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.,

$$E_b = k \int (H - c_0)^2 dx.$$  \hspace{1cm} (1)

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

$$W(\phi_1) = \int_{\Omega} \left( \frac{1}{2} |\nabla \phi_1|^2 + \frac{1}{2c_0^2}(\phi_1^2 - 1)^2 \right) dx,$$  \hspace{1cm} (2)

with surface area

$$A(\phi_1) = \int_{\Omega} \frac{1}{2} |\nabla \phi_1|^2 dx$$  \hspace{1cm} (3)

and volume difference

$$V(\phi_1) = \int_{\Omega} \phi_1 dx.$$  \hspace{1cm} (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 tasks when modeling the adhesion is to represent the adhesive potential energy between them. We propose a formula denoting this energy

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

which approaches the sharp interface limit

$$E_p = \int W ds$$  \hspace{1cm} (6)

as $\epsilon \to 0$. This requires a decomposition from an integral 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

$$E(\phi_1, \phi_2) = W(\phi_1) + W(\phi_2) - \sigma S(\phi_1, \phi_2),$$  \hspace{1cm} (7)

whereas the constraints are given by

$$V(\phi_1) = a_1, \quad A(\phi_1) = \beta_1, \quad V(\phi_2) = a_2, \quad A(\phi_2) = \beta_2,$$  \hspace{1cm} (8)

with $a_1, a_2$ and $\beta_1, \beta_2$ 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

$$E_M(\phi_1, \phi_2) = W(\phi_1) + W(\phi_2) - \sigma S(\phi_1, \phi_2)$$

$$+ \frac{1}{2} M_{A1}(V(\phi_1) - a_1)^2 + \frac{1}{2} M_{B1}(A(\phi_1) - \beta_1)^2$$

$$+ \frac{1}{2} M_{A2}(V(\phi_2) - a_2)^2 + \frac{1}{2} M_{B2}(A(\phi_2) - \beta_2)^2.$$  \hspace{1cm} (9)

We use gradient flow method to carry out our computational process. For each step we update both $\phi_1$ and $\phi_2$,

$$\partial_t \phi_i = -\frac{\delta E_M}{\delta \phi_i}, \quad i = 1, 2.$$  \hspace{1cm} (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 $M_{A1}$ and $M_{B1}$ 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 rigidity is always fixed at 1.00 otherwise indicated. The coefficient $\gamma$ 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