Phase Field method for Equilibrium Vesicle Shapes



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Cell membrane shapes

Most part of the biological membranes is composed by lipid, a molecule with one polar head and one or more tails. On a cell membrane lipids form a bilayer structure, which is a basic building block of almost all the cell membranes. Put the isolated lipids into the water, they will spontaneously form a variety of structures.



With constraints:

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

$$B(\Phi) = \int_{\Omega} \frac{\epsilon}{2} |\nabla \Phi|^2 + \frac{1}{4\epsilon} (\Phi^2 - 1)^2 dx = \beta$$
(5)

over the admissible set:

$$L = \{ \Phi \in H^2 | \Phi |_{\partial \Omega} = -1, \nabla \Phi \cdot n |_{\partial \Omega} = 0 \}$$
 (6)

Numerical Results

The purpose of our research is to study the deformation and interaction of vesicle membranes in equilibrium shapes or under external fields.

Elastic Bending Energy

One simplistic model of vesicle membranes was first studied by Canham, Evans and Helfrich (see reference 1), in which the equilibrium shape of biomembranes is mainly determined by the curvature of the surface.

The basic assuption in this model is that the equilibrium shape of such a membrane is determined by minimizing the elastic bending energy:

$$E = \int_{\Gamma} a_1 + a_2 (H - c_0)^2 + a_3 K ds, \qquad (1)$$

Where $H = \frac{k_1 + k_2}{2}$ is the mean curvature of the membrane surface.

a_1	surface tension
<i>a</i> ₂	bending rigidity
<i>a</i> ₃	bending rigidity
C_0	spontaneous curvature

Start from an ellipse disc flat enough, with time marching, it will pinch into a pancake. With enough calculating time until the energy reaches minimum, it will pinch off into a torus.



Future Work

Some people suggested another form of elastic bending energy:

$$E = \int_{\Gamma} a_1 + a_2 (H - c_0)^2 + a_3 K ds + k (\int_{\Gamma} H ds - h_0)^2$$
(7)

Whether the phase field function still holds for this form needs to be discussed.

Another topic is the interaction between two vesicle membranes. The energy model will be built and numerical results be presented.

Also considering a cell moving in a vein, we need to think about the pressure the cell gives to the fluid. Numerical results will be given for fluid coupled system although it would be more complicated.

Table 1: The explanation of the parameters.

Phase Field Model

The phase field function is chosen as a Tanh format to simulate the distance of points in the domain to the membrane surface. The nodes inside the cell are set to be 1 while outside to be -1:

$$\Phi(x) = \tanh(\frac{d(x)}{\sqrt{2}\epsilon})$$

Our phase field model is the variational problem:

$$\min_{\Phi \in L} E(\Phi) = \int_{\Omega} \frac{k}{2\epsilon} (\epsilon \triangle \Phi + (\frac{1}{\epsilon} + c_0 \sqrt{2})(1 - \Phi^2))^2 dx$$
(3)

Reference

P. G. Ciarlet

(2)

Introduction to linear shell theory,

vol. 1 of Series in Applied Mathematics (Paris), Gauthier-Villars, Editions Scientifiques et Medicales Elsevier, Paris, 1998.

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