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Surface Finite Elements for Membranes with Lateral Phase Separation

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Supported by

EPSRC

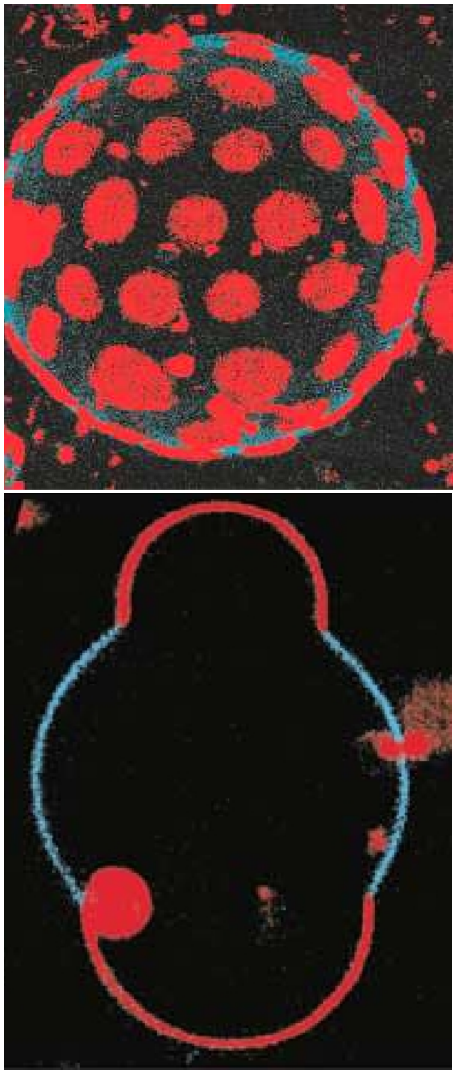
Introductory Example

Two-phase membranes:
Shape determined by elastic energy (bending energy),
phase separation of lipids (red and blue domains)
$\rightsquigarrow$ phase interface carrying energy (line energy).

Goal: Compute equilibrium shapes of vesicles,
define and study an appropriate relaxation dynamics,

- geometric evolution law for membrane,
- phase field methodology for phase separation,
- discretisation based on triangulated surfaces.

Example: Phase separation and formation of an interface
followed by a deformation due to the line energy.



[Baumgart, Hess, Webb 2005]

Outline

1. Biomembranes with Lipid Decomposition
   - membrane energy and equilibrium equations
   - phase field methodology for line energy
2. Relaxation Dynamics
   - dynamics of the surface
   - dynamics of the phase separation
3. Numerical Approach
   - triangulated surfaces, linear and quadratic finite elements
   - discretisation of the evolution equations
4. Simulation Results
   - convergence (in interfacial thickness)
   - influence of physical parameters

Lipid Decomposition

[Jülicher, Lipowsky 1996]:

The membrane Γ is split into two domains (phases) Γ_1, Γ_2 with a common smooth boundary $\gamma = \partial\Gamma_1 = \partial\Gamma_2$
Assumption: Γ is C^1 across γ.

Bending energy:

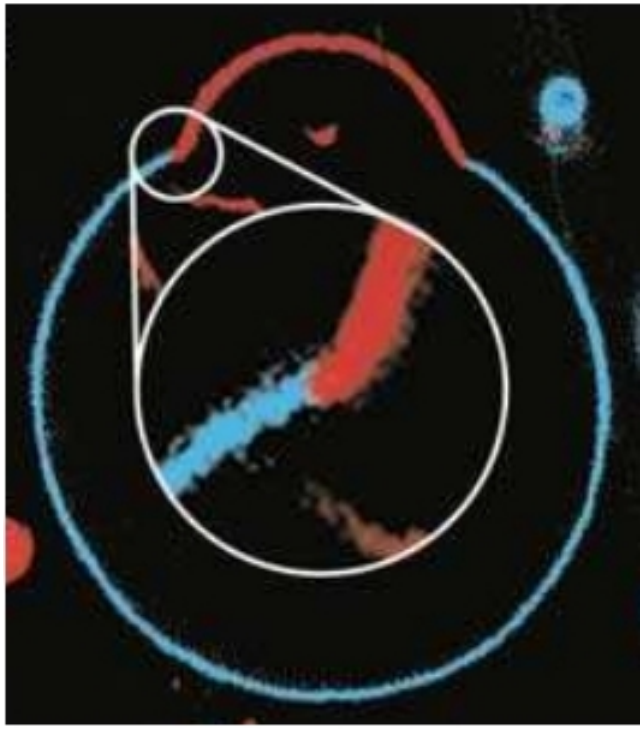
$$F_b = \sum_{i=1,2} \int_{\Gamma_i} \frac{k_i}{2}(\kappa - \bar{\kappa}_i)^2 \left[+ \int_{\Gamma_i} r_i \kappa_G \right]$$

k_i, r_i rigidities, $\bar{\kappa}_i$ spontaneous curvatures.
Assumption: $r_1 = r_2$.

Line energy:

$$F_l = \int_\gamma \sigma$$

σ line energy coefficient (constant).



[Baumgart, Hess, Webb 2003]

Calculus on Surfaces - Surface Gradient

$\boldsymbol{\nu}$ unit normal on Γ.

Surface gradient: ($c : \Gamma \to \mathbb{R}$ scalar field)

$$\nabla_\Gamma c = \nabla c - \nabla c \cdot \boldsymbol{\nu}\, \boldsymbol{\nu}.$$

With a local parametrisation $\boldsymbol{p}(\boldsymbol{y})$:

$$\nabla_\Gamma c = \sum_{i,j=1}^{2} \partial_{y_i} \boldsymbol{p} g^{ij} \partial_{y_j} (c \circ \boldsymbol{p}).$$

Mean curvature vector:

$$\boldsymbol{\kappa} = (-\nabla_\Gamma \cdot \boldsymbol{\nu})\boldsymbol{\nu} = \Delta_\Gamma \boldsymbol{x} \quad \text{where } \boldsymbol{x} : \Gamma \to \Gamma \text{ identical map.}$$

Calculus on Surfaces - Integration by Parts

$\gamma = \partial\Gamma$ smooth with outer co-normal $\boldsymbol{\mu}$.

Integration by parts: ($\boldsymbol{v} : \Gamma \to \mathbb{R}^3$ vector field)

$$\int_\Gamma \nabla_\Gamma c + c\boldsymbol{\kappa} = \int_\gamma c\boldsymbol{\mu},$$

$$\int_\Gamma \nabla_\Gamma \cdot \boldsymbol{v} + \boldsymbol{v} \cdot \boldsymbol{\kappa} = \int_\gamma \boldsymbol{v} \cdot \boldsymbol{\mu}.$$

Example (Γ closed):

$$\int_\Gamma \boldsymbol{\kappa} \cdot \boldsymbol{w} = \int_\Gamma \Delta_\Gamma \boldsymbol{x} \cdot \boldsymbol{w} = \int_\Gamma \sum_i (\nabla_\Gamma \cdot \nabla_\Gamma \boldsymbol{x}_i)\boldsymbol{w}_i$$

$$= \int_\Gamma \sum_i -\nabla_\Gamma \boldsymbol{x}_i \cdot \nabla_\Gamma \boldsymbol{w}_i = \int_\Gamma -\nabla_\Gamma \boldsymbol{x} : \nabla_\Gamma \boldsymbol{w}$$

Calculus on Surfaces - Evolving Surfaces

$\{\Gamma(t)\}_t$ evolving surfaces with **material velocity field** $\boldsymbol{v}(\cdot,t) : \Gamma(t) \to \mathbb{R}^3$.
Splits into normal and tangential portion: ($\boldsymbol{P} = I - \boldsymbol{\nu} \otimes \boldsymbol{\nu}$ projection onto tangent space)

$$\boldsymbol{v} = (\boldsymbol{v} \cdot \boldsymbol{\nu})\, \boldsymbol{\nu} + \boldsymbol{P}\boldsymbol{v}$$

Material (time) derivative: ($c(t) : \Gamma(t) \to \mathbb{R}$ scalar field)

$$\partial_t^\bullet c(\boldsymbol{p}(y,t),t) = \frac{d}{dt} c(\boldsymbol{p}(y,t),t) = \partial_t c + \boldsymbol{v} \cdot \nabla c.$$

Leibniz formula:

$$\begin{aligned}\frac{d}{dt}\Big(\int_{\Gamma(t)} c(t)\Big)\Big|_{t=t_0} &= \int_{\Gamma(t_0)} \big(\partial_t^\bullet c + c\nabla_\Gamma \cdot \boldsymbol{v}\big)(t_0) \\ &= \int_{\Gamma(t_0)} \big(\partial_t^\circ c - c\boldsymbol{\kappa} \cdot \boldsymbol{v} + \int_{\partial\Gamma(t_0)} \big(c\boldsymbol{P}\boldsymbol{v} \cdot \boldsymbol{\mu}\big)\big)(t_0).\end{aligned}$$

Variation of the Membrane Energy

Problem: For prescribed $|\Gamma_1|$, $|\Gamma_2|$, and $|\Omega|$, minimise

$$F = F_b + F_l = \sum_{i=1,2} \int_{\Gamma_i} \frac{k_i}{2} (\kappa - \bar{\kappa}_i)^2 + \int_\gamma \sigma.$$

Deformation: given $\boldsymbol{w} : \Gamma \to \mathbb{R}^3$ let

$$\Gamma_t := \{\boldsymbol{y} + t\boldsymbol{w}(\boldsymbol{y}) \,|\, \boldsymbol{y} \in \Gamma\}$$

Then a minimiser fulfils

$$0 = \langle \delta F(\Gamma), \boldsymbol{w} \rangle = \frac{d}{dt} F(\Gamma_t)\big|_{t=0}.$$

Observe that $\{\Gamma_t\}_t$ can be considered as an evolving surface.

Euler-Lagrange Equations

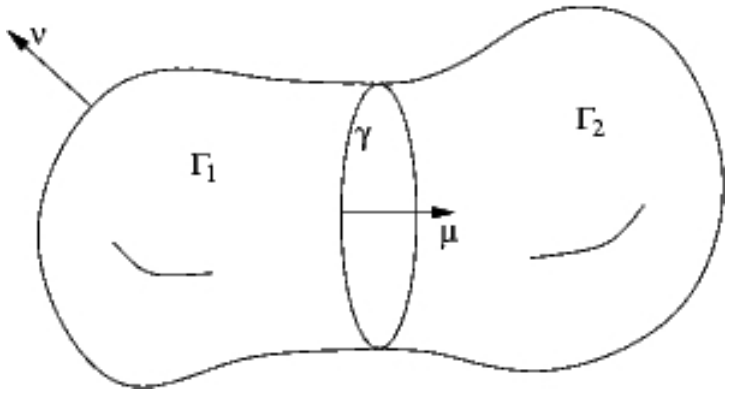
A minimiser of the membrane energy fulfils

$$
\begin{aligned}
0 &= k_i\big(\Delta_\Gamma\kappa + |\nabla_\Gamma \boldsymbol{\nu}|^2(\kappa-\bar\kappa_i) - \tfrac{1}{2}(\kappa-\bar\kappa_i)^2\kappa\big) - \lambda_\Omega + \lambda_{\Gamma_i}\kappa && \text{on } \Gamma_i,\ i=1,2,\\
0 &= \big[k(\kappa-\bar\kappa)\big]_2^1 && \text{on } \gamma,\\
0 &= \big[k\nabla_\Gamma\kappa\big]_2^1\cdot\boldsymbol{\mu} - \sigma\kappa_n && \text{on } \gamma,\\
0 &= -\big[\tfrac{k}{2}(\kappa-\bar\kappa)^2\big]_2^1 - \sigma\kappa_g - \big[\lambda_\Gamma\big]_2^1 && \text{on } \gamma,
\end{aligned}
$$

where λ_Ω, λ_{Γ_1}, and λ_{Γ_2} are Lagrange multipliers for the constraints.

Splitting of the curvature vector of γ:

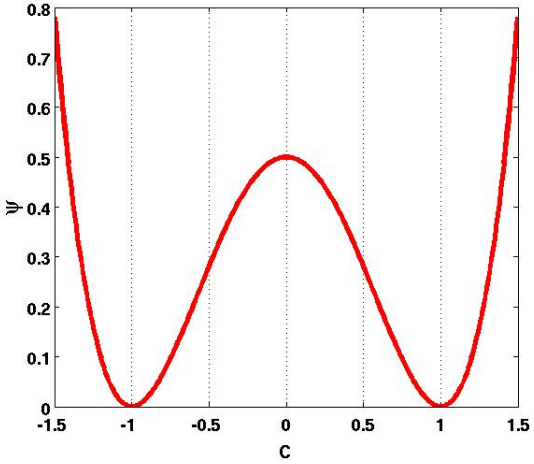
$$\boldsymbol{\kappa}_\gamma = \kappa_g\boldsymbol{\mu} + \kappa_n\boldsymbol{\nu}.$$



Line Energy in the Phase Field Approach

Γ smooth, $c : \Gamma \to \mathbb{R}$ order parameter. **Ginzburg-Landau Energy:**

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



In the flat case: $F_l^\varepsilon \overset{\varepsilon\to 0}{\longrightarrow} F_l = \int_\gamma \sigma$ in the sense of a Γ-limit.

Minima of ψ energetically are favourable
$\rightsquigarrow \Gamma_1 \sim \{c \approx 1\}$, $\Gamma_2 \sim \{c \approx -1\}$.

Total membrane energy:

$$F(\Gamma, c : \Gamma \to \mathbb{R}) = \int_\Gamma \underbrace{\frac{k(c)}{2}(\kappa - \bar{\kappa}(c))^2}_{\text{bending energy}} + \underbrace{\tilde{\sigma}\left(\frac{\varepsilon}{2}|\nabla_\Gamma c|^2 + \frac{1}{\varepsilon}\psi(c)\right)}_{\text{line energy}}$$

Relaxation Dynamics - Ideas and Methods

Goal: set up a dynamics which reduces the energy such that:

- The phase separation is described by a surface pde:
  Parabolic equation for the order parameter $c(t)$, [Chen 2002].
  Use [Dziuk, Elliott 2006] for solving pdes on evolving surfaces .
- The membrane evolves according to a geometric evolution law: Roughly

$$\text{normal velocity} \;=\; -\ \text{variation of the energy.}$$

  Overview article: [Deckelnick, Dziuk, Elliott 2005].
  Here of Willmore flow type; relevant work (triangulated surfaces):
  [Mayer, Simonett 2002], [Clarenz, Diewald, Dziuk, Rumpf, Rusu 2004],
  [Bänsch, Morin, Nochetto 2005], [Barrett, Garcke, Nürnberg 2007], [Dziuk 2008].
- The areas of the two phases and the enclosed volume are preserved:
  Newton method for computing Lagrange multipliers.

Some Other Work of Relevance

[Jülicher, Lipowsky 1996], equilibrium shapes and budding, axisymmetric case,
[Taniguchi, 1996, 1997], sphere-like membranes, diffuse interface model for phase separation,
[Jiang, Lookman, Saxena 1999], other symmetries, diffuse interface model for phase separation.
[Du, Wang 2004, 2006], diffuse interface model for representation of the membrane,
[Campelo, Saxena 2006], FD methods, no intermembrane domains,
[Lowengrub, Xu, Voigt 2007], IIM, phase separation on vesicles in 2D flow,
[Ma, Klug 2008], C^1 FE, direct minimisation, mesh regularisation.

Phase Separation

Postulate a law for the order parameter c such that the energy decreases if Γ is stationary.

- **Cahn-Hilliard** equation, c conserved quantity:

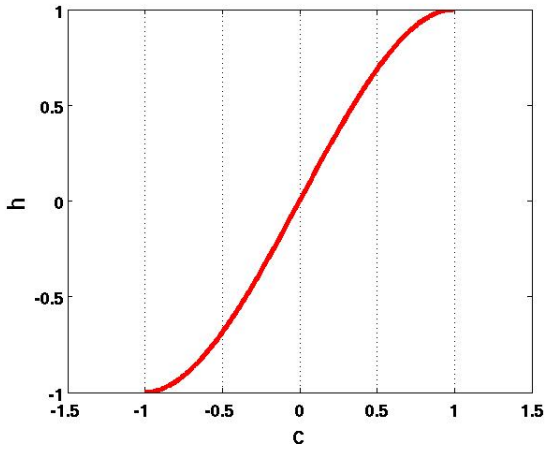
$$\partial_t^\bullet c + c\nabla_\Gamma \cdot \boldsymbol{v} = \nabla_\Gamma \cdot \left(D_c \nabla_\Gamma \mu\right).$$

- **Allen-Cahn** equation:

$$\varepsilon \partial_t^\bullet c = -\mu - \lambda_c h'(c)$$

with Lagrange multiplier λ_c to preserve $\int_\Gamma h(c)$.

Area constraints:



$\int_\Gamma h(c) \xrightarrow{\varepsilon \to 0} |\Gamma_1| - |\Gamma_2|,$

$\rightsquigarrow$ preserve $|\Gamma| = |\Gamma_1| + |\Gamma_2|$ and $\int_\Gamma h(c)$.

Chemical potential:

$$\mu = \frac{\delta F}{\delta c} = \frac{k'(c)}{2}(\kappa - \bar{\kappa}(c))^2 - k(c)(\kappa - \bar{\kappa}(c))\bar{\kappa}'(c) - \tilde{\sigma}\varepsilon\Delta_\Gamma c + \frac{\tilde{\sigma}}{\varepsilon}\psi'(c)$$

Evolution of the Surface

Deduced by computing the time derivative of the energy and using the law for c.

Exemplary for $k(c) = k_1 = k_2$ constant, $\bar{\kappa}(c) = \bar{\kappa}_1 = \bar{\kappa}_2 = 0$, Allen-Cahn equation for c:

$$
\begin{aligned}
V = & - k\Delta_\Gamma \kappa - k|\nabla_\Gamma \boldsymbol{\nu}|^2 \kappa \\
& + \tilde{\sigma}\varepsilon \nabla_\Gamma c \otimes \nabla_\Gamma c : \nabla_\Gamma \boldsymbol{\nu} - \frac{\int_\Gamma \mu h'(c)}{\int_\Gamma (h'(c))^2} h(c)\kappa \\
& + \left(\tfrac{k}{2}\kappa^2 + \tfrac{\tilde{\sigma}\varepsilon}{2}|\nabla_\Gamma c|^2 + \tfrac{\tilde{\sigma}}{\varepsilon}\psi(c)\right)\kappa \\
& + \lambda_\Omega - \lambda_\Gamma \kappa
\end{aligned}
$$

with Lagrange multipliers λ_Ω and λ_Γ for preserving the enclosed volume and the membrane area.

Stationary Solutions, Sharp Interface Limit

Using **matched asymptotic expansions** [Caginalp, 1989]
the Euler-Lagrange equations are obtained from the stationary equations as $\varepsilon \longrightarrow 0$.

Stationary problem:

$$
\begin{aligned}
0 = {} & k\Delta_\Gamma \kappa + k|\nabla_\Gamma \boldsymbol{\nu}|^2 \kappa - \tfrac{k}{2}\kappa^3 \\
& - \lambda_\Omega + \lambda_\Gamma \kappa + \lambda_c h(c)\kappa \\
& - \tilde{\sigma}\varepsilon \nabla_\Gamma c \otimes \nabla_\Gamma c : \nabla_\Gamma \boldsymbol{\nu} \\
& - \left(\tfrac{\tilde{\sigma}\varepsilon}{2}|\nabla_\Gamma c|^2 + \tfrac{\tilde{\sigma}}{\varepsilon}\psi(c)\right)\kappa, \\
0 = {} & \tilde{\sigma}\varepsilon\Delta_\Gamma c + \tfrac{\tilde{\sigma}}{\varepsilon}\psi'(c) - \lambda_c h'(c).
\end{aligned}
$$

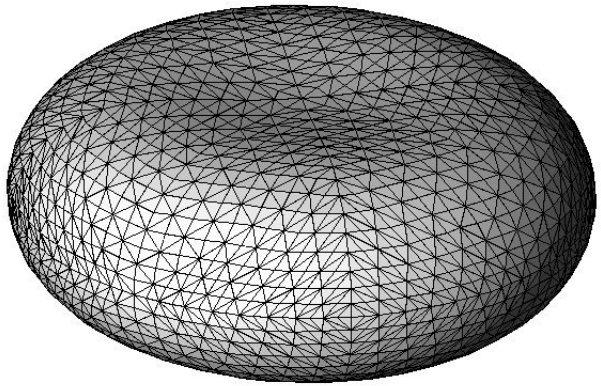
Euler-Lagrange equations:

$$
\begin{aligned}
0 &= k\left(\Delta_\Gamma \kappa + |\nabla_\Gamma \boldsymbol{\nu}|^2 \kappa - \tfrac{1}{2}\kappa^3\right) \\
&\quad - \lambda_\Omega + \lambda_{\Gamma_i}\kappa && \text{on } \Gamma_i, \\
0 &= k\left[\kappa\right]_2^1 && \text{on } \gamma, \\
0 &= k\left[\nabla_\Gamma \kappa\right]_2^1 \cdot \boldsymbol{\mu} - \sigma\kappa_n && \text{on } \gamma, \\
0 &= \sigma\kappa_g + \left(\lambda_{\Gamma_1} - \lambda_{\Gamma_2}\right) && \text{on } \gamma.
\end{aligned}
$$

Surface Finite Elements

Approximation of Γ by a triangulated surface Γ_h,

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

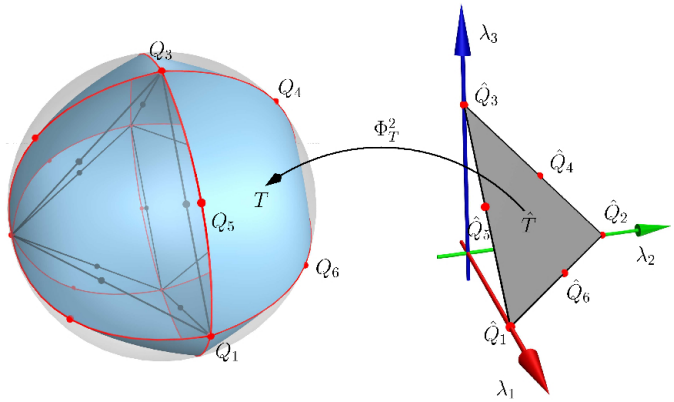


$(\hat{T}, \hat{P}, \hat{N})$ reference element, e.g. standard simplex.

Element domains $T \in \mathcal{T}_h$ parameterised by maps Φ_T, admissible functions on T by retraction,

$$p(\boldsymbol{y}) := \hat{p}(\Phi_T^{-1}(\boldsymbol{y})), \quad \hat{p} \in \hat{P},\ \boldsymbol{y} \in T.$$

Element is **isoparametric** if Φ_T belongs to $(\hat{P})^{dim}$ $\Leftrightarrow$ the identical map on T is admissible.



[Heine 2003]

Isoparametric linear finite elements: $\left\{ \phi_h \in C^0(\Gamma_h) \,\middle|\, \phi_h\big|_T \text{ linear for all } T \in \mathcal{T}_h \right\}$.

Weak Formulation, Surface Evolution

Employ discretisation scheme for Willmore flow as in [Dziuk 2008]:
The curvature identity is used to compute the variation of the bending energy, can be done on Γ_h (with $\boldsymbol{x}_h$, $\boldsymbol{\kappa}_h$ etc.) as well.

$$
\begin{aligned}
0 &= \int_\Gamma \boldsymbol{\kappa} \cdot \boldsymbol{\zeta} + \nabla_\Gamma \boldsymbol{x} : \nabla_\Gamma \boldsymbol{\zeta}, \\
\int_\Gamma \partial_t \boldsymbol{x} \cdot \boldsymbol{w} &= \int_\Gamma k\big(\nabla_\Gamma \boldsymbol{\kappa} : \nabla_\Gamma \boldsymbol{w} + \nabla_\Gamma \cdot \boldsymbol{\kappa}\, \nabla_\Gamma \cdot \boldsymbol{w} + \tfrac{1}{2}|\boldsymbol{\kappa}|^2 \nabla_\Gamma \cdot \boldsymbol{w}\big) \\
&\quad - k\big((\nabla_\Gamma \boldsymbol{\kappa})^T : \nabla_\Gamma \boldsymbol{w} - \boldsymbol{P} \nabla_\Gamma \boldsymbol{\kappa} : \nabla_\Gamma \boldsymbol{w}\big) \\
&\quad + \tilde{\sigma} \varepsilon \nabla_\Gamma c \otimes \nabla_\Gamma c : \nabla_\Gamma \boldsymbol{\nu}\, \boldsymbol{\nu} \cdot \boldsymbol{w} - \frac{\int_\Gamma \mu h'(c)}{\int_\Gamma (h'(c))^2} h(c) \boldsymbol{\kappa} \cdot \boldsymbol{w} \\
&\quad + \tilde{\sigma}\big(\tfrac{\varepsilon}{2}|\nabla_\Gamma c|^2 + \tfrac{1}{\varepsilon}\psi(c)\big)\boldsymbol{\kappa} \cdot \boldsymbol{w} - \lambda_\Omega \boldsymbol{\nu} \cdot \boldsymbol{w} + \lambda_\Gamma \boldsymbol{\kappa} \cdot \boldsymbol{w}.
\end{aligned}
$$

Issue: discretisation of the shape operator $\nabla_\Gamma \boldsymbol{\nu}$.
For quadratic elements there is a method converging in L^2 (on given surfaces).

Discrete Surface Evolution

Given data at time t^m we compute the new vertex positions and the curvature at time t^{m+1}.

$$\begin{pmatrix} \frac{1}{\Delta t}\boldsymbol{M}^m & -k\boldsymbol{A}^m \\ \boldsymbol{A}^m & \boldsymbol{M}^m \end{pmatrix} \begin{pmatrix} \underline{\boldsymbol{x}}^{m+1} \\ \underline{\boldsymbol{\kappa}}^{m+1} \end{pmatrix} = \begin{pmatrix} \underline{\boldsymbol{r}}^m - \lambda_\Omega^{m+1}\underline{\boldsymbol{n}}^m + \lambda_\Gamma^{m+1}\underline{\boldsymbol{k}}^m \\ 0 \end{pmatrix}$$

Resolving second equation w.r.t. $\underline{\boldsymbol{\kappa}}^{m+1}$ yields

$$\underbrace{\left(\tfrac{1}{\Delta t}\boldsymbol{M}^m + k\boldsymbol{A}^m(\boldsymbol{M}^m)^{-1}\boldsymbol{A}^m\right)}_{=:\boldsymbol{I}^m}\underline{\boldsymbol{x}}^{m+1} = \underline{\boldsymbol{r}}^m - \lambda_\Omega^{m+1}\underline{\boldsymbol{n}}^m + \lambda_\Gamma^{m+1}\underline{\boldsymbol{k}}^m.$$

Algorithm:

1. solve $(\boldsymbol{I}^m)^{-1}\underline{\boldsymbol{r}}^m$, $(\boldsymbol{I}^m)^{-1}\underline{\boldsymbol{n}}^m$, $(\boldsymbol{I}^m)^{-1}\underline{\boldsymbol{k}}^m$,
2. compute λ_Ω^{m+1} and λ_Γ^{m+1} with a Newton method,
3. find the new curvature values $\underline{\boldsymbol{\kappa}}^{m+1}$.

(similar to ideas of [Bonito, Nochetto])

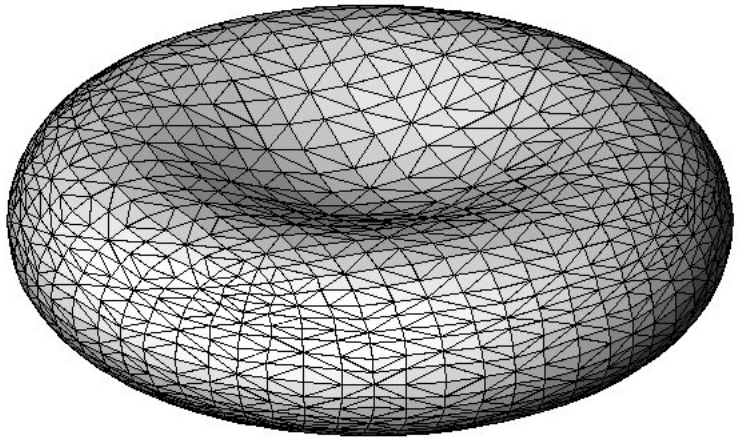
Example, Membrane Shapes without Phase Separation

No line energy but only bending energy, constraints on membrane area and enclosed volume.

Relaxed flat ellipsoids to discocyte
and prolate ellipsoids to dumbbells.

Final energies:

shape \ reduced volume	0.62111	0.79205
discocyte	47.7782	36.9878
dumbbell	49.1430	35.3023



Time step: $\Delta t^{m+1} \sim h^2 / \|\boldsymbol{v}_h^m\|_\infty$.

Weak Formulation, Phase Separation

Ideas taken from discretisation as is [Dziuk, Elliott 2006] for surface conserved quantities.

Continuum equation:

$$\int_\Gamma \varepsilon \partial_t^\bullet c \chi + \tilde{\sigma}\varepsilon \nabla_\Gamma c \cdot \nabla_\Gamma \chi = \int_\Gamma -\frac{\tilde{\sigma}}{\varepsilon}\psi'(c)\chi - \lambda_c h'(c)\chi.$$

Discrete system:

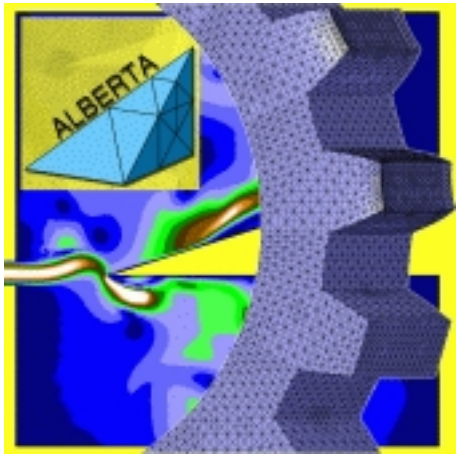
$$\left(\frac{\varepsilon}{\Delta t}\boldsymbol{M}^{m+1} + \tilde{\sigma}\varepsilon \boldsymbol{A}^{m+1}\right)\underline{c} = \underline{w}^{m+1}(c_h^m) - \lambda_c^{m+1}\underline{h}^{m+1}(c_h^m).$$

Algorithm analogous to the one for surface evolution.

Implementation

Implementation with the ALBERTA finite element toolkit,
`http://www.alberta-fem.de/`
[Schmidt, Siebert 2005].

Isoparametric linear and quadratic surface finite elements provided.



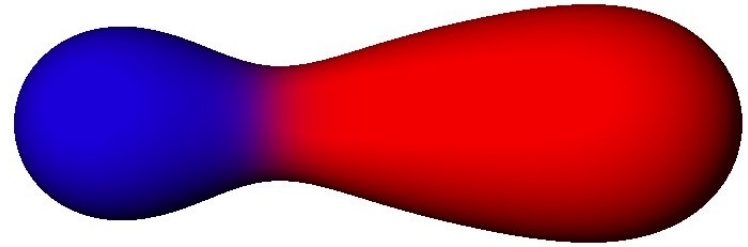
Grid adaption based on bisection, subsequent refinement edge a priori determined,
no other mesh adaptions as edge flipping etc.

$\rightsquigarrow$ eventually a drawback when vertices are moving.

Convergence Test, Quadratic Elements

Initial shape

Relaxed shape



Parameters:

$\lvert\Omega\rvert$	2.8798	k	1.0000
$\lvert\Gamma\rvert$	12.5664	$\bar{\kappa}$	0.0000
$\int_\Gamma h(c)$	4.7100	σ	2.6666
$R_c := \sqrt{\lvert\Gamma\rvert/4\pi}$	1.0000	$\lambda := R_c\sigma/k$	2.6666
$\bar{v} := \lvert\Omega\rvert/\frac{4}{3}\pi R_c^3$	0.6875	$x := \lvert\Gamma_1\rvert/\lvert\Gamma\rvert$	0.6874

$\int_\Gamma h(c) \approx 2|\Gamma_1| - |\Gamma|$,
$\sigma = \frac{4}{3}\tilde{\sigma}$ for our choice of ψ.

Results:

ε	F_h	eoc
0.3000	49.920194	–
0.2121	49.830931	1.7543
0.1500	49.782332	1.3634
0.1061	49.752034	–

$$eoc(\varepsilon) = \log\left(\frac{F_h(\sqrt{2}\varepsilon) - F_h(\varepsilon)}{F_h(\varepsilon) - F_h(\varepsilon/\sqrt{2})}\right) \Big/ \log\left(\sqrt{2}\right).$$

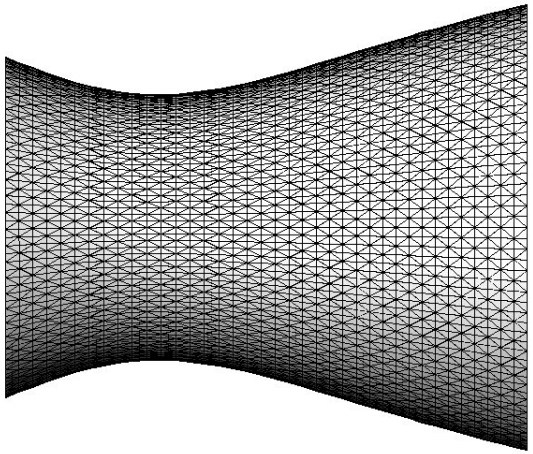
Adaptive Refinement, Linear Elements

Adaptively refined grid:

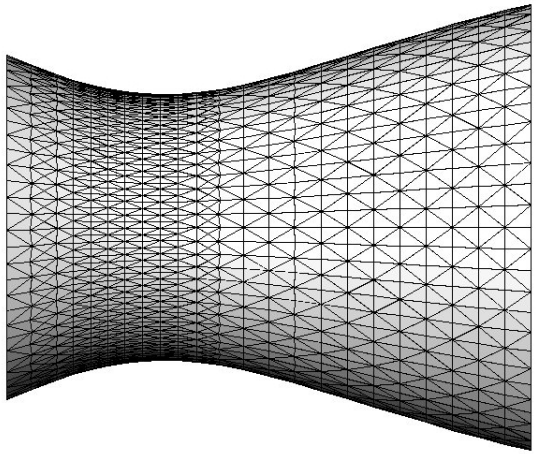
ε	F_h	eoc	comment
0.2121	51.270		
0.1500	51.199	1.6556	
0.1061	51.159	3.0291	
0.0750	51.145		
0.2121	51.280		finer mesh
0.2121	51.244		globally refined

Parameters slightly different, e.g. $\lambda = 3.3319$.

18434 vertices

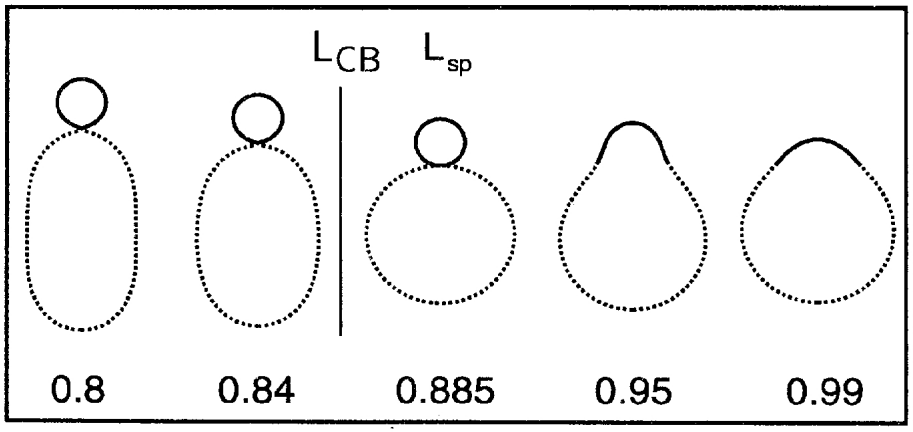


$\approx$ 5314 vertices

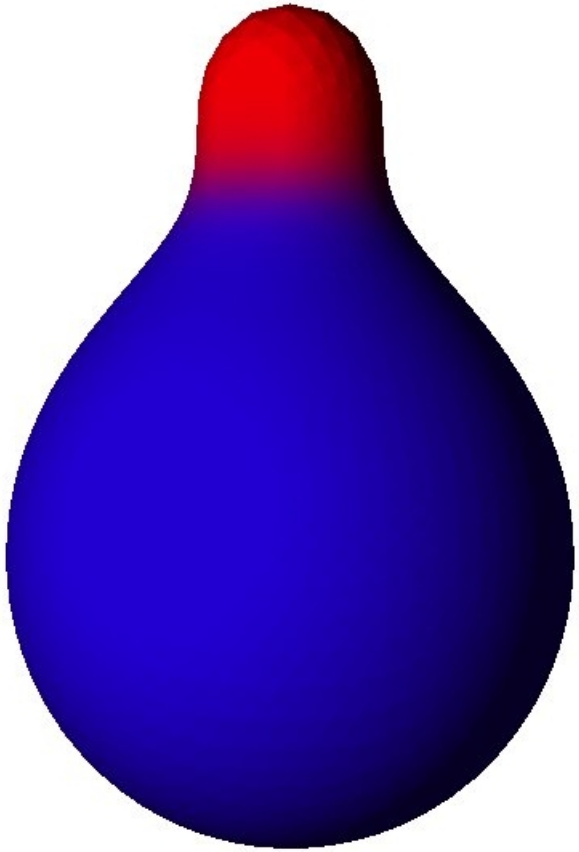


Quantitative Example

[Jülicher, Lipowsky 1996]:



Computed shape:



$\bar{v} = 0.92$, $\lambda = 9$, $x = 0.1$.

Predicted energy: $[54.915, 55.047]$.

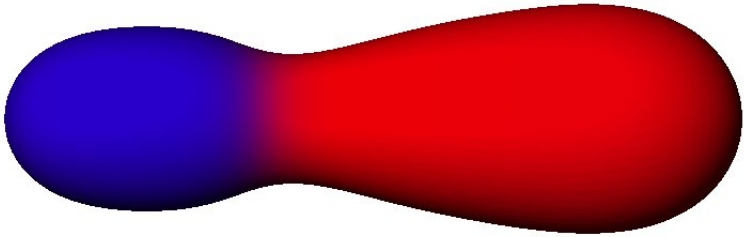
Measured energy: 55.019.

Effect of Different Bending Rigidities

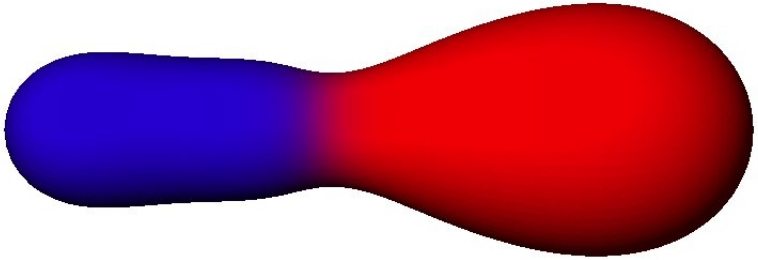
$k(\text{red}) = 2.0$, $k(\text{blue}) = 0.4$ and interpolation with a polynomial of degree three in between.

$t = 0.00$

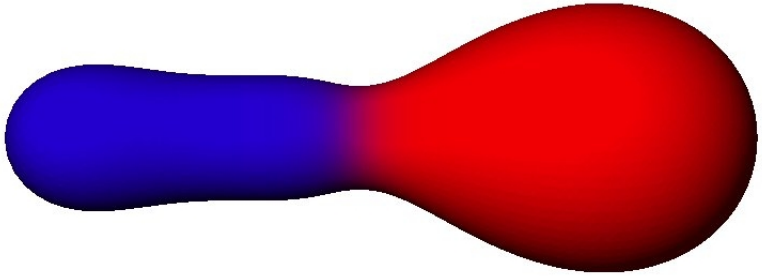
$t = 0.05$



$t = 0.15$

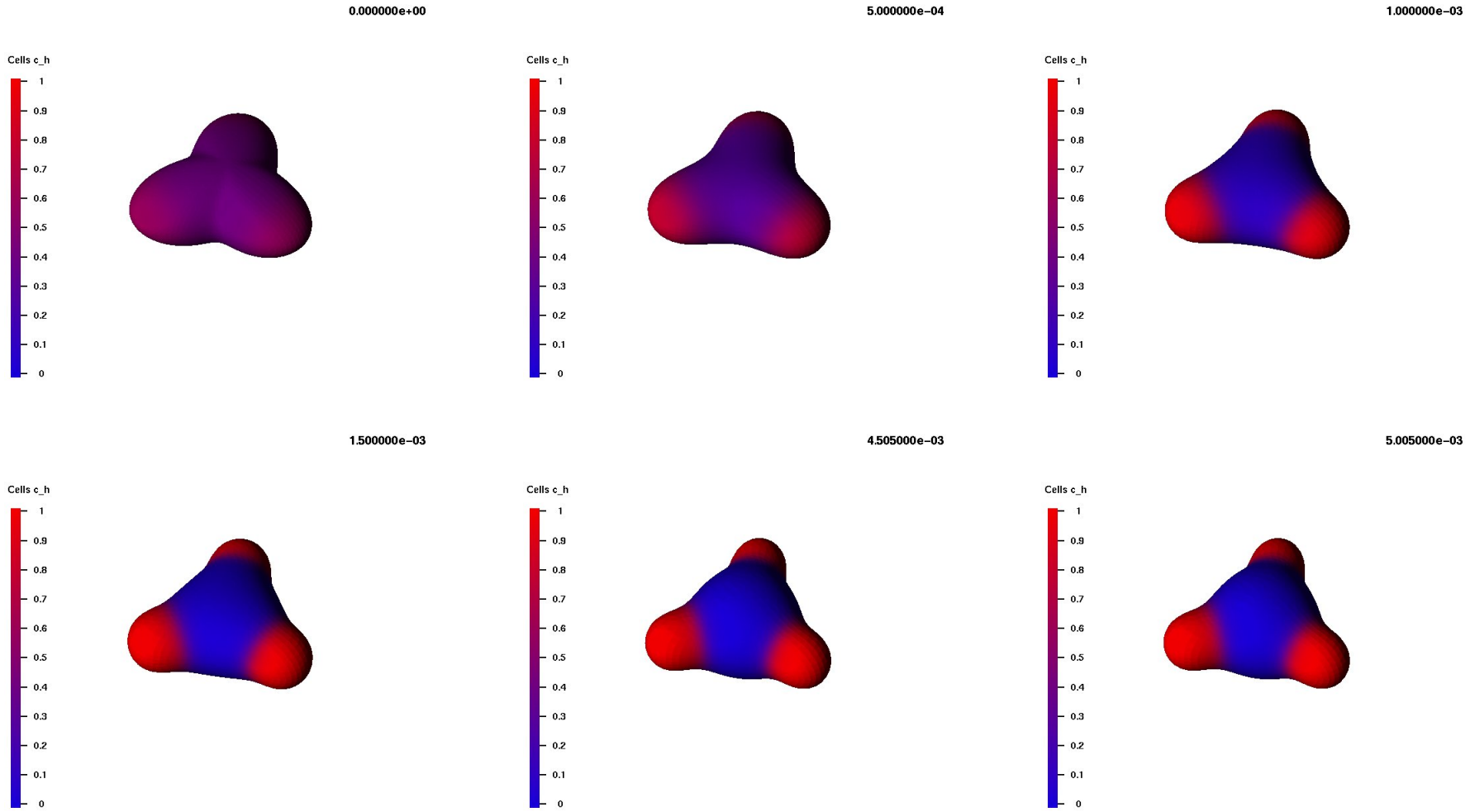


$t = 0.65$



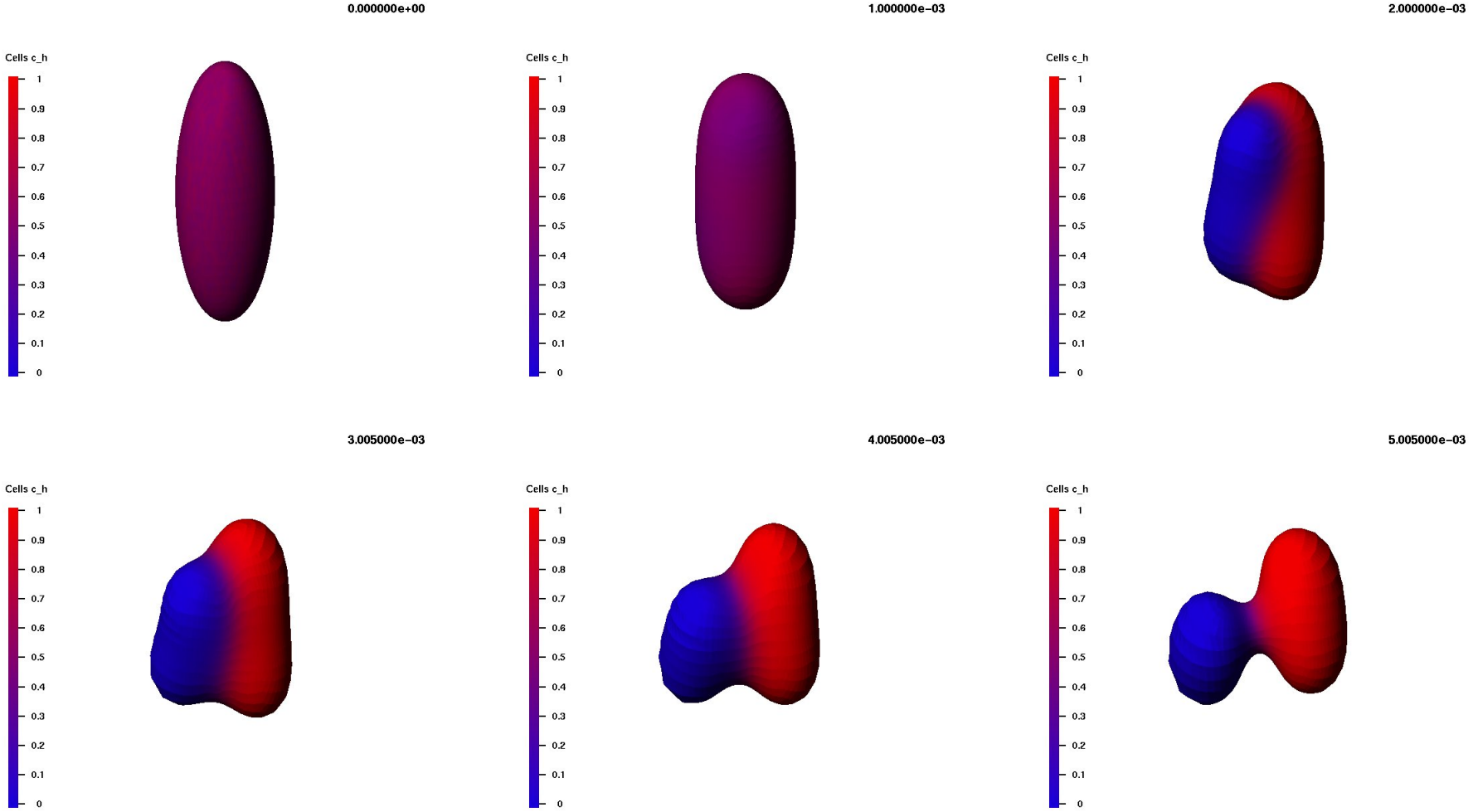
Non-Axisymmetric Structure

$\bar{v} \approx 0.9$, $\lambda \approx 9.0$, $x \approx 0.45$, $\bar{\kappa} = 0.0$.

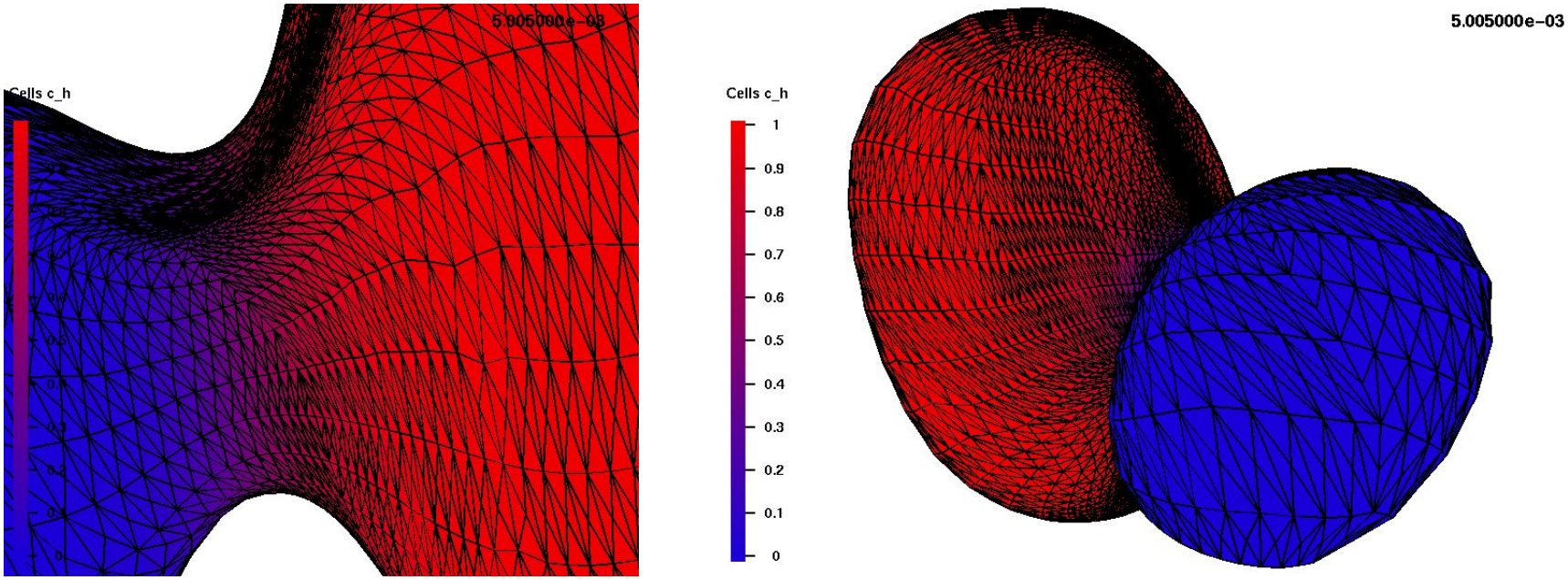


Random Order Parameter

$\bar{v} \approx 0.85$, $\lambda \approx 14.85$, $x \approx 0.55$ (random initial field c), $\bar{\kappa} = 0.0$.



Necessity for Grid Adaption



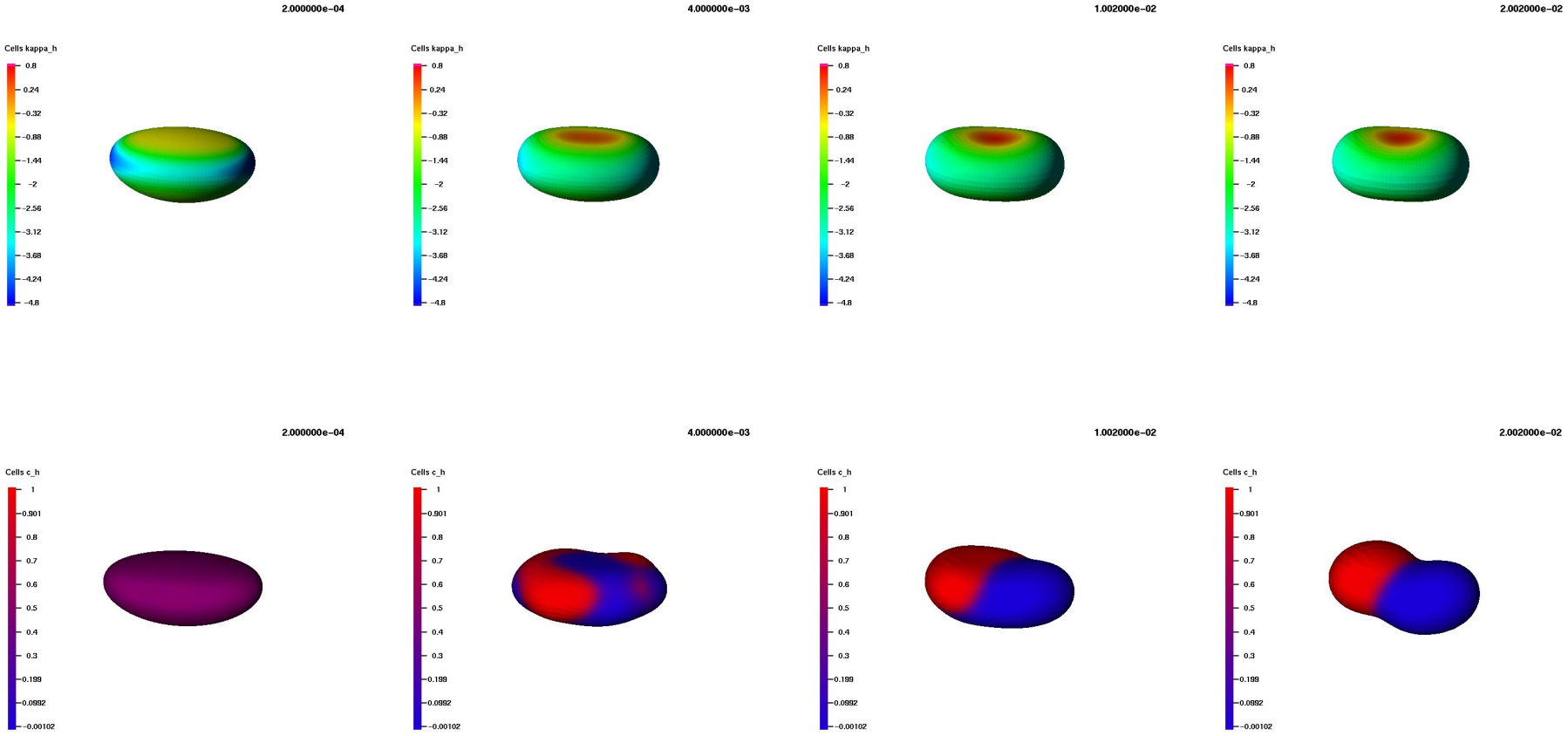
Evolution of the Surface

Deduced by computing the time derivative of the energy and using the law for c.

Exemplary for $k(c) = k_1 = k_2$ constant, $\bar{\kappa}(c) = \bar{\kappa}_1 = \bar{\kappa}_2 = 0$, Allen-Cahn equation for c:

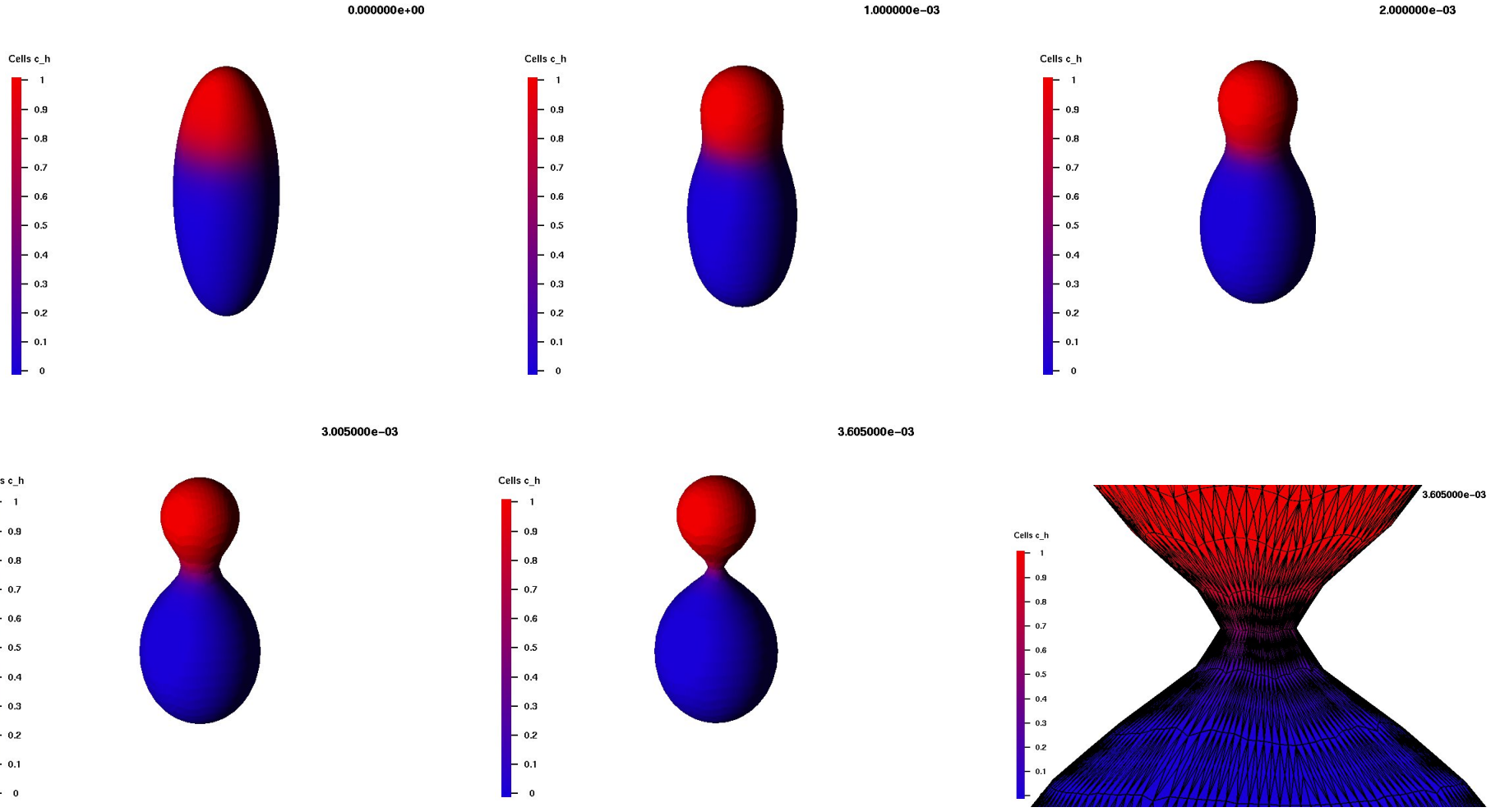
$$
\begin{aligned}
\frac{d}{dt}F = & \int_\Gamma \partial_t^\bullet \Big(\frac{k}{2}\kappa^2 + \tilde{\sigma}\varepsilon |\nabla_\Gamma c|^2 + \frac{\tilde{\sigma}}{\varepsilon}\psi(c) \Big) \\
& + \int_\Gamma \Big(\frac{k}{2}\kappa^2 + \tilde{\sigma}\varepsilon |\nabla_\Gamma c|^2 + \frac{\tilde{\sigma}}{\varepsilon}\psi(c) \Big) \nabla_\Gamma \cdot \boldsymbol{v} \\
= & -\frac{1}{\varepsilon}\int_\Gamma |\mu|^2 + \frac{1}{\varepsilon}\frac{\left(\int_\Gamma \mu h'(c)\right)^2}{\int_\Gamma (h'(c))^2} \\
& + \int_\Gamma \boldsymbol{v}\cdot\boldsymbol{\nu}\Big(k\Delta_\Gamma\kappa + k|\nabla_\Gamma \boldsymbol{n}|^2\kappa - \tilde{\sigma}\varepsilon \nabla_\Gamma c \otimes \nabla_\Gamma c : \nabla_\Gamma \boldsymbol{\nu} + \frac{\int_\Gamma \mu h'(c)}{\int_\Gamma (h'(c))^2} h(c)\kappa \Big) \\
& + \int_\Gamma \boldsymbol{v}\cdot\boldsymbol{\nu}\Big(- \big(\tfrac{k}{2}\kappa^2 + \tfrac{\tilde{\sigma}\varepsilon}{2}|\nabla_\Gamma c|^2 + \tfrac{\tilde{\sigma}}{\varepsilon}\psi(c) \big)\kappa \Big)
\end{aligned}
$$

Discocyte Without and With Phase Separation



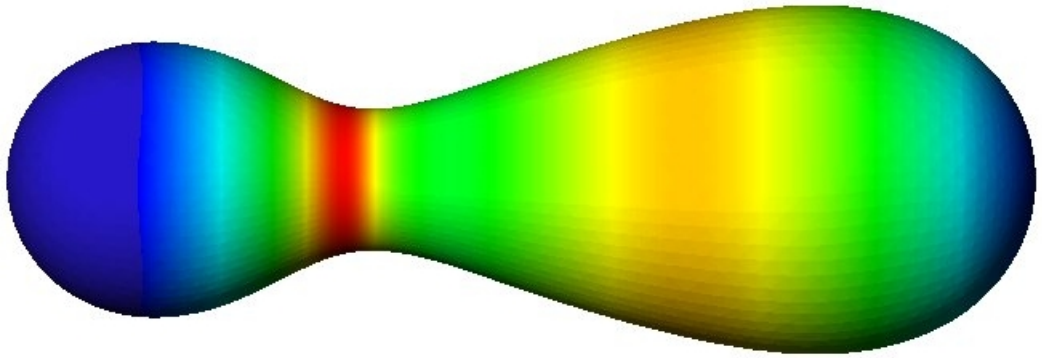
Budding?

Budding due to high line energy coefficient σ.
$\bar{v} \approx 0.85$, $\lambda \approx 14.7$, $x \approx 0.275$, $\bar{\kappa} = 0.0$.

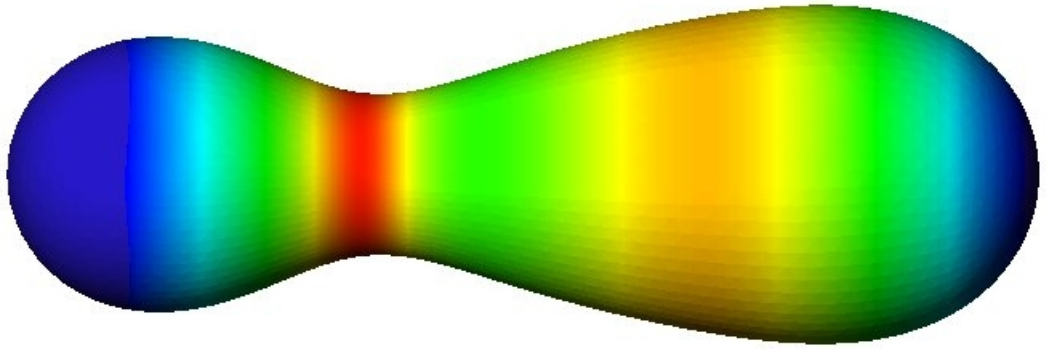


Spontaneous Curvature Effect

With spontaneous curvature:



No spontaneous curvature:



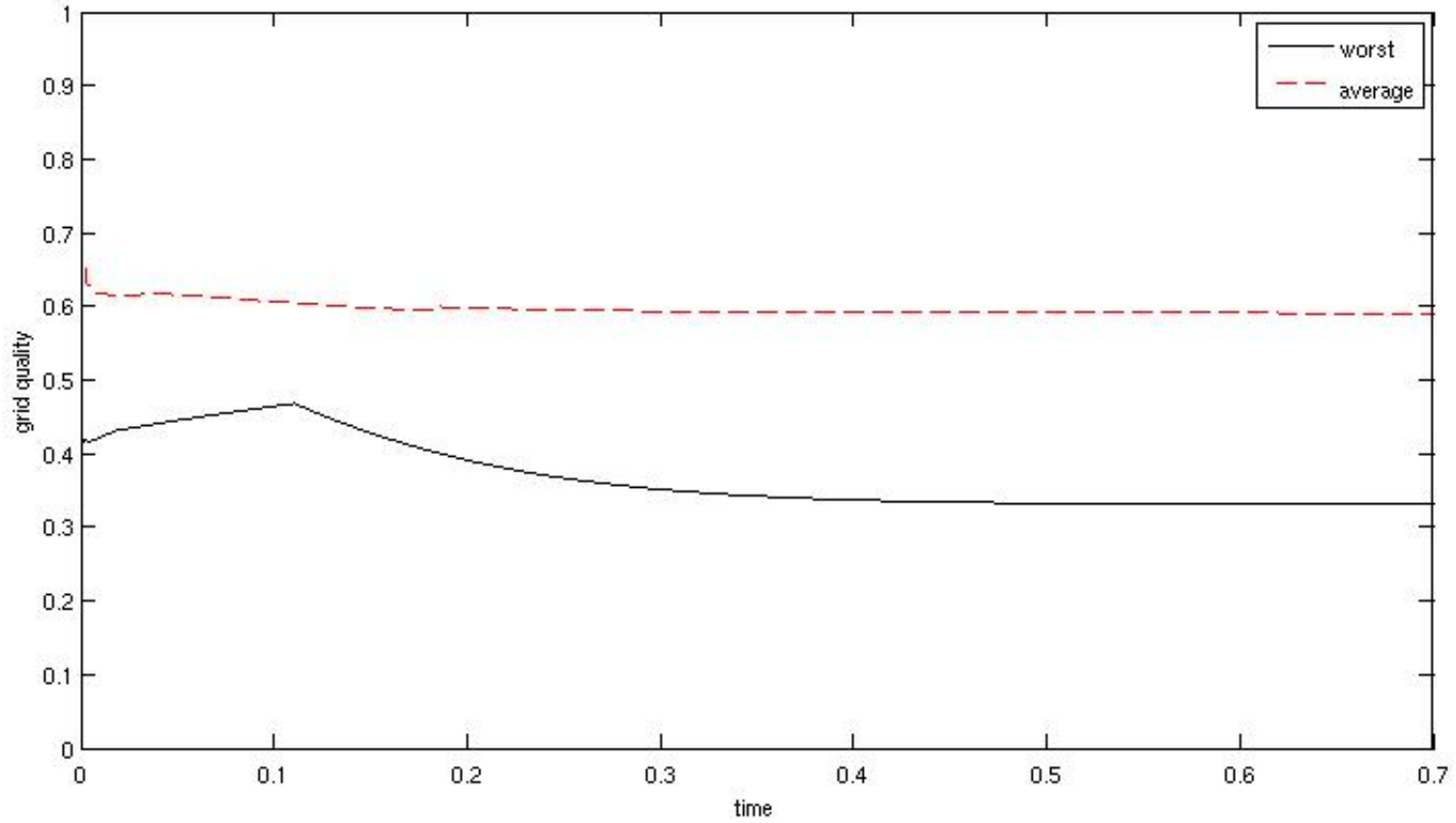
$\bar{\kappa}(c = 1) = -1.206061$,
$\bar{\kappa}(c = -1) = 0.0$,
interpolation with polynomial
of degree three in between.

Result:
neck more pronounced,
adjacent membranes
slightly more rounded.

Colour indicates the curvature between -0.35 (blue) and -0.15 (red).

Grid Quality

$q = \min\{\sin(\alpha) \mid \alpha \text{ inner angle}\}$.



Scale Invariance, Effective Parameters

Consider smooth hypersurfaces Γ in $\mathbb{R}^3$ of sphere-topology enclosing a domain Ω, as well as smooth, compact curves $\gamma \subset \Gamma$. Characteristic radius: $R = |\Gamma|/4\pi$.

System energy

$$F = \int_\Gamma \frac{k}{2}(\kappa - \bar{\kappa})^2 + \int_\gamma \sigma$$

is invariant under scaling $\boldsymbol{x} \mapsto \eta\boldsymbol{x}$, $\boldsymbol{x} \in \Gamma$, $\eta > 0$, provided that $\sigma \mapsto \sigma/\eta$ and $\bar{\kappa} \mapsto \bar{\kappa}/\eta$.

Equilibrium shapes / local minimiser are characterised by:

$v_r = \|\Omega\|/(4\pi/3)R^3$	reduced volume,
$q_r = \|\Gamma_1\|/\|\Gamma\|$	relative domain size,
$\sigma_r = \sigma R/k$	reduced line tension,
$c_r = \bar{\kappa}R$	reduced spontaneous curvature.

Effective Parameters, Phase Diagram

Example from [Jülicher, Lipowsky 1996].

$q_r = 0.1$ fixed, $c_r = 0.0$.

Top: variation of $\lambda = \sigma_r$ and $v = v_r$.
Bottom: $\sigma_r = 0.9$ fixed, variation of v_r.

Limit shapes:
L_{CB}: prolate and a spherical bud,
L_{sp}: two cut spheres.

Axisymmetric shapes only.