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

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

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

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

1. Introduction

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

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

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

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

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

its corresponding form in the phase field model is given by

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

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The surface area and volume constraints can be specified as

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

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

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

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

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

2. Spatial discretization of the equilibrium problem

We begin with the spatial discretizations of the equilibrium problem. The numerical schemes developed in [12] and subsequently in [10, 13] include standard finite difference, finite element and Fourier spectral methods, which were shown to have their own advantages and limitations in the practical implementation, depending on the boundary conditions and the problems to be simulated. Here, we focus mainly