Tracking Vesicle-Vesicle Adhesions Using Multiple Phase Field Functions

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Abstract

A phase field model for simulating the adhesion between two vesicles is constructed. Two phase field functions are introduced to simulate each of the two vesicles. An energy model is defined which accounts for the elastic bending energy of each vesicle, the contact potential energy between the two vesicles, and the vesicle volume and surface area constraints through a penalty method.

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.,

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

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

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

with surface area

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

and volume difference

$$V(\phi_1) = \int_\Omega \phi_1\, dx. \tag{4}$$

Adhesive Potential Energy

Due to various forces between the membranes, adhesion will take place when they come close enough. Therefore, 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

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

which approaches the sharp interface limit

$$E_p = \int_\Gamma W ds \tag{6}$$

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-vesicle adhesion is given by

$$E(\phi_1,\phi_2) = W(\phi_1) + W(\phi_2) - \sigma S(\phi_1,\phi_2), \tag{7}$$

whereas the constraints are given by

$$V(\phi_1) = \alpha_1, \quad A(\phi_1) = \beta_1, \quad V(\phi_2) = \alpha_2, \quad A(\phi_2) = \beta_2, \tag{8}$$

with α_1, α_2 and β_1, β_2 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

$$\begin{aligned} E_M(\phi_1,\phi_2) = {} & W(\phi_1) + W(\phi_2) - \sigma S(\phi_1,\phi_2) \\ & + \frac{1}{2}M_{A1}(V(\phi_1)-\alpha_1)^2 + \frac{1}{2}M_{B1}(A(\phi_1)-\beta_1)^2 \\ & + \frac{1}{2}M_{A2}(V(\phi_2)-\alpha_2)^2 + \frac{1}{2}M_{B2}(A(\phi_2)-\beta_2)^2. \end{aligned} \tag{9}$$

We use gradient flow method to carry out our computational process. For each step we update both ϕ_1 and ϕ_2.

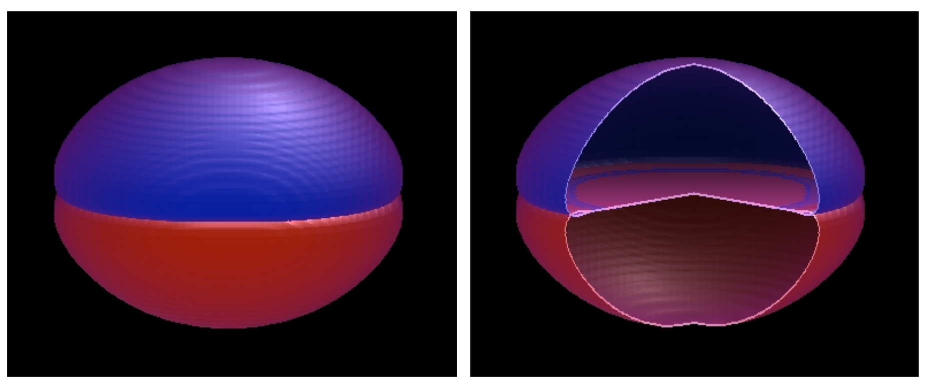
$$\partial_t\phi_i = -\frac{\delta E_M}{\delta\phi_i}, \quad i = 1, 2. \tag{10}$$

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_{Ai} and M_{Bi} both tend to infinity.

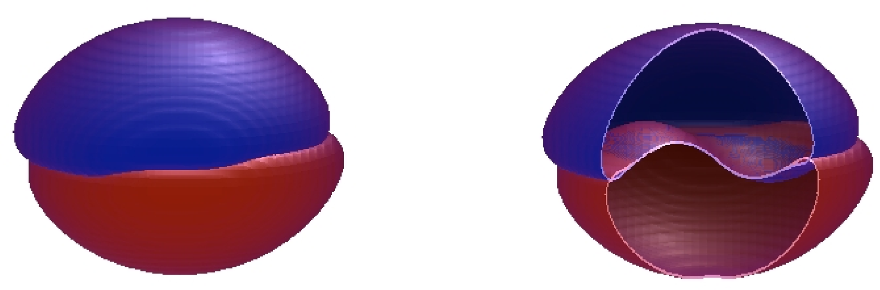
Numerical Results

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 otherwise indicated. The coefficient γ before the variation is always set at 0.50.

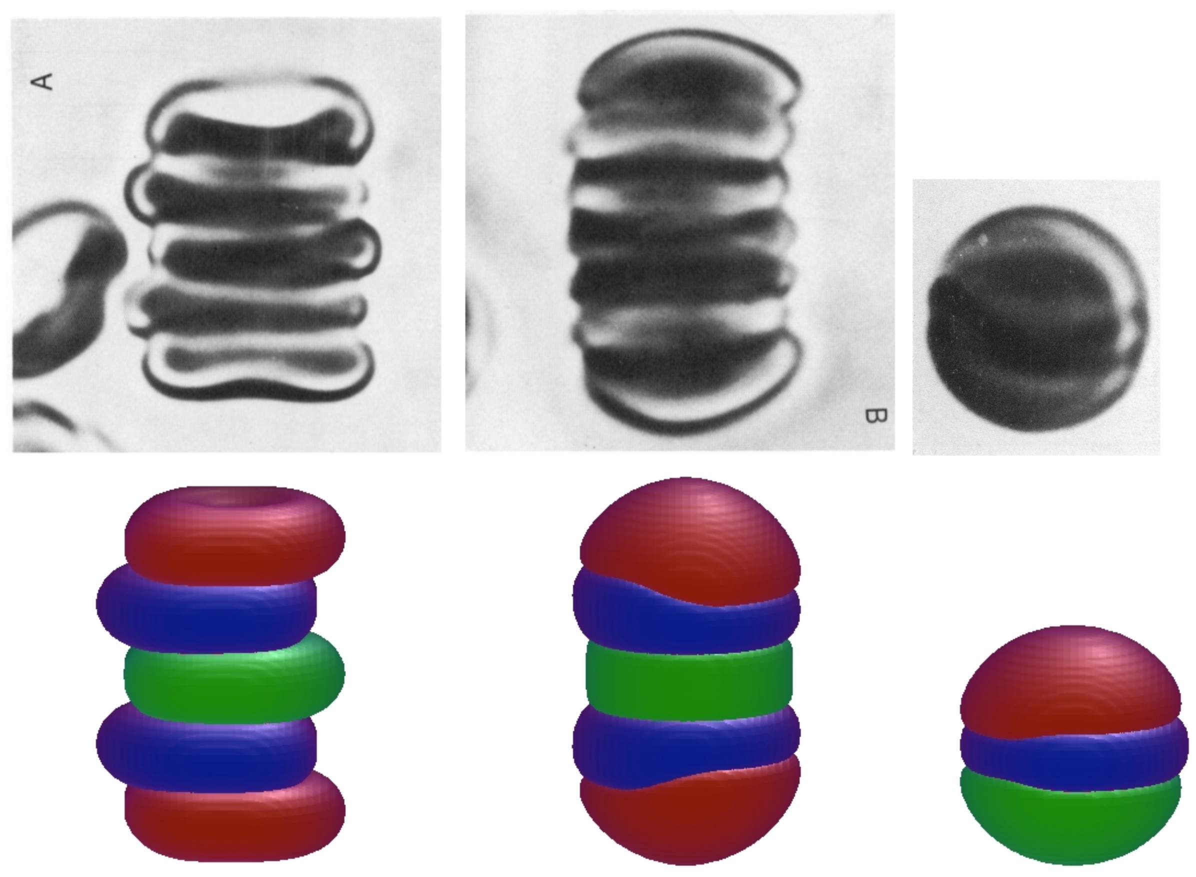
Flat contact of a doublet



Sigmoidal contact of a doublet



Contact of a rouleaux



The pics on the first row 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] Skalak R. et al. *Mechanics of rouleau formation.* Biophysical journal 35.3 (1981): 771-781.