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Computation of Two-Phase Biomembranes with Phase Dependent Material Parameters Using Surface Finite Elements

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Abstract. The shapes of vesicles formed by lipid bilayers with phase separation are governed by a bending energy with phase dependent material parameters together with a line energy associated with the phase interfaces. We present a numerical method to approximate solutions to the Euler-Lagrange equations featuring triangulated surfaces, isoparametric quadratic surface finite elements and the phase field approach for the phase separation. Furthermore, the method involves an iterative solution scheme that is based on a relaxation dynamics coupling a geometric evolution equation for the membrane surface with a surface Allen-Cahn equation. Remeshing and grid adaptivity are discussed, and in various simulations the influence of several physical parameters is investigated.

AMS subject classifications: 49Q10, 65M60, 74S05, 74G15, 74L15, 82B26, 92C10

Key words: Biomembrane, surface finite elements, relaxation dynamics.

1 Introduction

The basic components of cell boundaries and organelles are bilayers consisting of phospholipids that spontaneously form when introduced into an aqueous environment in appropriate concentration. Vesicles or bags formed by such biomembranes show a great variety of shapes and have been attracting interest from various fields. First, the geometry and composition are conjectured to contribute to and interact with cell processes. Second, the lipid bilayers possess intricate mechanical properties which partially are solid-like, namely they reveal a stiffness against stretching and bending, but are unable to sustain

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shear stress and so also behave like a viscous fluid within each of the monolayers. Mathematicians finally are attracted by the geometric properties of the membrane but also by the patterns that phases within the membrane may form. Such phase separation phenomena are due to the different types of lipids of which the membrane consists. Here we wish to consider computational simulations and modeling in the context of a partial differential equation model which couples the geometric equation for the membrane surface to a diffusion equation on the surface which defines the surface phase separation. We begin by describing the model.

The classical biomembrane mechanics theory developed in [10, 27, 32] models the vesicle boundary as a hypersurface on which the following elastic energy functional is defined:

$$\mathcal{F}_{CEH}(\Gamma)=\int_\Gamma \frac{k_\kappa}{2}(\kappa-\kappa_s)^2+\int_\Gamma k_g g. \tag{1.1}$$

Here, the mean curvature (sum of the principal curvatures) of the membrane is denoted by κ and the Gaussian curvature by g and $k_\kappa>0$ (bending rigidity) and k_g (Gaussian bending rigidity) are material dependent elasticity parameters while the number κ_s is known as the spontaneous curvature. A lateral phase separation due to a decomposition of the different lipid molecules has been observed and recently been made visible [5,6,43]. Line tension is observed at the phase interfaces and in [34,35] an energy functional of the form

$$\mathcal{F}_{SI}(\Gamma,\gamma)=\mathcal{F}_B(\Gamma,\gamma)+\mathcal{F}_L(\Gamma,\gamma)=\sum_{i=1}^{2}\Big(\int_{\Gamma_i}\frac{k_\kappa^{(i)}}{2}(\kappa-\kappa_s^{(i)})^2+\int_{\Gamma_i}k_g^{(i)}g\Big)+\int_\gamma\bar{\sigma} \tag{1.2}$$

was proposed. The two-phase membrane, $\Gamma=\Gamma_1\cup\Gamma_2\cup\gamma$, consists of two smooth, not necessarily connected surfaces Γ_i with a common boundary γ which is the phase interface. The constant parameter $\bar{\sigma}$ denotes the energy density of the interfacial energy. An intricate issue is the smoothness across the phase interface. As in [35], Section II.B, we assume a C^1 surface which means that the external unit normal of the enclosed vesicle domain is continuous. This assumption is motivated by the fact that the lipid bilayer should be intact across the interface. However, higher order derivatives in general are discontinuous. For instance, we will see that the mean curvature is subject to a jump condition in equilibrium. But we want to mention that C^0 surfaces may be considered [33], motivated from the pictures in [6] which, on a macroscopic scale, reveal kinks at the phase interfaces.

In order to deal with the line energy we consider a phase field approach and introduce an order parameter c to distinguish the two phases. The states $c=-1$ and $c=1$ then correspond to the two phases and the phase interfaces are replaced by thin layers across which c changes is value rapidly but smoothly. To achieve this we replace the line energy $\mathcal{F}_L$ by a Ginzburg-Landau energy of the form

$$\mathcal{F}_{GL}(\Gamma,c)=\int_\Gamma\sigma\Big(\frac{\varepsilon}{2}|\nabla_\Gamma c|^2+\frac{1}{\varepsilon}\psi(c)\Big). \tag{1.3}$$

The function $\psi(c):=(1-c^2)^2/2$ is a double-well potential with minima in $c=1$ and $c=-1$ which favors the two phases. Denoting by $\boldsymbol{\nu}$ the external unit normal to Γ and