Investigating Vesicle-substrate Adhesion Using Two Phase Field Functions

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Adhesion of Vesicle to Substrate

Vesicle-substrate adhesion is a ubiquitous phenomenon in our world. Various Application of this kind of adhesion in bio-medical science happens in:

- target plasma
- stem cells
- leukocytes rolling

It is interesting and also necessary to understand the behavior of a cell membrane (phospholipid bilayer structured) interacting with a hard wall such as vessel wall. and

$$A(\Phi_1) = \int_{\Omega} \frac{\epsilon}{2} |\nabla \Phi_1|^2 + \frac{1}{4\epsilon} (\Phi_1^2 - 1)^2 dx = \beta.$$
 (5)

Gradient Flow method is used to carried out the computational work on this problem:

$$\frac{d\Phi_1}{dt} = -\gamma \frac{\delta E(\Phi_1, \Phi_2)}{\delta \Phi_1} \tag{6}$$

Numerical Results





Bending Energy and Contact Potential

The sharp interface model describing the vesicle substrate system is a combination of elastic bending energy of a membrane and contact potential energy between the membrane and the substrate:

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

Where $H = \frac{k_1 + k_2}{2}$ is the mean curvature of the membrane surface and W = W(d(x)) is the potential depending on the distance to the susbtrate.

Phase Field Model

Our phase field function has a tanh profile with the

Listed below are three adhesion situations due to different substrate shapes, the first one with a straight flat substrate, the second one with a convex cylindrical substrate and the third one with a concave cylindrical substrate.



Also the effect of transitional layer width is shown on a sliced view of vesicle, left figure with small width and right figure with large width.



Reference

P. G. CIARLET, *Introduction to linear shell theory*, vol. 1 of Series in Applied Mathematics (Paris), Gauthier-Villars, Editions Scientifiques et Medicales Elsevier, Paris, 1998.

value outside the membrane being -1 and inside the membrane being +1. The width of the transitional layer simulating the membrane surface is controlled by the small parameter ϵ :

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

Our phase field model is the variational problem:

$$\min E(\Phi_{1}, \Phi_{2}) = \frac{k}{2\epsilon} \int_{\Omega} (\epsilon \bigtriangleup \Phi_{1} + (\frac{1}{\epsilon} + c_{0}\sqrt{2})(1 - \Phi_{1}^{2}))^{2} dx \qquad (3)$$
$$+ \frac{1}{2\epsilon} \int_{\Omega} (1 - \Phi_{1}^{2})(1 - \Phi_{2}^{2}) dx$$

With constraints of prescribed volume and surface area of the vesicle:

$$V(\Phi_1) = \int_{\Omega} \Phi_1 dx = \alpha, \tag{4}$$

X. WANG, *Phase Field Models And Simulations Of Vesicle Biomembranes*, Thesis for Doctor of Philosophy, August 2005.

B. ALBERTS, A. JOHNSON, J. LEWIS, M. RAFF, K. ROBERTS AND P. WALTER, *Molecular Biology of the Cell*, 4th ed. Garland Science, New York, 2002.

P. S. SWAIN AND D. ANDELMAN, *The influence of substrate structure on membrane adhesion*, Langmuir 15, pp. 8902-8914, 1999.

S. DAS, Q. DU, *Adhesion of vesicles to curved substrates*, Physical Review E 77, 011907, 2008.

J. ZHANG, S. DAS, Q. DU, *A phase field model for vesicle-substrate adhesion*, Journal of Computational Physics 228, 7837-7849, 2009.