Investigation on Vesicle-Substrate Adhesion by Using Two Phase Field Functions

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Abstract

A phase field model for simulating the adhesion of a cell membrane to a substrate is constructed. The model features two phase field functions which are used to simulate the membrane and the substrate. An energy model is developed considering both elastic bending energy and adhesive potential energy as well as, through a penalty method, volume and surface area constraints.

Elastic Bending Energy

The sharp interface model of the elastic bending energy involves the integral of the squared mean curvature along a membrane surface, i.e.,

$$E_b = k\int_\Gamma (H - c_0)^2 ds. \quad (1)$$

The phase field formula for the elastic bending energy of the vesicle (1) is given by

$$W(\phi_1) = \int_\Omega \frac{k}{2\epsilon}\Big(\epsilon\Delta\phi_1 + (\frac{1}{\epsilon}\phi_1 + c_0\sqrt{2})(1-\phi_1^2)\Big)^2 dx, \quad (2)$$

with surface area

$$A(\phi_1) = \int_\Omega \Big(\frac{\epsilon}{2}|\nabla\phi_1|^2 + \frac{1}{4\epsilon}(\phi_1^2 - 1)^2\Big) dx \quad (3)$$

and volume difference

$$V(\phi_1) = \int_\Omega \phi_1\, dx. \quad (4)$$

Adhesive Potential Energy

Due to various forces between the membrane and the substrate, adhesion will take place when those two structures come close. One of our crucial task when modeling the adhesion is to represent the adhesive potential energy between them. We propose a formula denoting this energy

$$S(\phi_1, \phi_2) = \frac{1}{2\epsilon}\int_\Omega (\phi_1^2 - 1)(\phi_2^2 - 1) dx, \quad (5)$$

which approaches the sharp interface limit

$$E_p = \int_\Gamma W ds \quad (6)$$

as $\epsilon \to 0$. This requires a decomposition from an intergral in 3D space to a composite of an integral on the membrane surface and an integral along the integral curve (see [1, Lemma 2.1]).

Total Energy and Gradient Flow

The total energy for our phase field model to simulate vesicle-substrate adhesion is given by

$$E(\phi_1, \phi_2) = W(\phi_1) - \sigma(\phi_1, \phi_2), \quad (7)$$

whereas the constraints are given by

$$V(\phi_1) = \alpha_1, \quad A(\phi_1) = \beta_1, \quad (8)$$

with α_1 and β_1 denoting the prescribed values for the volume difference and surface area, respectively. We use a penalty formulation to impose the constraints into the total energy

$$E_M(\phi_1, \phi_2) = W(\phi_1) - \sigma S(\phi_1, \phi_2) + \frac{1}{2}M_A(V(\phi_1) - \alpha_1)^2 + \frac{1}{2}M_B(A(\phi_1) - \beta_1)^2. \quad (9)$$

We use gradient flow method to carry out our computational process. We keep ϕ_2 fixed while ϕ_1 is updated for each time step,

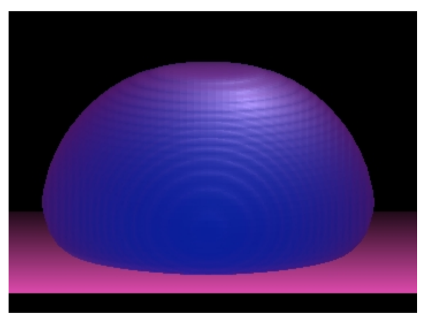
$$\phi_t = -\gamma\frac{\delta E_M(\phi_1, \phi_2)}{\delta\phi_1}. \quad (10)$$

Theoretical analysis [2, Theorem 2.6] shows that as the penalty energy E_M reaches its local minimum, the total energy E is also minimized if the penalty coefficients M_A and M_B both tend to infinity.

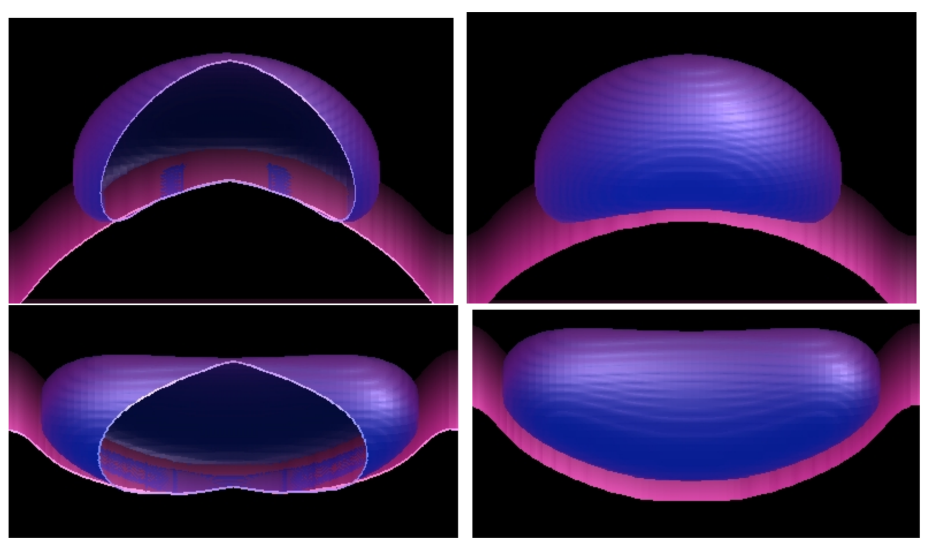
Numerical Results

Our computational domain is set to be $[-\pi, \pi]^3$. The mesh size is always set as 65x65x64. The Bending regidity is always fixed at 1.00. The coefficient γ before the variation is always set at 0.50.

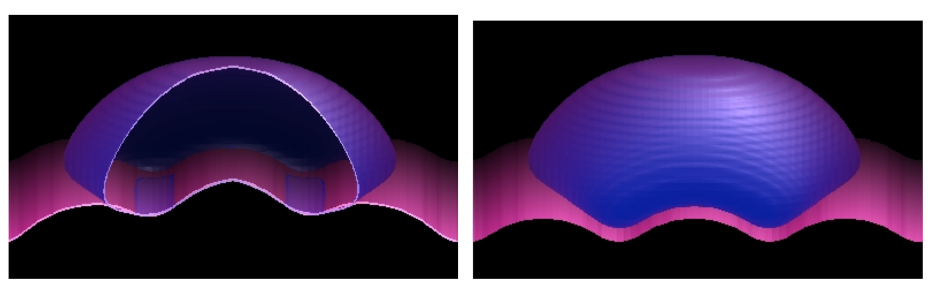
Adhesion to A Flat Substrate



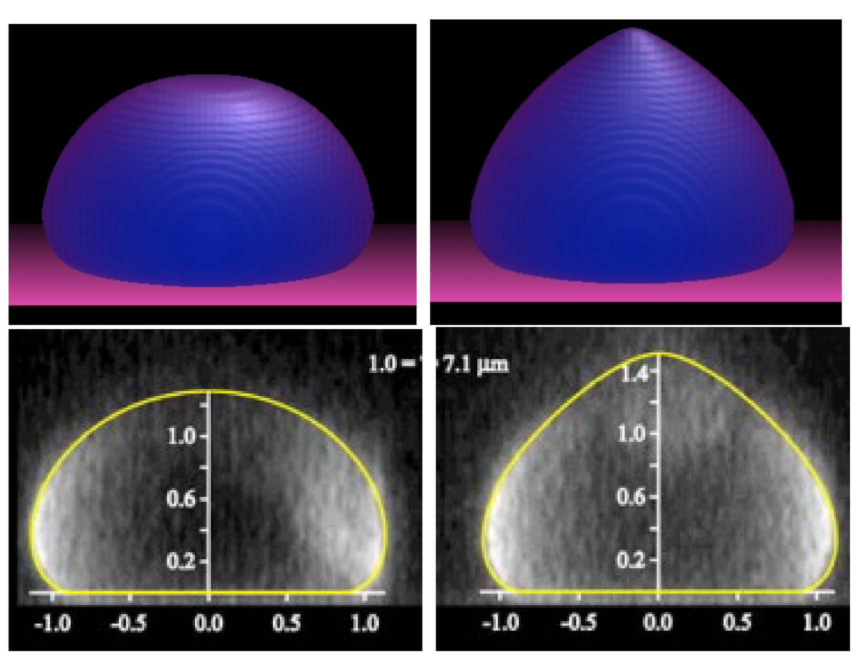
Adhesion to A Bending Substrate



Adhesion to A Perturbed Substrate



Adhesion with A Pulling Force



The bottom two pics are from [3].

References

[1] Q. Du, C. Liu, R. Ryham, and X. Wang, *A phase field formulation of the Willmore problem*, Nonlinearity, 18, pp. 1249-1267, 2005.

[2] X. Wang, *Phase field models and simulations of vesicle biomembranes. Diss.*, The Pennsylvania State University, 2005.

[3] A. Smith, B. Lorz, S. Goennenwein, and E. Sackmann, *Force-Controlled Equilibria of Specific Vesicle-Substrate Adhesion*, Biophysical Journal, Volume 90, Issue 7, 1 April 2006, Pages L52-L54.