorithm can be used to select the best $b$. A bi-section method can be adopted to make the auto-selection more efficient. The resulting $a$ and $b$ are used to compute the correct Euler numbers. As verified in the earlier theorems, the above algorithms are assured to terminate with suitable $a$ and $b$ if the step size $h$ and the tolerance $\nu$ are choosing to be reasonably small.
6.2.5 Formulae simplification

The formulae given in the above discussion of the Euler number are computable numerically, but for many practical situations, they can be further simplified if some appropriate ansatz can be taken. We now discuss some of these simplifications.

**Theorem 6.3.** If the variational problem (2.10)-(2.12) satisfies (A1) and (A2) with the minimizer \( \phi \), let

\[
M_{ij}(\phi) = \sqrt{\frac{35\epsilon}{64\sqrt{2\pi}}} (1 - \phi^2)\nabla^2 \phi + 2\phi \nabla_i \phi \nabla_j \phi), \tag{6.10}
\]

The Euler number of \( \Gamma \)

\[
\frac{\chi}{2} = \int_{\Omega} \Lambda(M(\phi)) \, dx + o(\epsilon) \tag{6.11}
\]

**Proof.** From theorem (2.2), we know \( \phi = \Phi + g \) where \( \Phi = \tanh(d/(\sqrt{2}\epsilon)) \),

\[
g = \epsilon^2 O(1).
\]

Since

\[
\int_{-\infty}^{+\infty} (1 - \tanh^2(\frac{x}{\sqrt{2}\epsilon}))^4 \, dx = \sqrt{2\epsilon} \int_{-\infty}^{+\infty} (1 - \tanh^2(x))^4 \, dx = \frac{32\sqrt{2}\epsilon}{35},
\]

\[
\int_{-\infty}^{+\infty} (1 - \tanh^2(\frac{x}{\sqrt{2}\epsilon}))^4 \, dx = \frac{32\sqrt{2}\epsilon}{35},
\]

\[
\frac{\chi}{2} = \int_{\Omega} \Lambda(M(\phi)) \, dx + o(\epsilon)
\]

Fig. 6.7. \( \Gamma_0, \Gamma_b \) have different Euler number.
\[ \int_\Gamma K \, ds = \frac{35}{32\sqrt{2\epsilon}} \int_{-\infty}^{+\infty} (1 - \tanh^2(\frac{\tau}{\sqrt{2\epsilon}}))^4 \, d\tau \int_\Gamma K \, ds \]

\[ \approx \frac{35}{32\sqrt{2\epsilon}} \int_\Omega 2e^2 \Lambda ((1 - \Phi^2)^2\Phi + 2\Phi \nabla_i \Phi \nabla_j \Phi) \, dx \]

\[ = \frac{35\epsilon}{16\sqrt{2}} \int_\Omega \Lambda ((1 - \Phi^2)^2\Phi + 2\Phi \nabla_i \Phi \nabla_j \Phi) \, dx \]

The second approximation in above equation is from formula (2.6) and Lemma (2.1).

And for \( \tanh \) function, this approximation is in the order of \( O(e^{-1/\epsilon}) \). Thus we have

\[ \frac{\chi}{2} = \frac{1}{4\pi} \int_\Gamma K \, ds \]

\[ = \frac{35\epsilon}{64\sqrt{2\pi}} \int_\Omega \Lambda ((1 - \Phi^2)^2\Phi + 2\Phi \nabla_i \Phi \nabla_j \Phi) \, dx + O(e^{-1/\epsilon}). \]

Define the matrix function \( M \) as

\[ M(\phi) = \sqrt{\frac{35\epsilon}{64\sqrt{2\pi}}} \left((1 - \phi^2)^2 \phi + 2\phi \nabla_i \phi \nabla_j \phi\right). \]

Now we need compare \( M(\phi) \) and \( M(\Phi) \).

\[ M(\phi) = C \left\{ [1 - (\Phi + g)^2](\nabla^2(\Phi + g)) + 2(\Phi + g)(\nabla_i \Phi + \nabla_i g)(\nabla_j \Phi \nabla_j g) \right\} \]

\[ = C \left\{ (1 - \Phi^2)^2 \Phi + (1 - \Phi^2)^2 g - g(2\Phi + g) \nabla^2 \Phi + 2\Phi \nabla_i \Phi \nabla_j \Phi + 2g \nabla_i \Phi \nabla_j \Phi \right. \]

\[ + 2\Phi \nabla_i g \nabla_j \Phi + \nabla_i \Phi \nabla_j g \}

\[ = M(\Phi) + C \left\{ [1 - \Phi^2]^2 g - g(2\Phi + g) \nabla^2 \Phi + 2g \nabla_i \Phi \nabla_j \Phi + 2g \nabla_i g \nabla_j \Phi + \nabla_i \Phi \nabla_j g \right\} \]

where \( C = \sqrt{\frac{35\epsilon}{64\sqrt{2\pi}}} \). Since \( g(x, \epsilon) = e^2 O(1), \| \nabla g(x, \epsilon) \| = \epsilon O(1) \) and \( \| \nabla^2 g(x, \epsilon) \| = O(1), \) together with \( \Phi(x, \epsilon) = O(1), \| \nabla \Phi(x, \epsilon) \| = O(1/\epsilon) \) and \( \| \nabla^2 \Phi(x, \epsilon) \| = O(1/\epsilon^2) \)
we have
\[ \|M_2 - M_1\| = \sqrt{\frac{35\epsilon}{64\sqrt{2\pi}}} O(1) = O(\sqrt{\epsilon}) \]

Since \(\Lambda(M)\) denote the coefficient of the linear term of the characteristic polynomial of \(M\), then \(\Lambda(M(\phi)) - \Lambda(M(\Phi)) = O(\epsilon)\) and we have

\[ \chi \frac{x}{2} = \int_{\Omega} \Lambda(M(\phi)) \, dx + o(\epsilon) \]

Because of this theorem, we can get the phase field formulation of the Elastic bending energy in the general form (1.1):

\[
E(\phi) = \int_{\Omega} \left[ \frac{3a_1}{4\sqrt{2\epsilon}} (1 - \phi^2)^2 + \frac{3a_2}{8\sqrt{2\epsilon}} (\epsilon \Delta \phi + \left( \frac{1}{\epsilon} \phi + c_0 \sqrt{2} \right)(1 - \phi^2))^2 \right. \\
\left. + \frac{35a_3\epsilon}{16\sqrt{2}} \Lambda((1 - \phi^2)\nabla^2 \phi + 2\phi \nabla_i \phi \nabla_j \phi) \right] \, dx
\]

(6.12)

And in the proof of this theorem, we use \((1 - \tanh^2(x))^4\) to concentrate the Gaussian curvature to the surface. If you use \((1 - \tanh^2(x))^2\), we can use another formula to define \(M(\phi)\).

**Theorem 6.4.** With the same notation as in the Theorem (6.1), if \(\phi = \tanh\left( \frac{d}{\sqrt{2\epsilon}} \right) = p\left( \frac{d}{\sqrt{2\epsilon}} \right)\), we have

3d case: let

\[
M_{ij} = \sqrt{\frac{3\epsilon}{8\sqrt{2\pi}}} \left( \nabla^2_{ij} \phi + \frac{2\phi}{1 - \phi^2} \nabla_i \phi \nabla_j \phi \right).
\]

(6.13)
The Euler number of $\Gamma$

$$\frac{\chi}{2} = \lim_{\epsilon \to 0} \int_{\Omega} \Lambda(M(\phi)) \, dx$$  \hspace{1cm} (6.14)

2d case: The Euler number of $\Gamma$

$$\chi = \lim_{\epsilon \to 0} \frac{1}{4\pi} \int_{\Omega} -\Delta \phi + \frac{1}{\epsilon^2} (\phi^2 - 1) \phi \, dx .$$  \hspace{1cm} (6.15)

Proof. Simple calculation yields that

$$\int_{-\infty}^{+\infty} (1 - \phi^2)^2 \, dx = \sqrt{2} \int_{-\infty}^{+\infty} (1 - \tanh^2(x))^2 \, dx = \frac{4\sqrt{2}\epsilon}{3},$$

With sufficient small $\epsilon$, the function $\phi$ goes to 1 or $-1$ very quickly (exponentially) away from $\Gamma$. Thus, we can just take $a = -b = 1$ with $\epsilon \to 0$. From formula (2.5), the matrix in the formula (6.2) becomes:

$$M = \sqrt{\frac{3\epsilon}{8\sqrt{2}\pi}} \left( \nabla^2 \phi + \frac{2\phi}{1 - \phi^2} \nabla_i \phi \nabla_j \phi \right).$$

and (6.14) holds.

For the two dimensional cases, by taking a similar ansatz, and putting

$$|\nabla \phi|^2 = \frac{1}{2\epsilon^2} (1 - \phi^2)^2$$

into the formula (6.7), we finally have (6.15).
Remark 6.1. If the variational problem (2.10)-(2.12) satisfies (A1) and (A2) with the minimizer $\phi$, let $M$ defined in (6.13), similar to Theorem 6.3, the Euler number of $\Gamma$

$$\frac{\chi}{2} = \int_{\Omega} \Lambda(M(\phi)) \, dx + o(\epsilon).$$

More simplifications can be made for problems where periodic boundary conditions are used, since $\int_{\Omega} \Delta \phi = 0$, the above formula can be further simplified to

$$\chi \approx \frac{1}{4\pi \varepsilon^2} \int_{\Omega} (\phi^2 - 1) \phi \, dx. \quad (6.16)$$

The above formula can be compared with the formula (6.7) (with $a = -b = 1$) applied to the periodic boundary condition case:

$$\chi = \frac{1}{4\pi} \int_{\Omega} \frac{\nabla|\nabla \phi|^2 \cdot \nabla \phi}{2|\nabla \phi|^2} \, dx = \frac{1}{8\pi} \int_{\Omega} \nabla \ln |\nabla \phi|^2 \cdot \nabla \phi \, dx$$

$$= -\frac{1}{8\pi} \int_{\Omega} \Delta \phi \ln |\nabla \phi|^2 \, dx. \quad (6.17)$$

where we only need $p$ being monotone from $-1$ to $1$ in $\Omega$ instead of being a strictly tanh function.

The previous formula (6.16) has no derivative terms while the latter one on (6.17) involves no bulk part.

We note that the approximations in (6.14), (6.15) and (6.16)) are of spectral accuracy with $\epsilon \to 0$. 
6.2.6 Formulae for cylindrically symmetric membranes

In Chapter 3, we use the energetic phase field models to compute three dimensional vesicle membranes minimizing the bending elastic energy. The numerical examples are for cylindrically symmetric membranes with various different topologies. We now present the Euler number computation in such situations.

In the numerical simulations of Chapter 3, where \( \phi(x) \rightarrow \tanh\left(\frac{d(x)}{\sqrt{2}\epsilon}\right) \) as \( \epsilon \rightarrow 0 \), the conventional cylindrical coordinates \((r, \theta, z)\) are used. Suppose the membrane is rotationally invariant with respect to the \(z\)-axis, i.e., \( \phi = \phi(z, r, \theta) = \phi(z, r) \), then

\[
\nabla \phi = \begin{pmatrix}
\partial_z \phi \\
\partial_r \phi \\
0
\end{pmatrix}, \quad \nabla_i \phi \nabla_j \phi = \begin{pmatrix}
(\partial_z \phi)^2 & \partial_z \phi \partial_r \phi & 0 \\
\partial_z \phi \partial_r \phi & (\partial_r \phi)^2 & 0 \\
0 & 0 & 0
\end{pmatrix}, \quad (6.18)
\]

and

\[
\nabla^2 \phi = \begin{pmatrix}
\partial^2_{zz} \phi & \partial^2_{zr} \phi & 0 \\
\partial^2_{zr} \phi & \partial^2_{rr} \phi & 0 \\
0 & 0 & \frac{1}{r} \partial_r \phi
\end{pmatrix}. \quad (6.19)
\]

If we substitute (6.18) and (6.19) into (6.13), we have that

\[
M = \sqrt{\frac{3\epsilon}{8\sqrt{2}\pi}} \begin{pmatrix}
\partial^2_{zz} \phi + \frac{2\phi}{1-\phi^2}(\partial_z \phi)^2 & \partial^2_{zr} \phi + \frac{2\phi}{1-\phi^2}\partial_z \phi \partial_r \phi & 0 \\
\partial^2_{zr} \phi + \frac{2\phi}{1-\phi^2}\partial_z \phi \partial_r \phi & \partial^2_{rr} \phi + \frac{2\phi}{1-\phi^2}(\partial_r \phi)^2 & 0 \\
0 & 0 & \frac{1}{r} \partial_r \phi
\end{pmatrix}.
\]
Hence $F$, the sum of the determinants of all principal $2 \times 2$ minors is equal to

$$F(r, z) = \frac{3\epsilon}{8\sqrt{2\pi r}} \partial_r \phi \{ \partial_{zz}^2 \phi + \partial_{rr}^2 \phi + \frac{2\phi}{1-\phi^2}[(\partial_z \phi)^2 + (\partial_r \phi)^2]\}, \quad (6.20)$$

and

$$\frac{\chi}{2} \approx \int \int 2\pi r F(r, z) \, drdz$$

$$\approx \frac{3\epsilon}{4\sqrt{2}} \int \int \partial_r \phi \{ \partial_{zz}^2 \phi + \partial_{rr}^2 \phi + \frac{2\phi}{1-\phi^2}[(\partial_z \phi)^2 + (\partial_r \phi)^2]\} \, drdz$$

$$\approx \frac{3\epsilon}{4\sqrt{2}} \int \int \partial_r \phi \{ \Delta \phi + \frac{2\phi}{1-\phi^2} |\nabla \phi|^2 \} \, drdz . \quad (6.21)$$

where the operators $\nabla$ and $\Delta$ are taken in the $r$-$z$ plane.

If we do not take the ansatz $\phi = \tanh(\frac{d}{\sqrt{2\epsilon}})$, but simply take (6.18) and (6.19) into the formula (6.2), we get a similar formula in the more general case:

$$\frac{\chi}{2} = \frac{1}{4\pi(a-b)} \int_{\Omega(a,b)} \frac{1}{r} \frac{1}{|\nabla \phi|} \partial_r \phi \{ \partial_{zz}^2 \phi + \partial_{rr}^2 \phi - \frac{\nabla|\nabla \phi|^2 \cdot \nabla \phi}{2|\nabla \phi|^4}[(\partial_z \phi)^2 + (\partial_r \phi)^2]\} \, dx ,$$

or

$$\frac{\chi}{2} = \frac{1}{2(a-b)} \int \int_{\Omega(a,b)} \frac{1}{|\nabla \phi|} \partial_r \phi \{ \Delta \phi - \frac{\nabla|\nabla \phi|^2 \cdot \nabla \phi}{2|\nabla \phi|^2} \} \, drdz . \quad (6.22)$$

We remark here that in the three dimensional cylindrically symmetric case, the two curvatures can be calculated by

$$k_1 = \Delta \phi - \frac{\nabla|\nabla \phi|^2 \cdot \nabla \phi}{2|\nabla \phi|^2} \quad (6.23)$$

$$k_2 = \frac{\partial_r \phi}{r(a-b)|\nabla \phi|} , \quad (6.24)$$
respectively. One can also use them to derive the formula for the Euler number directly.

Using the partial derivatives, (6.22) can be written as

\[
\frac{\chi}{2} = \int \int_{\Omega(a,b)} \frac{\partial_r \phi \left( \frac{\partial_{rr} \phi (\partial_z \phi)^2 + \partial_{zz} \phi (\partial_r \phi)^2 - 2 \partial_r \phi \partial_z \phi \partial_{rz} \phi}{2(a-b)((\partial_r \phi)^2 + (\partial_z \phi)^2)^{\frac{3}{2}}} \right) dr dz .
\]  

(6.25)

Using the difference approximation as described in section 3.2.2, the above integrals can be readily evaluated numerically on a spatial grid.

6.3 Numerical fulfillment

In section (6.2), various formulae were presented for calculating the Euler number in 2d and 3d under different kinds of conditions. In general, we can apply finite difference or spectral method directly to those formulae to calculate the Euler number. However, as discussed in the section (6.2.3), the singular cases often happen in the process with topology changes, such as the surface entanglement. When we apply the Euler number formulae to those singular cases, the numerical values at the singular vertices are always very large which make the final results inaccurate.

Figure (6.8 illustrate a 3-d singular case. The right most one is the graph shows the function \( F(r, z) \) in formula (6.20) with the \( r \) and \( z \) coordinates. From the right most graph, we see the numerical value may even go up to 10,000. If the Euler number is calculated directly by formula (6.22), although the theoretical value for this shape is 0.7500, we get 1.0671 which is close to the value 1, the Euler number of a sphere. This phenomenon is due to the so called singularity compensation as discussed earlier. Because of the finite discrete grid adopted in numerical scheme, the curvature value at
a singular vertex is always regularized from $\infty$ to a finite number. And in our case, such a change to the finite number provides certain compensation to the total Euler number, which can be viewed as putting a small elbow with a large curvature to complement the shape so that the singular shape changes to a regular shape.

A simple but effective way for getting rid of this singularity compensation is to avoid integrating over those singular vertices which are easy to detect because the numerical values of the integrand at those locations are very big relative to other points. From the formula (6.4), we know

$$F(x) = \frac{1}{4\pi(a - b)} p'(d(x)) K(x)$$

where $K(x)$ is the Gaussian curvature at a point $x$. If $p(x) = \tanh\left(\frac{x}{\sqrt{2}\epsilon}\right)$, $p'(d(x)) = \frac{1}{\sqrt{2}\epsilon}(1 - p^2(d(x)))$, then

$$|F(x)| \leq \frac{1}{4\sqrt{2}\pi\epsilon(a - b)} K(x).$$
In most cases, it is easy to estimate the possible largest Gaussian curvature value. In the phase field models, the radius of the smallest ball should be at least larger than the band width $\epsilon$. Thus it is natural to choose $K < 1/\epsilon^2$ for the regular points and regard the singular points as those satisfying the condition $F(x) > \frac{1}{4\epsilon^2\sqrt{2\pi\epsilon(a-b)}}$.

We verify the above argument using the examples shown in Figure 6.9 which represent the same cylindrically symmetric membrane with a singularity at the upper tip whose Euler number can be calculated by formula (6.25). By excluding the singular points with $F(x) > 200$, based on a $100 \times 200$ grid with $h = 0.01$, $\epsilon = 2h = 0.02$, and $\alpha = \frac{\pi}{6}$, the computed Euler number we get is 0.7498 which is a very good approximation of the theoretical value 0.7500 obtained from the formula (6.9). For $\alpha = \frac{\pi}{4}$, the computed Euler number 0.8534 is again an accurate approximation of the theoretical value 0.8536.

Fig. 6.9. A special cylindrically symmetric membrane with a singular point.

In the following section, we apply this technique to all our experiments.
6.4 Applications to some phase field models

In this section, we present two applications of the Euler number developed in the earlier sections for general phase field models. The special examples include the deformation of vesicle membrane configurations minimizing the bending elastic energy and the coarsening of two Newtonian bubbles in another Newtonian fluids. We expect that our formula can be equally applied to other more complicated and physical examples involving the phase field models as well.

6.4.1 The model for equilibrium membrane shapes

First we apply the Euler number formulae in the numerical experiments in Chapter 3. Figure 6.10 shows the deformation of a gourd (the first row, computed with a $40 \times 375$ grid and $\epsilon = 1.5h = 0.03$) and a torus (the second row, $100 \times 100$ grid, $\epsilon = 1.5h = 0.03$) with increasing surface areas while volumes being fixed at $1.1000$. The gourd becomes thinner and the torus moves further away from its axis. It is obvious that there is no topological change for both the gourd and the torus. This can be seen from the graph of the Euler numbers (Figure 6.11) with the value be kept at 1 for the gourd and 0 for the torus. On the other hand, in the same figure, the graphs of their energy are two intersecting curves which illustrates the existence of two shapes with totally different topologies but the same energy.

In the next set of numerical simulations, a rectangular domain with a $100 \times 200$ Cartesian grid having $h = 0.01$ is used and $\epsilon = 2h = 0.02$. Figure 6.12 shows the shape deformations with a decreasing area from $11.2960$ to $5.0912$ while fixing the volume at...
1.1000. The left picture in Figure 6.13 shows the corresponding change of the bending energy with different surface areas. Good resolutions of the interfaces based on the above choices of the computational grid and the parameter values have been demonstrated in section 3.3 for such a solution branch.

In the whole energy minimizing processing, the shape always jumps from one branch to another which results a discontinuous energy curve. Here the shape of the vesicle changes from a shell to a bangle (with no obvious energy jump), then to a torus (with a noticeable energy jump at the surface area $\beta = 6.6822$), then a longan (with an energy jump at around $\beta = 5.3563$) and finally to a spherical ball ( an energy jump at around $\beta = 5.1442$). There are 3 topological changes during the shape deformation: 1) from shell to a bangle; 2) from torus to a longan; and 3) from longan to a spherical ball. The energy can hardly detect the change from shell to bangle despite of the occurrence of the topology change.
The right picture in Figure 6.13 shows the change of the computed Euler numbers. The graph has exactly 3 jumps corresponding the three topological changes. We can see the corresponding Euler numbers 2, 0, 2, and 1 for shell, torus, longan and ball shapes respectively.

The calculation of the Euler numbers used the auto-selection algorithm for the best parameters $a$ and $b$. Observing the second, third and sixth graph of Figure (6.12) carefully, it is not hard to understand why we need such an algorithm here based on the theory stated in section 6.2.4. As different shapes have different best values of $a$ and $b$, we thus have different integration areas for the Euler numbers. It may be noticeable that some values are not exactly 0 when the vesicle surface area belongs to the interval $[5.3, 9.8]$. Such small errors are mainly due to the approximation errors of the finite difference scheme and the integration scheme. Fortunately, those errors are always sufficient small (less that 0.1 in this case) to be discriminated from the Euler number.
jumps which are at least 1. And this makes our method very stable and sensitive in detecting the topology changes.

In summary, the above experiments demonstrate that our formula for the Euler number can be successfully used to retrieve topological information and to capture topological events. Of course, the Euler number alone does not determine completely the topology of the interface.

### 6.4.2 The model for phase field model of fluid bubble motion

In the study of the coarsening of the Newtonian bubbles in another Newtonian fluid, the following two dimensional simple problem has been considered:

$$
\begin{align*}
\frac{\partial u}{\partial t} + (u \cdot \nabla)u - \nu \nabla \cdot D(u) + \nabla p + \lambda \nabla \cdot (\nabla \phi \odot \nabla \phi) &= 0, \quad (x, t) \in Q_T, \\
\nabla \cdot u &= 0, \quad (x, t) \in Q_T, \\
\frac{\partial \phi}{\partial t} + (u \cdot \nabla)\phi - \gamma \Delta (\Delta \phi + f(\phi)) &= 0, \quad (x, t) \in Q_T,
\end{align*}
$$

(6.26)
with the initial values $u(x, 0) = u_0(x), d(x, 0) = d_0(x)$ and periodic boundary conditions. Here $f(\phi) = (1 - \phi^2)/\epsilon^2$, $D(u) = (\nabla u + (\nabla u)^T)/2$, $\nabla \phi \odot \nabla \phi$ is the induced elastic tensor with the $(j, k)$-th entry being $\partial x_j \phi \partial x_k \phi$. The above equations have been used in [38] to analyze the motion of bubbles in a Newtonian fluid. These phase field models are also very similar to the liquid crystal model studied in [26, 37, 41].

The above simple system was used to study the free interface motion under the surface tension in the mixture of two Newtonian fluids with same density and viscosity constants. And we can think it is simple case of the fluid systems studied in Chapter 5. And the system similarly satisfies the following energy law:

$$
\frac{d}{dt} \int_{\Omega} \left\{ \frac{1}{2} |u|^2 + \frac{\lambda}{2} |\nabla \phi|^2 + \lambda F(\phi) \right\} dx = - \int_{\Omega} \left\{ \nu |\nabla u|^2 + \gamma \lambda (\Delta \phi - f(\phi))^2 \right\} dx. \quad (6.27)
$$

Moreover, the whole system can be viewed as the approximation of the classical sharp interface model with the kinematic and traction free boundary condition on the free
interface [38]. As the transition width $\epsilon$ approach zero, the induced bulk elastic stress term converges to the corresponding surface tension.

To test our formula for computing the Euler number, we solve the above system in two space dimension via a spectral spatial discretization coupled with a second order semi-implicit in time scheme for $\phi$ and a semi-implicit projection scheme for the Navier-Stokes equations as those in [26, 38].

Figure 6.14 shows a special example of the deformation of two Newtonian bubbles in another Newtonian fluid. In this experiment, we take the $128 \times 128$ grid, period boundary condition on area $[0, 2\pi] \times [0, 2\pi]$, and $\epsilon = 2.5h = 0.1227$, $\lambda = 10.0$, $\gamma = 3.0$, $\nu = 1.0$. In the simulation, the larger bubble grows at the expense of the shrinkage of the smaller one. In fact, the smaller bubble dissolves into the fluid while the bigger bubble absorbs from the fluid, similar to the well-known Oswald ripening effects (due to the Cahn-Hillard effect of the phase equation in (6.26)). The total volume of these two bubbles remains to a constant in time.

The topology change in this simulation can be characterized by the Euler number of the whole configuration. At the beginning, the Euler number of the configuration with the two bubbles is 2. And finally, after the smaller bubble is totally absorbed by the larger bubble, the Euler number of the bubble configuration becomes 1. Figure 6.15 shows the sharp change of Euler number in this procedure by using the formula (6.17).

6.5 Conclusion

While an important advantage of the Phase-field modelling of the interface variation and the interfacial motion is its ability to handle the change of interface topologies
in natural and physically meaningful ways, it has also come to our attention that in many practical problems, useful topological information may be in need and the effective control of the topological transformations may be important. In this chapter, mechanisms to retrieve relevant topological information based on the phase field formulations are discussed. In particular, some robust formulae for computing a generalized Euler number of the interface are proposed based on the phase field order parameter $\phi$. Using a special ansatz, we also get further simplified formulae. For smooth interfaces, our formulae give desired quantized characterization of the interface genus. When passing through singularities, they give fractional values that generalize the notion of the genus.

As a demonstration, numerical experiments are performed for the cases of a static deformation of a three dimensional axial symmetric membrane as well as a time dependent annihilation of fluid bubbles in two dimensional space. The experimental results show that the proposed methods for computing the Euler number is very effective and robust in detecting the topological changes. The ideas presented in this chapter are very natural and easy to implement for other phase field models also and may as well be equally applicable to other simulations methods for free boundary and interface problems including the standard level set methods.
Fig. 6.14. Deformation of two bubbles in a Newtonian fluid with the time valued at 0.00, 0.10, 0.18, 0.22, 0.24, 0.28.

Fig. 6.15. A plot of the Euler number in time with the annihilation of the small bubble.
Chapter 7

Conclusions and Current Work

7.1 Conclusion and remaining problems

A phase field approach for the deformation of a vesicle membrane minimizing the elastic bending energy is presented in both static and dynamic, axis-symmetric and non-symmetrical 3d cases. Theoretically and computationally, we verified the convergence of our phase field model to a sharp interface model. Furthermore, as a global method, our phase field model has advantage in avoiding tracking the free interfaces, and it can easily handle topological changes. Within the phase field framework, it is convenient to study the interaction of vesicle membranes with other external fields. Start from our phase field model, we can also recover the original sharp interface model in fluid fields. Some numerical schemes are discussed in all of these cases. A series of formulae for retrieving the Euler Number of the vesicles are given and discussed. We discover several axial symmetric configurations using numerical simulations and made a detailed examination of the energetic bifurcation landscape. The complete 3-d code for both the equilibrium shapes and the simulations in fluid fields realizes more complex experiments and gives more examples of the vesicle transformations in fluid fields.

There also are a number of issues that need further study, both analytically and computationally. In analysis, Theorem 2.2 proved the asymptotic limit of the phase field formulation in (2.10) under the ansatz (A1) and (A2) in section 2.4. one question
remained further is that how can we remove the ansatz. Theorem 2.8 verify the approximation of the penalty solution by numerical solutions for fixed transition layer width $\epsilon$. Theoretically, we need further $\epsilon \rightarrow 0$. It is another important issue to study for the relation between $\epsilon$ and grid mesh size $h$ when they go to 0 at the same time. This in fact related somehow to the error estimate of the approximation of the phase field function by numerical solutions.

Computationally, there are a lot work are in consideration. Experimentally, can we find more three dimensional non-symmetric shapes? At present, we already find the non-symmetric torus and some other structures with special topology structures such as that shows in Figure 4.15. Another important issue is the other global structure information besides the Euler number. Also how can we control the structures based on the Euler number and the other global information? Our current code are paralleled with OPENMP for shared memory clusters. The faster and even adaptive methods are required for simulating collective motion and interaction of multiple vesicles which requires higher resolution but with no added complexity.

### 7.2 On-going works

Although there is a lot of analytical and computational problems that need further consideration, there is a lot of works are already on the way. The first problem is the couple of our phase field formulation with other fields, such as the gravity field. Some preliminary vesicle equilibrium shapes already got and more works are on going to couple three systems together: phase field, fluids and gravity field.
Instead of merging together, another important issue is the study of the bumping and rebounding of two or several vesicles. Solving this problem need the combination of several phase field functions together instead of only one phase field function used in work already done. The zero level set of each phase field function represents a vesicle, we need add control avoiding their merging.

Also there are some problems are under going. The study of vesicle membranes interact with laser beams and electric fields; models for other lipid structures, such as micelles; multi-scale models for flows with large number of vesicles.

In all of these works, we are collaborating with biologists and trying to transfer the techniques here useful tools that can be applied broadly in biological studies.
References


Vita


Xiaoqiang Wang’s current research interest is in the fields of applied mathematics and scientific computation. His work at Penn State involves numerical simulation and analysis, algorithms for image processing, data mining, parallel algorithms and high-performance computing.