Mathematics Institute

Centre for Scientific Computing

Björn Stinner

Surface Finite Elements for Biological Membranes with Lateral Phase Separation

In cooperation with
Charles M. Elliott (Warwick)

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Biological Membranes with Lipid Decomposition

Elastic energy: Lipid bilayer resisting deformations.

[Canham, Evans, Helfrich 1970s]:
Represented by two-dimensional hypersurface Γ.

$$F_b = \int_\Gamma \frac{k_\kappa}{2}(\kappa - \kappa_s)^2 + \int_\Gamma k_g g.$$

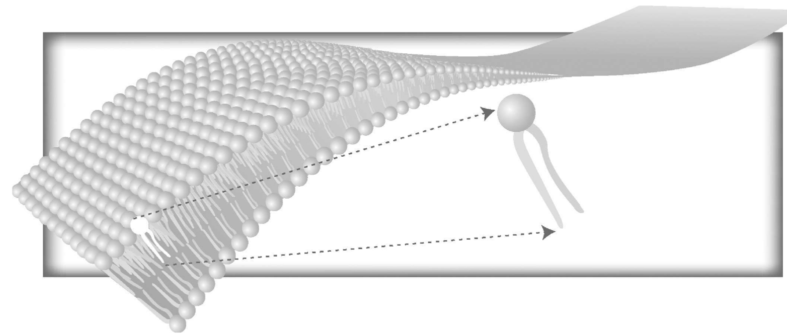
$\kappa = \kappa_1 + \kappa_2$ mean curvature, $g = \kappa_1 \kappa_2$ Gaussian curvature,
k_κ, k_g bending rigidities, κ_s spontaneous curvature.

Line energy: The lipid molecules may separate and form different phases.

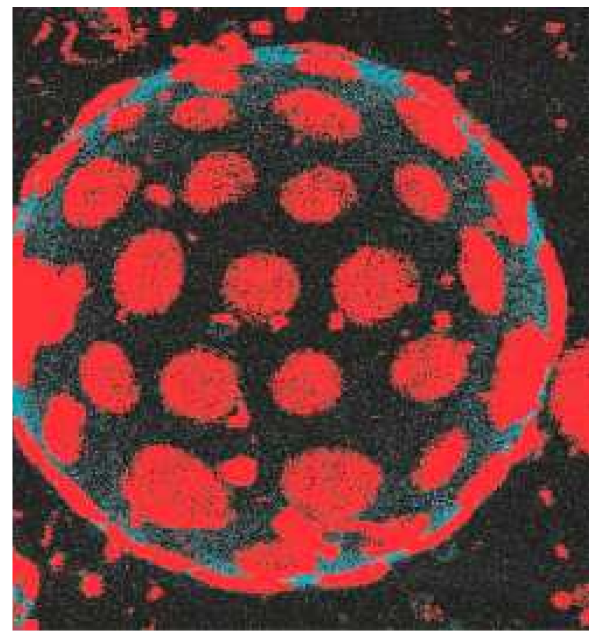
[Jülicher, Lipowsky 1993, 1996]:
Two smooth domains Γ_1 and Γ_2
with a common boundary $\gamma = \partial\Gamma_1 = \partial\Gamma_2$.

$$F_l = \int_\gamma \bar{\sigma}$$

$\bar{\sigma}$ line energy coefficient (constant).



[Peletier, Röger]



[Baumgart, Hess, Webb 2003]

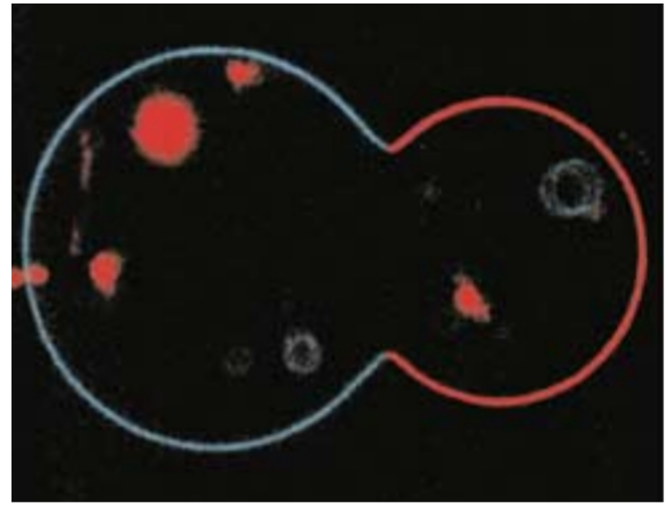
Relaxation Dynamics - Ideas and Methods

Aim: For given $|\Gamma_1|$, $|\Gamma_2|$ and $|\Omega|$, compute (local) minima of

$$F = \sum_{i=1,2} \int_{\Gamma_i} \Big(\frac{k_\kappa^{(i)}}{2} (\kappa - \kappa_s^{(i)})^2 + k_g^{(i)} g \Big) + \int_\gamma \bar{\sigma}.$$

Idea: Define an appropriate gradient flow dynamics and employ surface finite elements:

- **Geometric evolution law** for the membrane surface (Willmore flow type) . Methods:
  [Mayer, Simonett 2002],
  [Clarenz, Diewald, Dziuk, Rumpf, Rusu 2004],
  [Bänsch, Morin, Nochetto 2005],
  [Barrett, Garcke, Nürnberg 2008], [Dziuk 2008].
- **PDE on the evolving membrane surface** for the phase separation, using the phase field methodology. Method:
  [Dziuk, Elliott 2007].



[Baumgart, Hess, Webb 2003]

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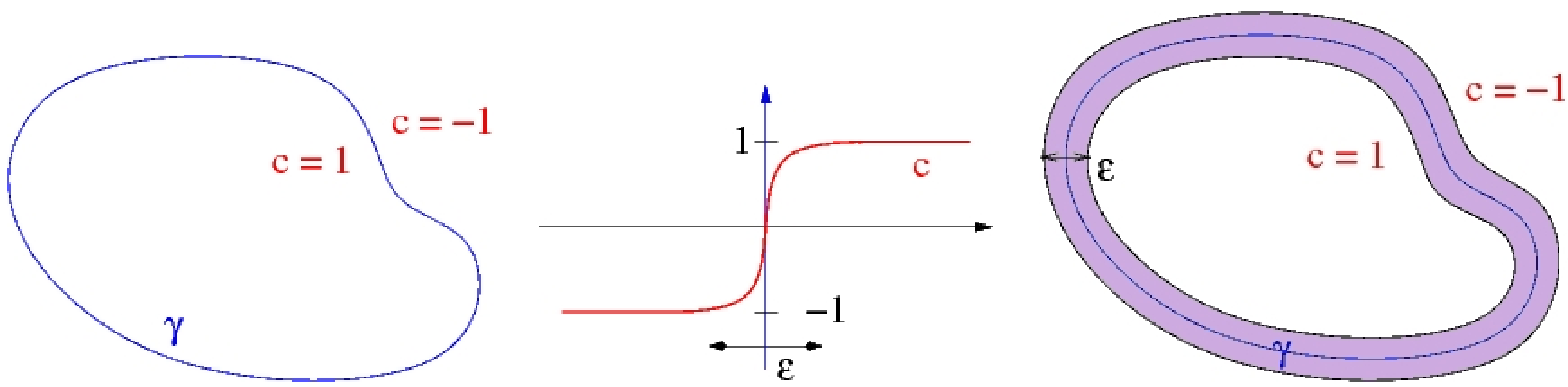
Phase Field Methodology

An order parameter (or phase field variable) $c : \Gamma \to [-1, 1]$ is introduced to distinguish two possible states (associated with phases).

Model with free boundary: c jumps over the phase boundary,
Phase field model: The profile of c is smoothed out, $\rightsquigarrow$ transition layers with a thickness $\sim \varepsilon$.



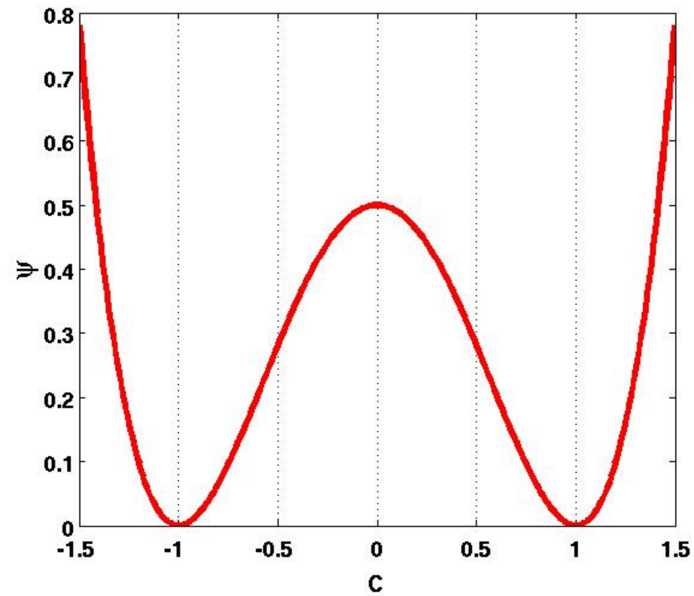
Line Energy in the Phase Field Approach

Ginzburg-Landau Energy:

$$F_l^\varepsilon = \int_\Gamma \sigma\Big(\frac{\varepsilon}{2}|\nabla_\Gamma c|^2 + \frac{1}{\varepsilon}\psi(c)\Big).$$

$\psi(c) = \frac{1}{2}(1-c^2)^2.$

$\Gamma_1 \sim \{c \approx 1\}$, $\Gamma_2 \sim \{c \approx -1\}$.



$F_l^\varepsilon \xrightarrow{\varepsilon\to 0} F_l = \int_\gamma \bar{\sigma}$
in the sense of *Gamma convergence*.

Total energy:

$$F(\Gamma, c:\Gamma\to\mathbb{R}) = \int_\Gamma \underbrace{\frac{k_\kappa(c)}{2}\big(\kappa-\kappa_s(c)\big)^2 + k_g(c)g}_{\text{bending energy}} + \underbrace{\sigma\Big(\frac{\varepsilon}{2}|\nabla_\Gamma c|^2 + \frac{1}{\varepsilon}\psi(c)\Big)}_{\text{line energy}}$$

Surface gradient: $\nabla_\Gamma c = (\underline{D}_i c)_{i,j=1}^3 = \sum_{i=1}^2 \partial_{y_i}\boldsymbol{p} g^{ij}\partial_{y_j}(c\circ\boldsymbol{p})$.

Gradient Flow

Dynamics: L^2 gradient flow, $(v, \partial_t^\bullet c) = -\delta F(\Gamma, c) - \boldsymbol{\lambda} \cdot \delta \boldsymbol{C}(\Gamma, c)$:

$$\begin{aligned}
v = &-\Delta_\Gamma\big(k_\kappa(c)(\kappa - \kappa_s(c))\big) - |\nabla_\Gamma \boldsymbol{\nu}|^2 k_\kappa(c)(\kappa - \kappa_s(c)) + \tfrac{1}{2}k_\kappa(c)(\kappa - \kappa_s(c))^2\kappa \\
&- \nabla_\Gamma \cdot \big(k_g'(c)(\kappa \boldsymbol{I} - \nabla_\Gamma \boldsymbol{\nu})\nabla_\Gamma c\big) \\
&+ \sigma\varepsilon \nabla_\Gamma c \otimes \nabla_\Gamma c : \nabla_\Gamma \boldsymbol{\nu} + \sigma\big(\tfrac{\varepsilon}{2}|\nabla_\Gamma c|^2 - \tfrac{1}{\varepsilon}\psi(c)\big)\kappa \\
&- \lambda_V + \big(\lambda_A - \lambda_c h(c)\big)\kappa, \\
\partial_t^\bullet c = &-\tfrac{1}{2}(\kappa - \kappa_s(c))^2 k_\kappa'(c) + k_\kappa(c)(\kappa - \kappa_s(c))\kappa_s'(c) - g k_g'(c) \\
&+ \varepsilon\sigma\Delta_\Gamma c - \tfrac{\sigma}{\varepsilon}\psi'(c) - \lambda_c h'(c),
\end{aligned}$$

plus constraints.

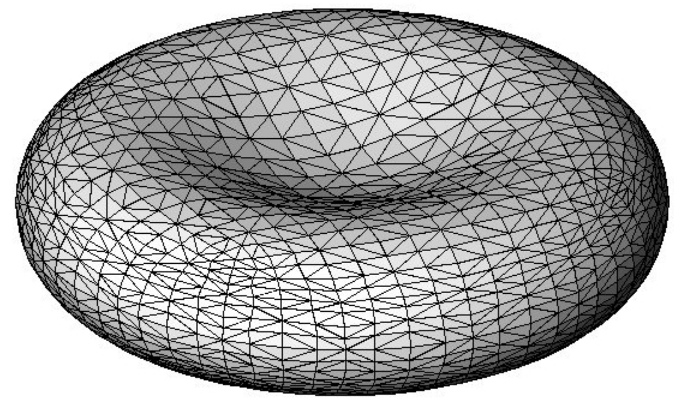
$\partial_t^\bullet c = \partial_t c + v\boldsymbol{\nu} \cdot \nabla c$ material derivative, $\boldsymbol{v} = v\boldsymbol{\nu}$ velocity, $\Delta_\Gamma c = \nabla_\Gamma \cdot \nabla_\Gamma c$, convenient formulation for approach with surface finite elements.

Theorem (asymptotic analysis): *In the limit as $\varepsilon \to 0$, solutions to the stationary phase field model converge to solutions to the (Euler-Lagrange equations of the) two-phase model.*

Isoparametric Quadratic Surface Finite Elements

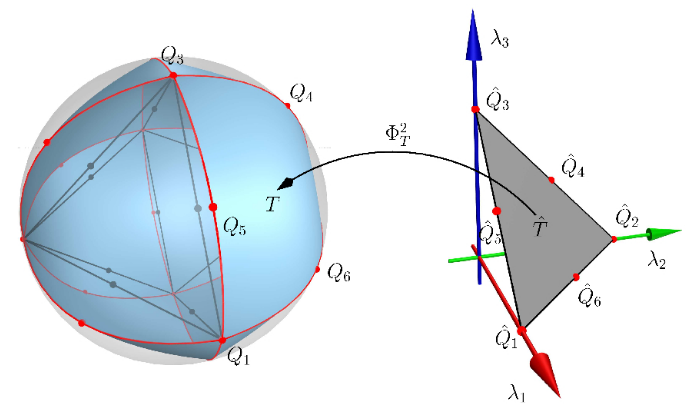
Approximation of Γ by a triangulated surface Γ_h,

$$\Gamma_h = \bigcup_{T \in \mathcal{T}_h} T.$$



The triangles are images of a
reference element $\hat{T}$ under a quadratic polynomial,

$$T = \Phi_T(\hat{T}) \quad \forall T \in \mathcal{T}_h.$$



[Heine 2003]

Finite element space:

$$\mathcal{S}_h(\Gamma_h) := \left\{ \phi_h \in C^0(\Gamma_h) \,\middle|\, \phi_h \circ \Phi_T \text{ quadratic for all } T \in \mathcal{T}_h \right\}.$$

Discretisation of Geometric Evolution Laws

Exemplary, **mean curvature flow** $v = \kappa$ with the method of [Dziuk 1988].

With $\boldsymbol{\kappa}$ mean curvature vector and $\boldsymbol{x}$ the identity map on Γ, based on the identity

$$\boldsymbol{\kappa} = \Delta_\Gamma \boldsymbol{x} \qquad \rightsquigarrow \quad \int_\Gamma \partial_t \boldsymbol{x} \cdot \boldsymbol{w} = - \int_\Gamma \nabla_\Gamma \boldsymbol{x} : \nabla_\Gamma \boldsymbol{w}.$$

Spatial discretisation: $\Gamma \longrightarrow \Gamma_h$ and $\boldsymbol{x} \longrightarrow \boldsymbol{x}_h$, using $\mathcal{S}_h(\Gamma_h)$.

Time discretisation: Parametrise the new surface over the old one.

$$\int_{\Gamma_h^m} \frac{1}{\tau}\left(\boldsymbol{x}_h^{m+1} - \boldsymbol{x}_h^m\right) \cdot \boldsymbol{w}_h + \nabla_{\Gamma_h^m} \boldsymbol{x}_h^{m+1} : \nabla_{\Gamma_h^m} \boldsymbol{w}_h = 0.$$

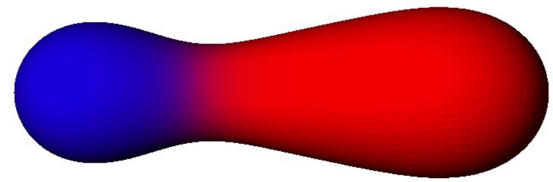
Willmore flow: $\quad v = -\Delta_\Gamma \kappa - |\nabla_\Gamma \boldsymbol{\nu}|^2 \kappa + \frac{1}{2}\kappa^3$,
keep κ (operator splitting) $\rightsquigarrow$ variational formulation with H^1 spaces.

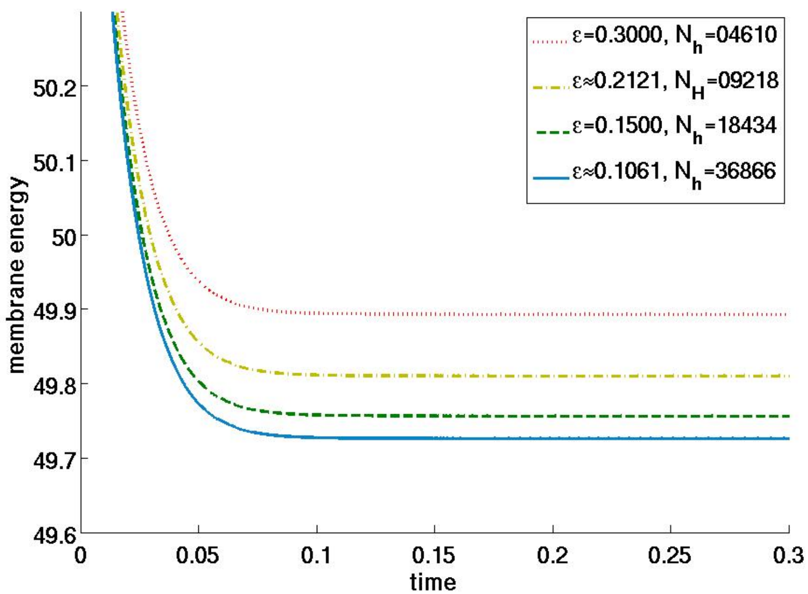
Approximation $\boldsymbol{Q}_h$ of $\nabla_\Gamma \boldsymbol{\nu}$ on Γ_h: [Heine 2003, 2004 (preprint)], [Demlow 2009].
Quadratic finite elements are sufficient for $\|\nabla_\Gamma \boldsymbol{\nu} - \boldsymbol{Q}_h\|_{L^2} \longrightarrow 0$.

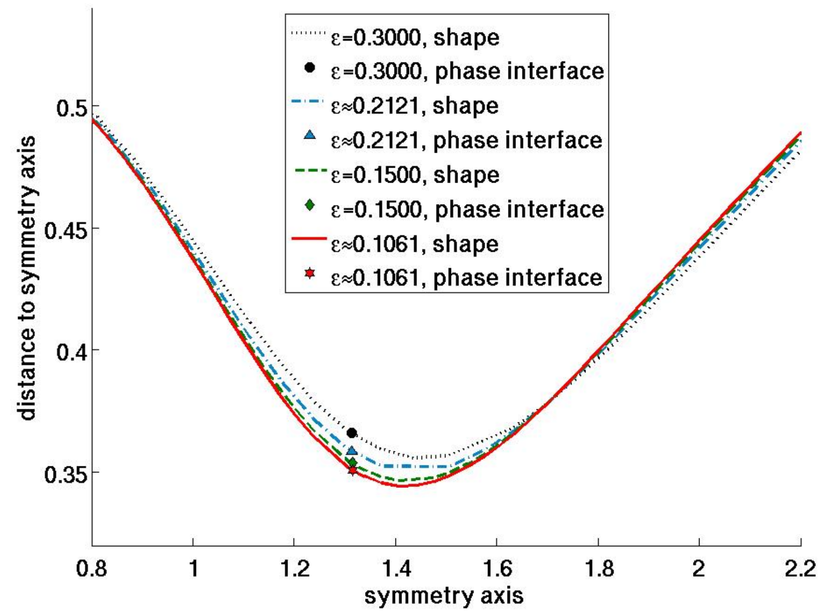
Convergence in ε

initial shape

relaxed shape





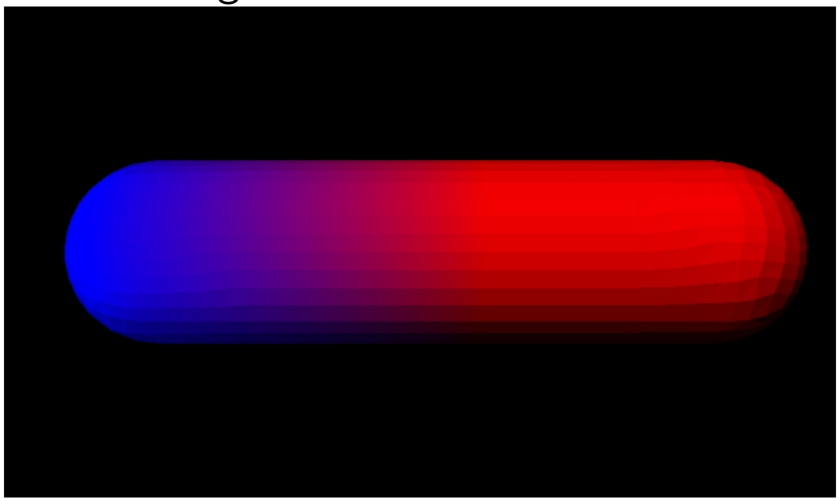


ε	$\mathcal{F}_h$	$eoc(\mathcal{F}_h)$	$\lambda_{c,h}$	$eoc(\lambda_{c,h})$	$\lambda_{V,h}$	$eoc(\lambda_{V,h})$
0.3	49.892651	—	-0.439907	—	17.572540	—
$0.3/\sqrt{2}$	49.809268	1.3213	-0.460235	1.6625	17.580688	2.3282
0.15	49.756520	1.5992	-0.471660	1.8007	17.584324	1.6989
$0.15/\sqrt{2}$	49.726216	—	-0.477781	—	17.586342	—

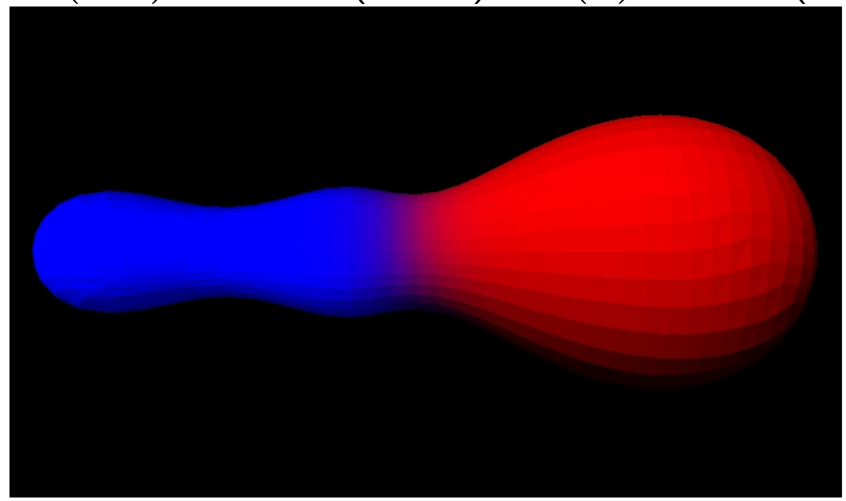
Different Bending Rigidities

$F = \sum_{i=1,2} \int_{\Gamma_i} \left(\frac{k_\kappa^{(i)}}{2} (\kappa - \kappa_s^{(i)})^2 + k_g^{(i)} g \right) + \int_\gamma \bar{\sigma}$

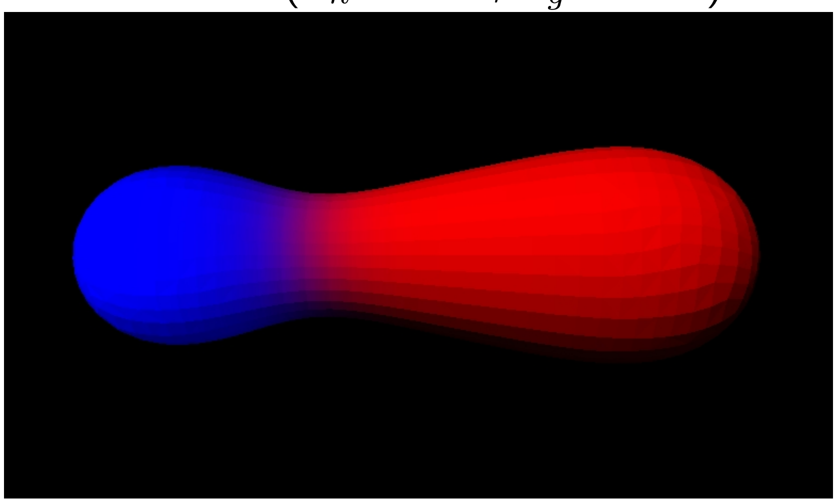
initial configuration



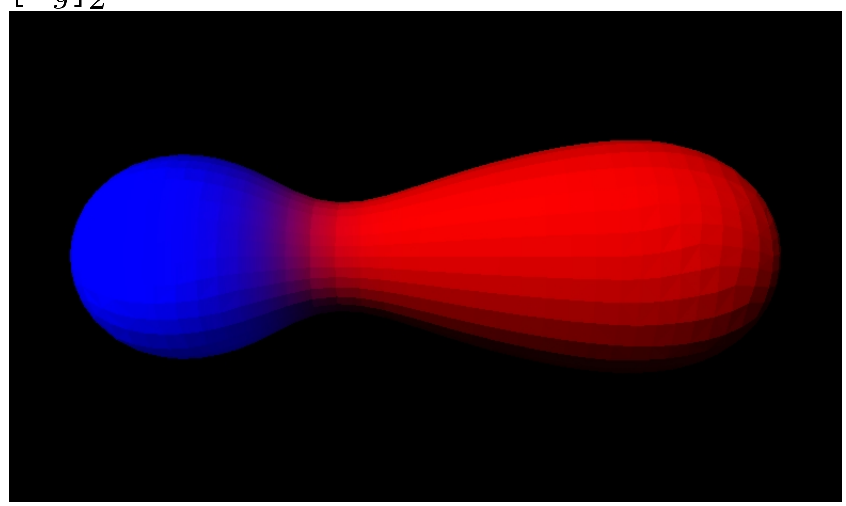
$k_\kappa(-1) = 0.25$ ('blue'), $k_\kappa(1) = 2.5$ ('red')



standard data ($k_\kappa = 1.0$, $k_g = 0.0$)



$[k_g]_2^1 = 1.0$



Spontaneous Curvature

$\kappa_s(-1) = 2.0$ ('blue' $\rightsquigarrow$ concave), $\kappa_s(1) = -2.0$ ('red' $\rightsquigarrow$ convex).

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[Agrawal, Steigmann 2008] (axisymmetric case)

Conclusion

Development of a method to compute equilibrium shapes
of vesicles formed by two-phase biomembranes:

- Phase field method to describe the interfacial energy from the phase interfaces.
- Asymptotic analysis, solutions to the phase field equations converge to solutions to the Euler-Lagrange equations, supported by numerical results.
- Formulation with a surface calculus that is convenient for surface finite elements.
- Computational approach involves
  - operator splitting and using H^1 conforming finite elements (for forth order equations),
  - quadratic finite elements on triangulated surfaces (for consistency),
  - iteration by semi-implicit time stepping.
- Numerical simulations, influence of parameters, comparison with results in the literature.