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ANALYSIS OF A MIXED FINITE ELEMENT METHOD FOR A PHASE FIELD BENDING ELASTICITY MODEL OF VESICLE MEMBRANE DEFORMATION *[1)]

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Dedicated to the 70th birthday of Professor Lin Qun

Abstract

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

Mathematics subject classification: 65N12, 65N12, 65N30, 49J45, 92C37, 92C05.
Key words: Bio-membrane, Elastic bending energy, Phase field, Finite element, Nested mixed saddle point formulation, Optimal error estimates.

1. Introduction

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

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

$$E = \int_\Gamma \left\{a_1 + a_2(H - c_0)^2 + a_3 G\right\} ds, \tag{1.1}$$

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where a_1 represents the surface tension, $H = \frac{k_1+k_2}{2}$ is the mean curvature of the membrane surface, with k_1 and k_2 as the principle curvatures, and $G = k_1k_2$ is the Gaussian curvature. The coefficient a_2 is the bending rigidity and a_3 the stretching rigidity, and c_0 is the spontaneous curvature that describes the asymmetry effect of the membrane or its environment. The equilibrium membrane configurations are the minimizers of the energy subject to given surface area and volume constraints [17].

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

$$E_{elastic} = \int_\Gamma H^2 ds \,, \tag{1.2}$$

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

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

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

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

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

The surface area and volume constraints can be specified as

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

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

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

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