Topology-preserving phase-field modeling of elastic bending energy

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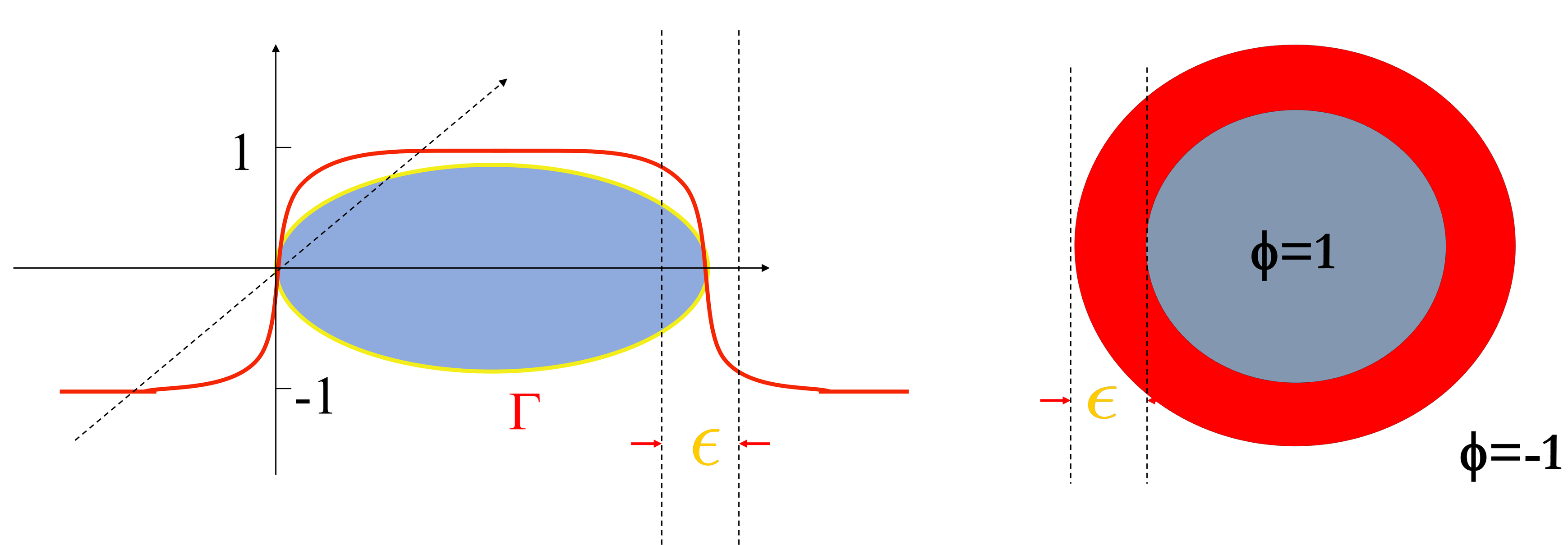
Abstract

In bio-membranes, the minimum of the elastic bending energy determines the equilibrium shape. We can formulate the energy using a phase-field function and optimize it using the standard gradient flow approach. In simulations, we impose surface area and volume constraints to force membranes to take on various shapes. Most previous works ignore the Gaussian curvature from the elastic bending energy, which allows the numerical simulations to automatically handle topological changes to the configurations of vesicle membranes. Our research recognizes that in some events (such as in the simulation of blood cells), it might be important to preserve the topological information. In this study, we add a topological constraint to the other constraints imposed on membranes and calculate the equilibrium shapes.

Formulation of the energy and the constraints

We use a phase-field function, $\phi(x) = \tanh\left(\frac{d(x,\Gamma)}{\sqrt{2}\epsilon}\right)$, defined on a computational domain Ω, to track the surface of the membrane. The level set $\{x: \phi(x) = 0\}$ is the membrane, $\{x: \phi(x) > 0\}$ is inside of the membrane and $\{x: \phi(x) < 0\}$ is outside of the membrane.



The elastic bending energy is given by

$$E_0 = \int_\Gamma a_1 + a_2(H - c_0)^2 + a_3 G \, ds,$$

where: a_1 = surface tension, H = mean curvature of the surface
a_2 = bending rigidity, G = Gaussian curvature of the surface
a_3 = stretching rigidity, c_0 = spontaneous curvature

We simplify the energy E_0 to

$$E = \int_\Gamma H^2 \, ds.$$

Now, using the phase-field function $\phi(x)$, the energy E is

$$E(\phi) = \int_\Omega \frac{\epsilon}{2}\left|\Delta\phi + \frac{1}{\epsilon^2}(\phi^2 - 1)\phi\right|^2 d\mathbf{x}.$$

We optimize the energy using the standard gradient flow approach,

$$\frac{\partial E(\phi)}{\partial t} = -\frac{\delta E(\phi)}{\delta\phi} = -\epsilon\Delta f(\phi) + \frac{1}{\epsilon}(3\phi^2 - 1) f(\phi),$$

with $f(\phi) = \Delta\phi - \frac{1}{\epsilon^2}(\phi^3 - \phi)$.

Constraints

1. Volume:
The inside volume of the membrane is

$$V(\phi) = \int_\Omega \frac{1}{2}(\phi + 1)\, d\mathbf{x}.$$

In 2D, $V(\phi)$ = the area of the membrane.

2. Surface area:

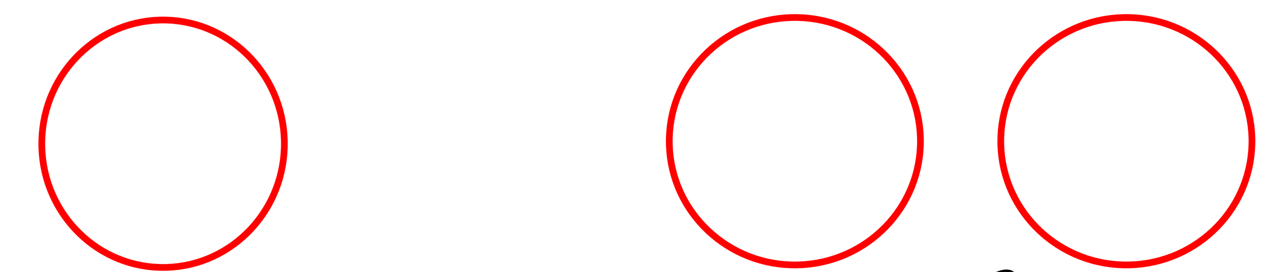
$$A(\phi) = \frac{3}{2\sqrt{2}}\int_\Omega \frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{4\epsilon}(\phi^2 + 1)\, dx.$$

In 2D, $A(\phi)$ = the circumference of the membrane.

3. Topology
In 2D, the total curvature is an integer multiple of 2π, called the index or turning number (χ) of the curve.

$$2\pi\chi = \int_\Gamma K \, dr,$$

where K is the curvature of the curve.



$\chi = 1$ $\chi = 2$

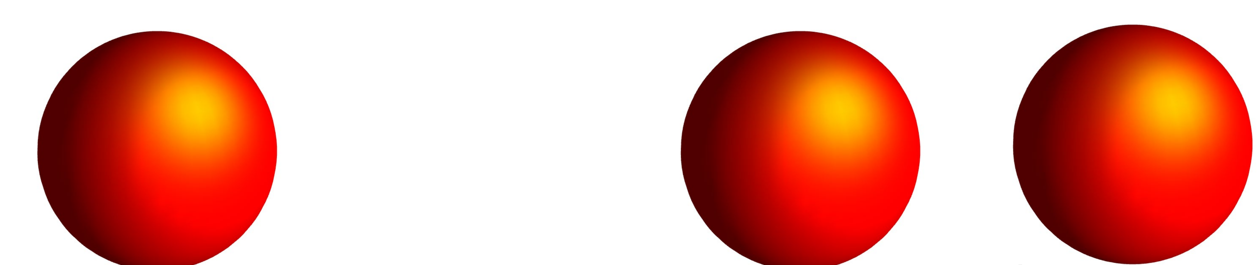
Using the phase-field function,

$$\chi(\phi) = \frac{1}{2\pi(a - b)}\int_{\Omega(a,b)} -\Delta\phi + \frac{\nabla|\nabla\phi|^2\,\nabla\phi}{2|\nabla\phi|^2}\, d\mathbf{x}$$

where, $\Omega(a, b) = \{x \in \Omega \mid b < \phi(x) < a\}$

Similarly, in 3D, the Euler characteristic is a topological invariant number.

$$2\pi\chi = \int_\Gamma G \, ds$$



$\chi = 2$ $\chi = 4$

Using the phase-field function,

$$\frac{\chi(\phi)}{2} = \int_{\Omega(a,b)} F(M)\, d\mathbf{x}$$

$$F(M) = M_{11}M_{22} + M_{11}M_{33} + M_{22}M_{33} - M_{12}^2 - M_{13}^2 - M_{23}^2$$

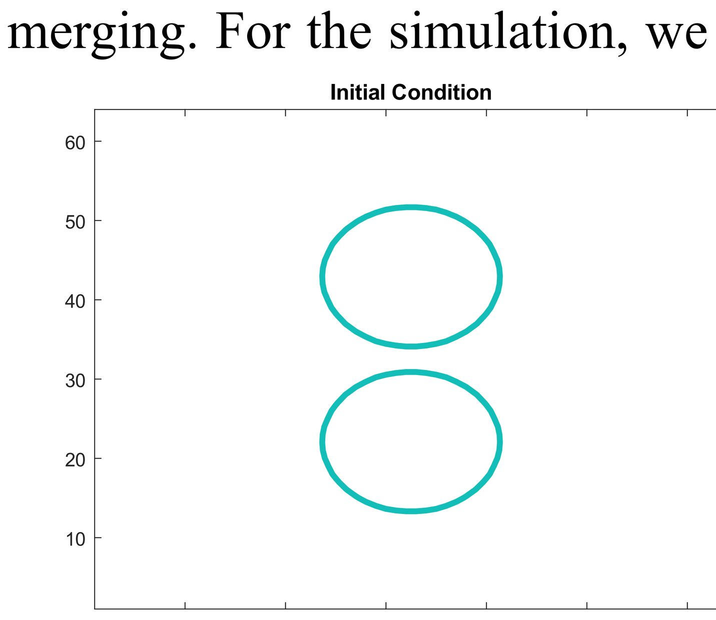
$$M_{ij}(\phi) = \frac{1}{2\sqrt{\pi(a - b)|\nabla\phi|}}\left(\nabla^2\phi - \frac{\nabla|\nabla\phi|^2\nabla\phi}{2|\nabla\phi|^4}\nabla_i\phi\nabla_j\phi\right)$$

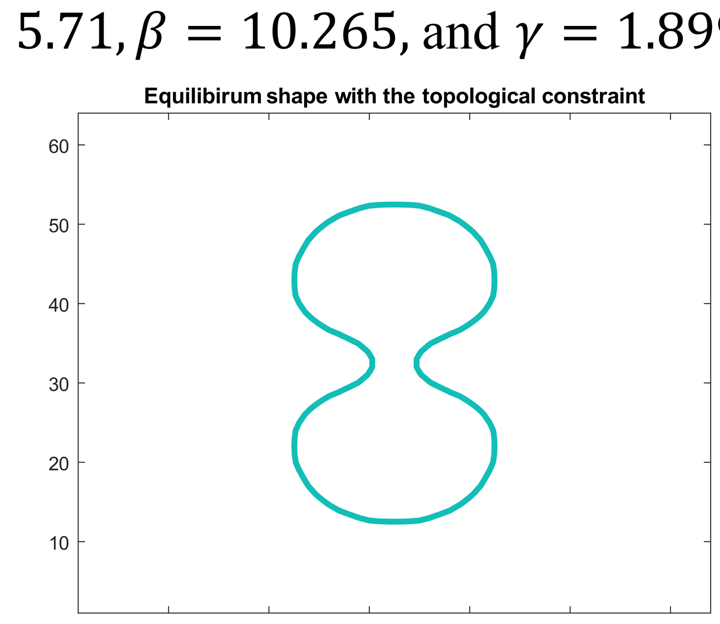
Results

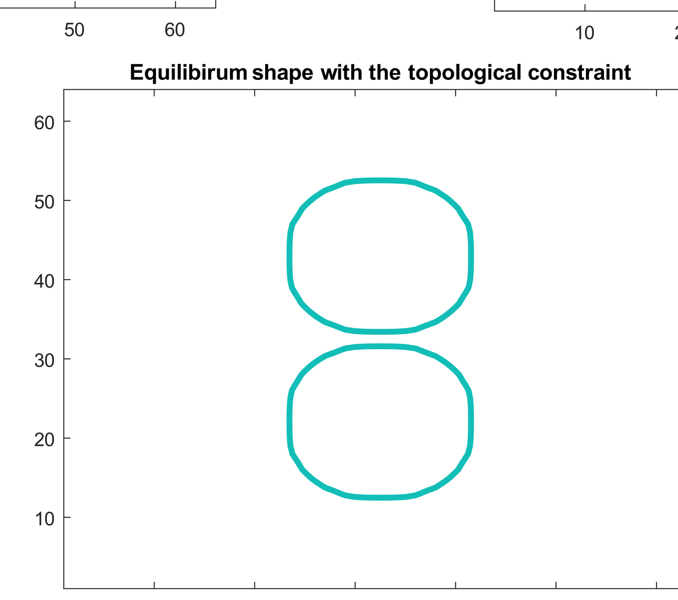
We formulated the constrained optimization problem using the penalty method and solved it with the standard gradient flow algorithm. Here, α, β, and γ are the required value of $V(\phi)$, $A(\phi)$, and $\chi(\phi)$, respectively.

$$\min E_M(\phi)$$
$$= E(\phi) + \frac{1}{2}M_1(A(\phi) - \alpha)^2 + \frac{1}{2}M_2(V(\phi) - \beta)^2 + \frac{1}{2}M_3(\chi(\phi) - \gamma)^2$$
$$\frac{\partial E_M}{\partial t} = -\frac{\delta E_M(\phi)}{\delta\phi}$$

We used the second-order centered difference approximation in space and first order forward Euler method in time. We initialized a 2D domain with two circles and initially solved the problem without the topological constraint; the two circles merge into one. The topological constraint, on the other hand, prevents the merging. For the simulation, we used $\alpha = 5.71, \beta = 10.265$, and $\gamma = 1.8991$.The







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