Surface phase separation and morphological transition of a multicomponent vesicle

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Introduction

Vesicle membranes usually have bilayer structures composed by lipid molecules with hydrophilic heads and hydrophobic tails (gathering together inside the structure). As the principal components of living cells, bilayer membranes play important roles in cell functions such as solute transport. Due to their highly flexible structures, the membranes exhibit rich shape transition behaviors. For example, recent experiments of giant unilamellar vesicles (GUV) [2] reveal that lipid bilayer membranes shows the formation of viscous fingering and budding (growth of a small vesicle from a larger one via shape transitions). Physical processes like phase separation and coarsening are usually coupled with these morphological changes [2].

A theory of equilibrium shapes of two-component vesicles was first developed by Julicher and Lipowsky [3] and was later used successfully by Baumgart et al. [2] to compare with experimental results on GUVs. In [7], a dynamical approach was developed that couples interface dynamics with a surface phase-field equation without flow. Reduced models (e.g. long-wave type approximations) were considered in [8, 5, 6, 9] and discrete methods (e.g. Monte-Carlo, dissipative particle dynamics) have been developed to evolve the coupled phase-field/membrane system[4, 1]. Note that the effects of flow were considered only in [5].

The model

We consider a simplified version of the Helfrich model [10] for fluid-like vesicle membranes. We focus on the effects of inhomogeneous surface tension and neglect bending and spontaneous curvature. Though simplified, the model is capable of describing the nonlinear coupling among the flow, vesicle morphology and the evolution of the surface phases.

The surface energy of the vesicle is assumed to depend on the concentration of the surface components. An additional energy is introduced to describe the chemical potential of surface phases (Cahn-Hilliard type). These yield generalized, thermodynamically consistent surface

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tension forces imparted to the flow. On the surface, the phases evolve according to a high-order, advection-reaction-diffusion equation of Cahn-Hilliard type.

The method and results

Because of the presence of high-order nonlinear interactions in these physical processes, it is highly challenging to simulate phase decomposition and motion of phase boundaries on a moving surface. Here we develop a method that combines the immersed interface method to solve the flow equations and the Laplace-Young jump conditions, the level-set method to represent and evolve the surface, and a non-stiff Eulerian algorithm to update the concentration on the surface.

As an example, we consider a long ellipse-like vesicle, half with the low concentration (i.e. high surface tension) and the other half with high concentration. As is typical in vesicle dynamics, the volume and surface area are conserved. During the evolution, surface tension drives the half with low concentration to a semi-circle; the other half, however, experiences a complicated morphological transition and forms a bud at later times, see Figure 1.

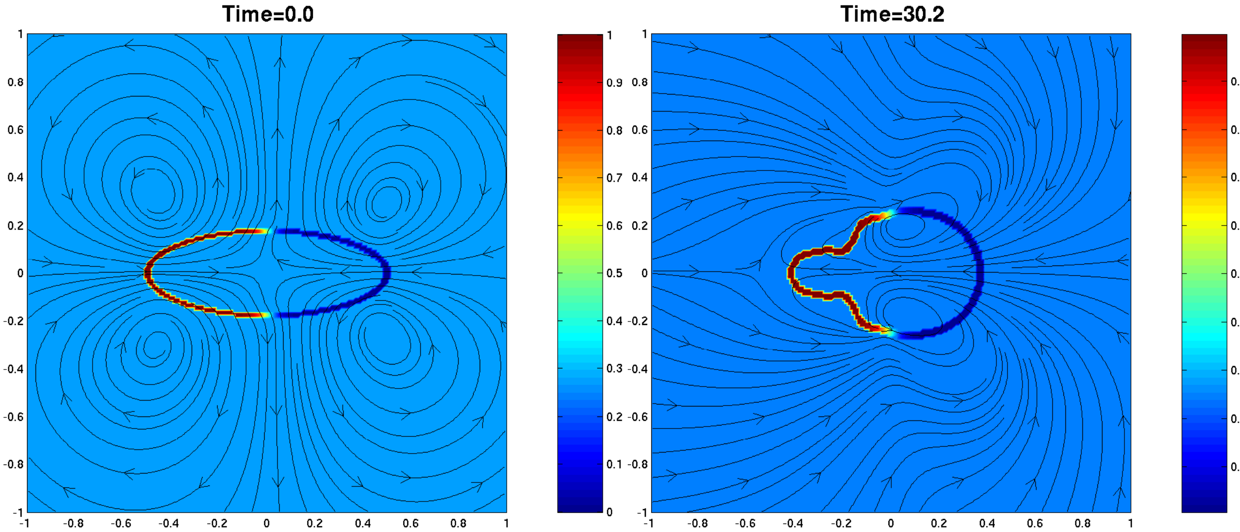

Figure 1: Bud formation without bending. Left: initial phase configuration and velocity field; Right: phase configuration and velocity field at later times.

Future work

We plan to include the effects of bending and spontaneous curvature. Also, we plan to connect our current algorithm with the boundary integral method to accurately compute the bending terms in surface tension, and we will extend our algorithms to three-dimension.

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