

Phase-field modeling and simulations of multicomponent cell membranes

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In this talk, we report some of recent works with current and former colleagues at Penn State (S. Das, M. Li, C. Liu, R. Ryham, X. Wang and J. Zhang) on the phase field modeling and simulations of the vesicle membrane deformation under elastic bending energy and the interaction with background fluid flows and other external fields. We discuss the relations between the phase field model and the sharp interface limits and numerical simulations of membranes with various topology and multiple components.

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1 Modeling and simulation of biomembranes

Biomembranes are a mixture of many different types of lipidic and protein components, and their relative amounts and composition differ between functionally distinct domains. In equilibrium membranes and in particular vesicles have been investigated intensively using a curvature-elastic model. However today curvature is no longer seen as a passive consequence of cellular activity but an active means to create membrane domains and to organize centres for membrane trafficking. Membrane curvature is thus a prime player in growth, division and movement of cells.

Recent advancements in applied mathematics allow the simulation of dynamic evolution of vesicles, with multiple components under the influence of flow. The underlying model includes the interaction of liquid with the elastic membrane, phase separation and coarsening of composition on the membrane and the geometric evolution of the membrane according to curvature effects. The problem is a highly nonlinear free boundary value problem for which various numerical methods have been developed including phase-field, level-set and immersed boundary methods.

2 Phase Field/Diffuse Interface Methods for Vesicle Membranes

Given an interface Γ , in the diffuse interface description, a smoothly defined phase field function (or order parameter) ϕ , which is defined in a computational domain Ω , and is nearly ± 1 on the two sides of Γ and has a thin *diffuse transition layer* (its thickness is typically characterized by a small parameter ϵ). The surface Γ is recovered as the zero level set of ϕ . To construct a diffuse interface or phase field model, a key question to be answered would then be: how can one use such a function ϕ to represent the various geometric features and physical properties associated with the interface Γ ?

For vesicle membranes, the bending elasticity model is a widely used model which postulates that the bending energy

$$E_b = \int_{\Gamma} \frac{k}{2} H^2 ds, \quad (1)$$

is minimized under given volume and surface area constraints. Here, k is the bending modulus and H is the mean curvature of the vesicle surface Γ . The corresponding phase field formulation of the bending energy is given by

$$\mathcal{E}_{\epsilon}^b(\phi) = \frac{k}{2\epsilon} \int_{\Omega} \left(\epsilon \Delta \phi + \frac{1}{\epsilon} \phi(1 - \phi^2) \right)^2 dx. \quad (2)$$

Such a formulation has been first established in [8], its various generalizations, the mathematical properties like the well-posedness and sharp interface limit, and numerical algorithms and simulations, have been subsequently studied in [3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 17]. Detailed presentation on the adaptive numerical methods is given in the talk ICIAM minisymposium talk 0156.

3 Multicomponent vesicle membranes

In recent experimental studies, multi-component vesicles with different lipid molecule compositions (and thus phases) have been shown to display even more complex morphology involving rafts and micro-domains [1, 14]. There is strong evidence suggesting that phase segregation and interaction contribute critically to the membrane signaling, trafficking and sorting processes [15].

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With the two phases co-existing on the membrane, it is natural to introduce a line tension on γ_0 to take into account the interfacial energy between the individual components [1]. Together with the bending elastic energy, this leads to the following energy for a two-component membrane

$$E = E_1 + E_2 + \int_{\gamma_0} \delta dl, \quad E_i = \int_{\Gamma_i} k_i (H - c_i)^2 ds, \quad (i = 1, 2) \quad (3)$$

with δ being the surface tension, γ_0 the phase boundary, and k_i, c_i the individual bending modulus and spontaneous curvature in each component Γ_i . The competition between the surface energies and the line tension gives rise to the complex morphology observed in the experiments.

In [17], diffuse interface (phase field) models are developed for multi-component vesicle membranes with different lipid compositions and membranes with free boundary, with the introduction of a second phase field function (order parameter) in addition to the function ϕ that describes the vesicle surface. These models are used to simulate the deformation of membranes under the elastic bending energy and the line tension energy with prescribed volume and surface area constraints. The model can be easily generalized to deal with single component membranes with a free boundary by viewing it as a special case of a two-component membrane with one virtual component having zero bending rigidity.

By comparing our numerical simulations with recent biological experiments, it is demonstrated that the diffuse interface models can effectively capture the rich phenomena associated with the multi-component vesicle transformation and thus offering great functionality in their simulation and modelling [17].

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