Natural Discretization of Gradient Flows

Applications to Viscous Thin Films and to Willmore Flow

Martin Rumpf, Universität Bonn

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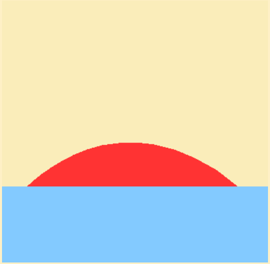
New Directions in Computational PDE
Warwick, January $12^{th} - 16^{th}$

joint work with

- thin film flow: Orestis Vantzos
- Willmore flow: Nadine Olischläger

Application: viscous thin films



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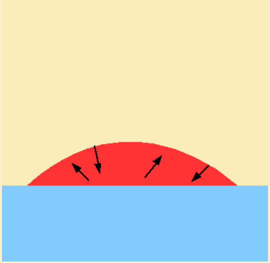

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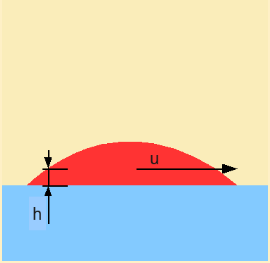

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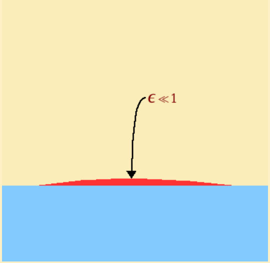

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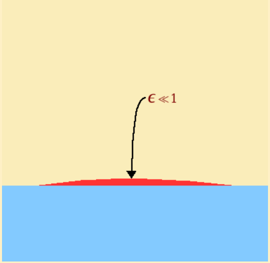

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governing PDE [Oron, Davis, Bankoff ´97]:

$$\partial_t h = -\operatorname{div}\left(\frac{h^3}{3\mu}\nabla \operatorname{div}(\sigma \nabla h)\right)$$

Application: viscous thin films (cont.)

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gradient flow perspective:

energy (surface tension):

$$e[h] = \int_\Omega \sigma \left(1 + \frac{|\nabla h|^2}{2} \right) \, \mathrm{d}x$$

Application: viscous thin films (cont.)

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metric:

$$\mathbf{g}_h(\delta h, \delta h) = g_h(u, u) = \int_\Omega \frac{3\mu}{h} |u|^2 \, \mathrm{d}x$$

derived as lubrication limit of dissipation based on friction:

$$\int_{\text{vol}} \mu \, |D_y \mathbf{u} + D_y \mathbf{u}^T|^2 \, \mathrm{d}y \quad , \; y = (x, x^\perp) \quad , \; u = \frac{1}{h} \int_0^h \mathbf{u} \, \mathrm{d}x^\perp$$

transport equation coupling δh and u:

$$\delta h + \operatorname{div}(hu) = 0$$

Application: viscous thin films (cont.)

Given energy and metric on the manifold (cf. [Giacomelli, Otto ´03]):

$$\mathcal{M} = \left\{ h \, : \, \int_\Omega h \, \mathrm{d}x = \text{const} \right\} \qquad \left(T_h\mathcal{M} = \left\{ \delta h \, : \, \int_\Omega \delta h \, \mathrm{d}x = 0 \right\} \right)$$

we consider the gradient flow [GF]:

$$\partial_t h = -\mathrm{grad}_{\mathbf{g}} e[h]$$

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$$\Rightarrow \mathbf{g}_h(\partial_t h, \theta) = -e'[h](\theta)$$

Application: viscous thin films (cont.)

[GF] ⇒ [PDE]:

$$0 = \mathbf{g}_h(\partial_t h, \delta h) + e'[h](\delta h)$$

Application: viscous thin films (cont.)

[GF] ⇒ [PDE]:

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\begin{aligned}
0 &= \mathbf{g}_h(\partial_t h, \delta h) + e'[h](\delta h) \\
&= g_h(u, v) + e'[h](\delta h) \\
&\quad \text{where } \partial_t h + \operatorname{div}(h\, u) = 0 \ \text{ and } \delta h + \operatorname{div}(h\, v) = 0
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Application: viscous thin films (cont.)

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&= \int_\Omega \frac{3\mu}{h} u \cdot v - \nabla \operatorname{div}(\sigma \nabla h) h\, v \,\mathrm{d}x \quad \text{(integration by parts)} \\
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Application: Willmore flow

We consider a compact surface $\mathcal{S} = \mathcal{S}[x]$ embedded in $\mathbb{R}^n$ $(n = 2, 3)$ and the **energy**:

$$w[x] = \frac{1}{2} \int_{\mathcal{S}} h^2 \, \mathrm{d}a$$

Here h is the mean curvature on $\mathcal{S}$.

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$$g_{\mathcal{S}}(v, v) = \int_{\mathcal{S}} v^2 \, \mathrm{d}a$$

be the L^2-**metric** on variations v of $\mathcal{S}$ generated by normal **motion**:

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Then, **Willmore flow** is the corresponding gradient flow (GF):

$$\partial_t x = -\mathrm{grad}_g w[x]$$

governing PDE ($n = 3$):

$$\partial_t x = \left(\Delta_{\mathcal{S}} h + h \left(|D_{\mathcal{S}} n|^2 - \frac{h^2}{2} \right) \right) n$$

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Remark: There is an inner variational principle, i.e.

$$h = \mathrm{grad}_{\mathcal{S}} a[x]\,, \quad \text{where } a[x] = \int_{\mathcal{S}} \mathrm{d}a$$

Numerical approaches:

[Rusu ´01], [Meyer, Simonett ´02], [Grzibovski, Heintz ´03], [Droske, M. ´04], [Bobenko, Schröder ´05], [Dziuk, Deckelnick ´06], [Barrett, Garcke, Nürnberg ´08], [Dziuk ´08] ...

Natural time discretization of gradient flows

For the gradient flow $\dot{x} = \mathrm{grad}_g e[x]$ on a manifold $\mathcal{M}$ and given x^0 define time discrete solutions $(x^k)_{k=0,\dots}$ $(x_k \approx x(k\tau))$:

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energy estimate as a direct consequence:

$$e[x^{k+1}] + \frac{1}{2\tau} \mathrm{dist}(x^{k+1}, x^k)^2 \le 0 + e[x^k]$$

[Luckhaus, Sturzenhecker ´95]

Natural time discretization (cont.)

Motivation (Euklidian case):

$$x^{k+1} \quad = \quad \arg\min_x \frac{1}{2\tau}|x - x^k|^2 + e[x]$$

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Generalization to the heat equation:

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Natural time discretization of thin film flow

Given h^0 define time discrete solutions $(h^k)_{k=0,\ldots}$:

$$h^{k+1} \quad = \quad \arg\min_h \frac{1}{2\tau} \operatorname{dist}(h, h^k)^2 + e[h]$$

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$$\text{and } h(t_k) = h^k$$

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$\longrightarrow$ PDE constraint optimization problem

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and $h(t_k) = h^k$

$\longrightarrow$ PDE constraint optimization problem

$$u^{k+1} = \arg\min_u \frac{\tau}{2}\inf_\gamma \left(\int_0^1 \sqrt{g_h(u(t_k+\tau s), u(t_k+\tau s))}\,\mathrm{d}s\right)^2 + e[h[u,h^k]],$$

where $\partial_t h + \operatorname{div}\,(h\,u)) = 0\,,$

$$h(t_k) = h^k, h(t_{k+1}) = h^{k+1}$$

Natural time discretization of thin film flow (cont.)

Approximation by numerical quadrature in the general case:

$$\mathrm{dist}(x, x^k)^2 \quad = \quad \inf_{\gamma} \left(\int_0^1 \sqrt{g_{\gamma(s)}(\dot{\gamma}(s), \dot{\gamma}(s))}\, \mathrm{d}s \right)^2$$

Natural time discretization of thin film flow (cont.)

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for some $r \in [0,1]$

numerical time discretization $(r = 1)$

$$u^{k+1} = \arg\min_u \frac{\tau}{2} g_{h^k}(u,u) + e[h[u,h^k]]$$

Natural time discretization of thin film flow (cont.)

space discretization:

- implicit Finite Volume scheme for the transport ($H^k, U^k \in \mathbb{R}^{\sharp\mathrm{dofs}}$):

$$L(U)H(U,H^k) = H^k$$

(constraint equation)

Natural time discretization of thin film flow (cont.)

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- discrete constraint variational problem in each time step:

$$U^{k+1} = \operatorname*{arg\,min}_{U \in \mathbb{R}^{\sharp\mathrm{dofs}}} \frac{\tau}{2} G_{H^k}(U,U) + E(H(U,H^k))\,,$$

where $G(\cdot,\cdot)$, $E(\cdot)$ are numerical quadrature evaluation corresponding to $g(\cdot,\cdot)$ and $e(\cdot)$.

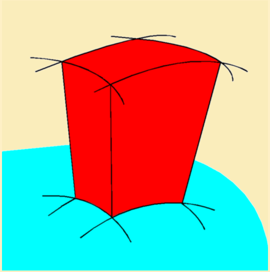
[Dohmen, Grunewald, Otto, R. ´06],

cf. also [Zhornitskaya, Bertozzi ´00], [Grün, R. ´00]

Thin film model in case of curved surface

We can not use the transport PDE

$$\partial_t h + \operatorname{div}_{\mathcal{S}}(h\,\mathbf{u}) = 0$$



The height h is not even conserved anymore!

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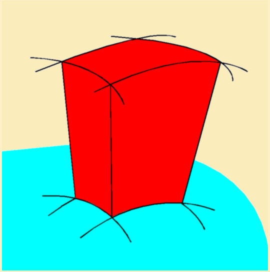

The correct transport PDE is

$$\partial_t \eta + \operatorname{div}_{\mathcal{S}}(\eta\, \mathbf{u}) = 0$$

where η is the fluid mass per unit surface

$$\eta = \int_0^h (1-\epsilon\xi\kappa_1)(1-\epsilon\xi\kappa_2)d\xi$$
$$= h + \frac{1}{2}\mathbf{h}h^2\epsilon + \frac{1}{3}\mathbf{k}h^3\epsilon^2$$

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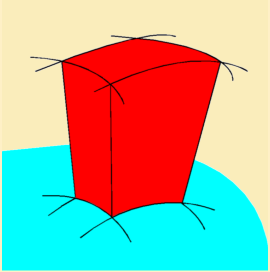

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and $\mathbf{u}$ is the transport velocity

$$u = \frac{1}{\eta}\int_0^h (1 - \epsilon\xi\kappa_2)\mathbf{u}_1 + (1 - \epsilon\xi\kappa_1)\mathbf{u}_2\, d\xi$$

, [Roy, Roberts, Simpson '02], [Meyer, Charpin, Chapman ´02]

Thin film model in case of curved surface (cont.)

Gradient flow perspective

transport equation (PDE constraint)

$$\delta\eta + \operatorname{div}_{\mathcal{S}}(\eta\mathbf{u}) = 0$$

Thin film model in case of curved surface (cont.)

Gradient flow perspective

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surface energy

$$e(h) = \int_{\mathcal{S}} \sigma\left(\mathbf{h}h + \mathbf{k}h^2\epsilon + \frac{\epsilon}{2}\left|\nabla_{\mathcal{S}}h\right|^2\right)$$

Thin film model in case of curved surface (cont.)

Gradient flow perspective

transport equation (PDE constraint)

$$\delta\eta + \operatorname{div}_{\mathcal{S}}(\eta\mathbf{u}) = 0$$

surface and gravitational energy

$$e(\eta) = \int_{\mathcal{S}} (\rho g z + \sigma\mathbf{h})\eta + \frac{\epsilon}{2}\Big((\rho g\cos\theta - \sigma(\mathbf{h}^2 - 2\mathbf{k})\eta^2 + \sigma\,|\nabla_{\mathcal{S}}\eta|^2\Big)$$

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metric (dissipation rate)

$$g_\eta(\mathbf{u},\mathbf{u}) = \int_{\mathcal{S}} \frac{3\mu}{\eta}\,\mathbf{u}\cdot\Big(1\!\!\mathrm{I} + \epsilon\frac{\eta}{2}(\mathbf{h}1\!\!\mathrm{I} + D_{\mathcal{S}}n)\Big)\,\mathbf{u}$$

Thin film model in case of curved surface (cont.)

Minimizing the Rayleigh functional, like in the planar case, yields the PDE:

$$\partial_t \eta - \mathrm{div}_{\mathcal{S}} \Big\{ \frac{\eta^3}{3\mu} \big(1\!\mathrm{I} - \epsilon \frac{\eta}{2} (\mathbf{h} 1\!\mathrm{I} + D_{\mathcal{S}} n) \big) \nabla_{\mathcal{S}} \big(\rho g z + \sigma \mathbf{h} + \epsilon ((\rho g \cos\theta - \sigma(\mathbf{h}^2 - 2\mathbf{k}))\eta - \sigma \Delta_{\mathcal{S}} \eta) \big) \Big\} = 0$$

Thin film model in case of curved surface (cont.)

Minimizing the Rayleigh functional, like in the planar case, yields the PDE:

$$\partial_t \eta - \operatorname{div}_{\mathcal{S}} \Big\{ \frac{\eta^3}{3\mu} \big(1\!\mathrm{I} - \epsilon \frac{\eta}{2} (\mathbf{h} 1\!\mathrm{I} + D_{\mathcal{S}} n) \big) \nabla_{\mathcal{S}} \big(\rho g z + \sigma \mathbf{h} + \epsilon ((\rho g \cos\theta - \sigma(\mathbf{h}^2 - 2\mathbf{k}))\eta - \sigma \Delta_{\mathcal{S}} \eta) \big) \Big\} = 0$$

- 4th order non linear PDE

Thin film model in case of curved surface (cont.)

Minimizing the Rayleigh functional, like in the planar case, yields the PDE:

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- 4th order non linear PDE
- Leading order term is hyperbolic, the correction is parabolic

Thin film model in case of curved surface (cont.)

Minimizing the Rayleigh functional, like in the planar case, yields the PDE:

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- 4th order non linear PDE
- Leading order term is hyperbolic, the correction is parabolic

Thin film model in case of curved surface (cont.)

Minimizing the Rayleigh functional, like in the planar case, yields the PDE:

$$\partial_t \eta - \mathrm{div}_{\mathcal{S}} \Big\{ \frac{\eta^3}{3\mu} \big(1\!\mathrm{I} - \epsilon \frac{\eta}{2} (\mathbf{h} 1\!\mathrm{I} + D_{\mathcal{S}} n) \big)$$
$$\nabla_{\mathcal{S}} \big(\rho g z + \sigma \mathbf{h} + \epsilon ((\rho g \cos\theta - \sigma(\mathbf{h}^2 - 2\mathbf{k}))\eta - \sigma \Delta_{\mathcal{S}} \eta) \big) \Big\} = 0$$

- 4th order non linear PDE
- Leading order term is hyperbolic, the correction is parabolic
- Mixture of transport, 2nd and 4th order diffusion terms

Thin film model in case of curved surface (cont.)

Minimizing the Rayleigh functional, like in the planar case, yields the PDE:

$$\partial_t \eta - \operatorname{div}_{\mathcal{S}} \Big\{ \frac{\eta^3}{3\mu} \big(1\!\mathrm{I} - \epsilon \frac{\eta}{2} (\mathbf{h} 1\!\mathrm{I} + D_{\mathcal{S}} n) \big) \nabla_{\mathcal{S}} \big(\rho g z + \sigma \mathbf{h} + \epsilon ((\rho g \cos\theta - \sigma(\mathbf{h}^2 - 2\mathbf{k}))\eta - \sigma \Delta_{\mathcal{S}} \eta) \big) \Big\} = 0$$

- 4th order non linear PDE
- Leading order term is hyperbolic, the correction is parabolic
- Mixture of transport, 2nd and 4th order diffusion terms
- It is in agreement, up to $\mathrm{O}(\epsilon^2)$, to the thin film equation in [Roy, Roberts, Simpson '02]

Alveoli in the lung

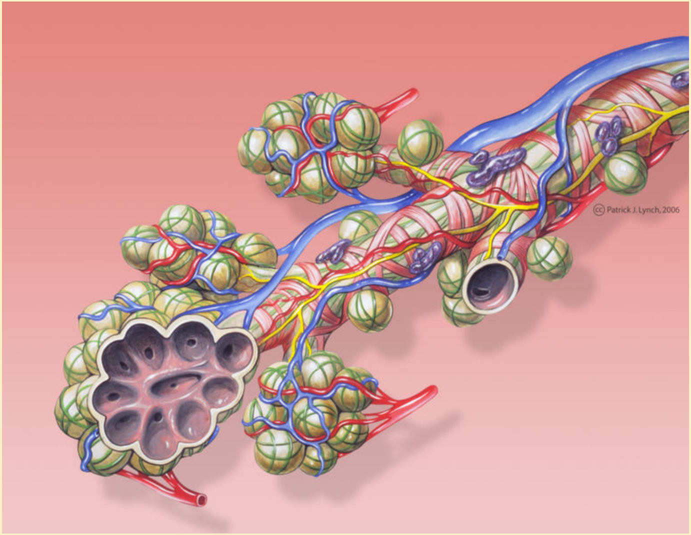
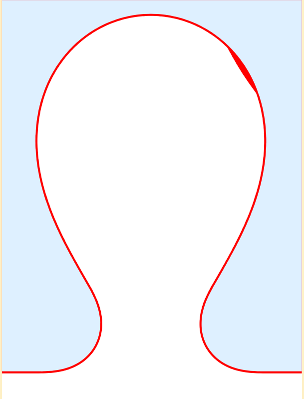


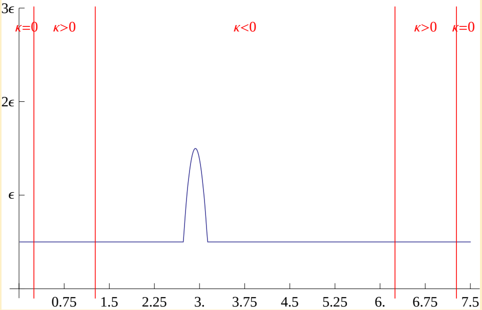
image by Patrick J. Lynch, medical illustrator; C. Carl Jaffe, MD, cardiologist

Evolution of a film with a local bump

liquid lining ($\epsilon = .03$) of alveolus-like shape with a bump on the upper left

$$t = 0$$

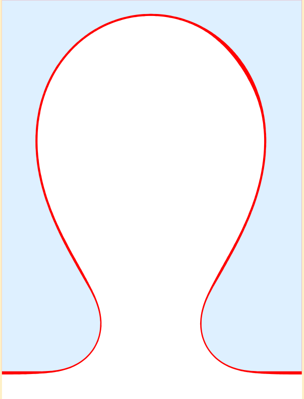


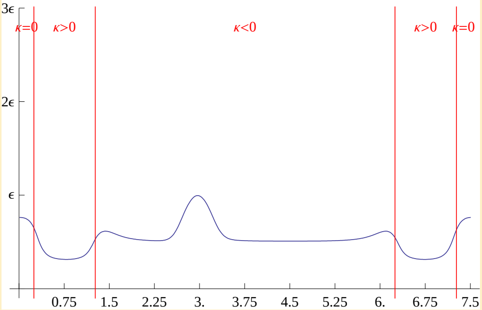


Evolution of a film with a local bump

liquid lining ($\epsilon = .03$) of alveolus-like shape with a bump on the upper left

$$t = 25\tau$$

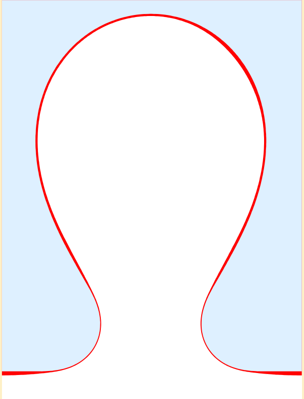


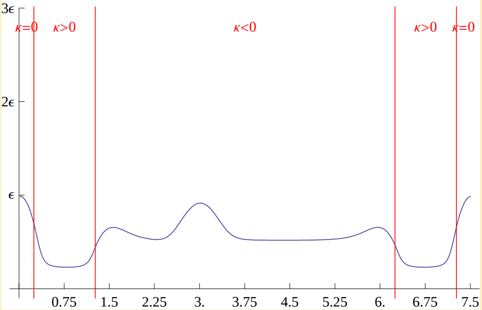


Evolution of a film with a local bump

liquid lining ($\epsilon = .03$) of alveolus-like shape with a bump on the upper left

$$t = 50\tau$$

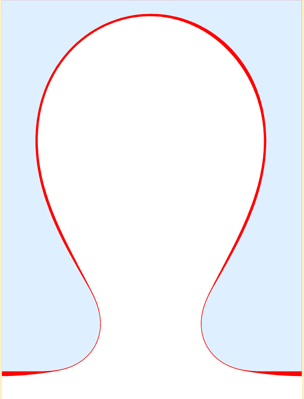


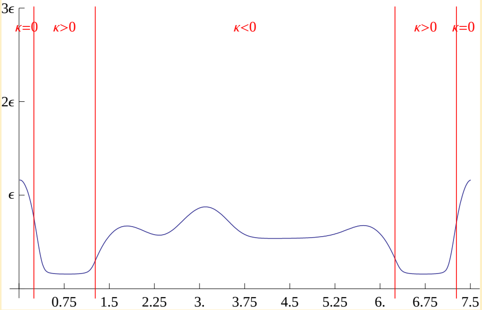


Evolution of a film with a local bump

liquid lining ($\epsilon = .03$) of alveolus-like shape with a bump on the upper left

$$t = 100\tau$$

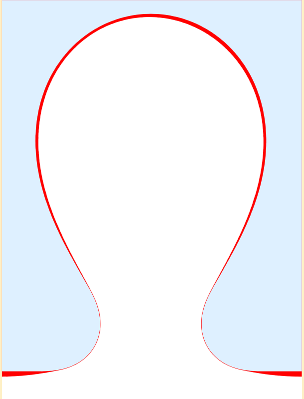


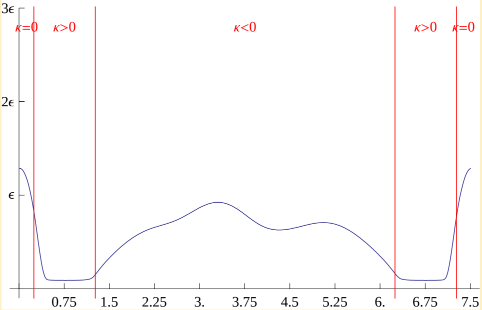


Evolution of a film with a local bump

liquid lining ($\epsilon = .03$) of alveolus-like shape with a bump on the upper left

$$t = 250\tau$$





Evolution of a film with a local bump

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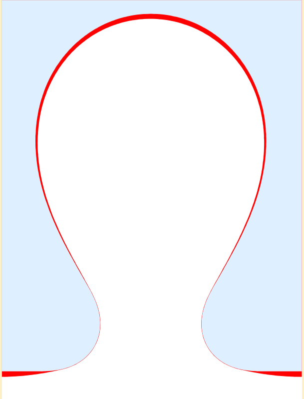
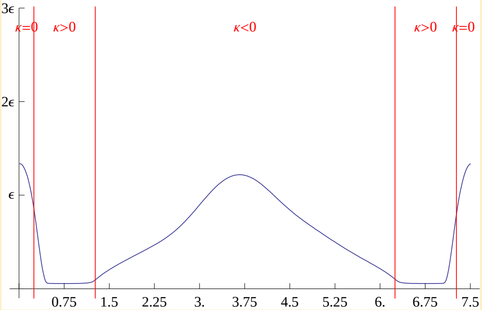
liquid lining ($\epsilon = .03$) of alveolus-like shape with a bump on the upper left

$$t = 500\tau$$

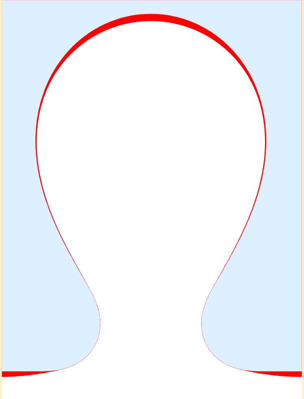


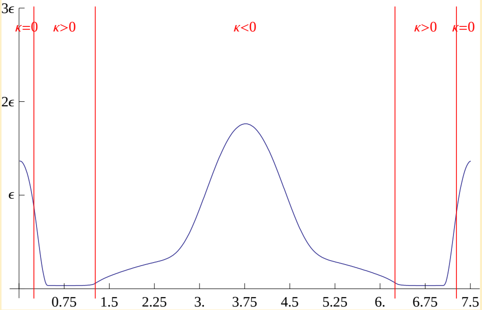


Evolution of a film with a local bump

liquid lining ($\epsilon = .03$) of alveolus-like shape with a bump on the upper left

$$t = 1000\tau$$

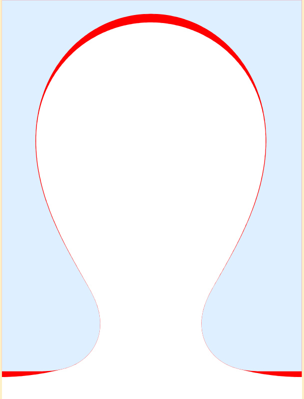


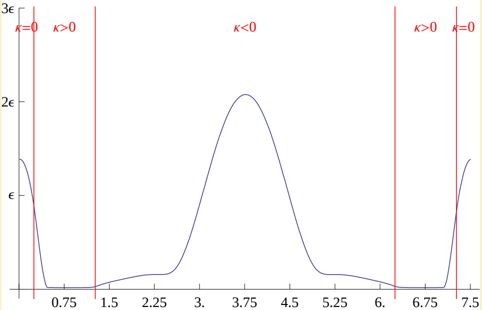


Evolution of a film with a local bump

liquid lining ($\epsilon = .03$) of alveolus-like shape with a bump on the upper left

$$t = 2500\tau$$

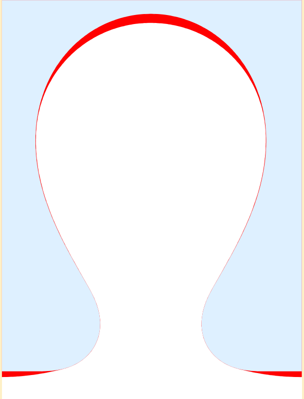


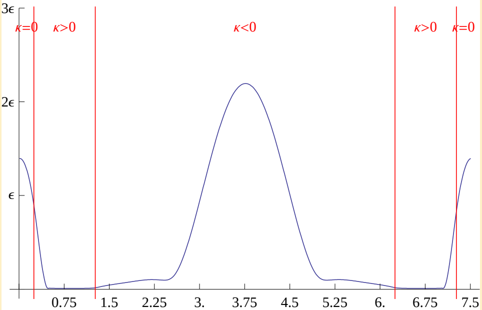


Evolution of a film with a local bump

liquid lining ($\epsilon = .03$) of alveolus-like shape with a bump on the upper left

$$t = 5000\tau$$

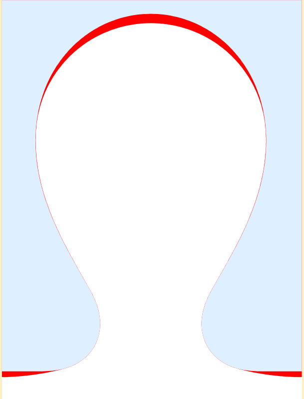


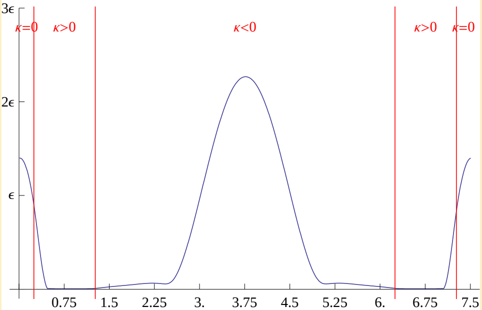


Evolution of a film with a local bump

liquid lining ($\epsilon = .03$) of alveolus-like shape with a bump on the upper left

$$t = 10000\tau$$

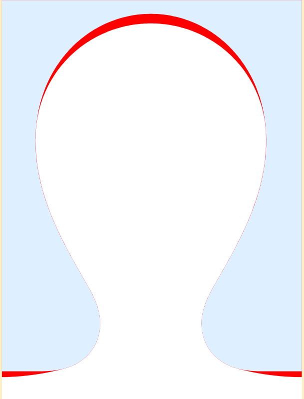


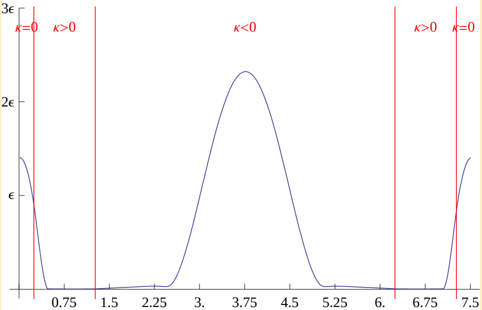


Evolution of a film with a local bump

liquid lining ($\epsilon = .03$) of alveolus-like shape with a bump on the upper left

$$t = 25000\tau$$

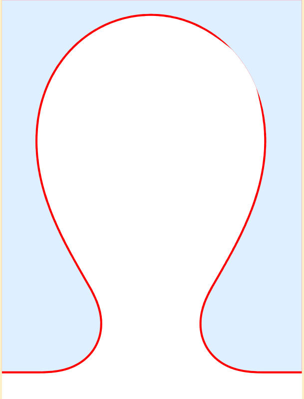


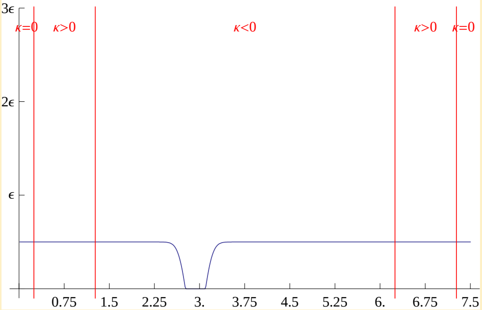


Evolution of a film with rupture

liquid lining ($\epsilon = .03$) of alveolus-like shape with a rupture on the top left

$$t = 0$$

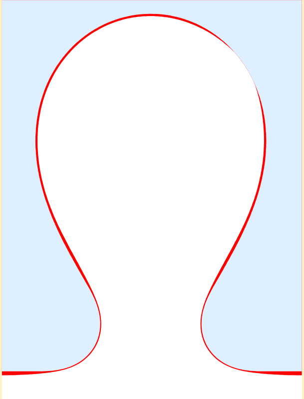


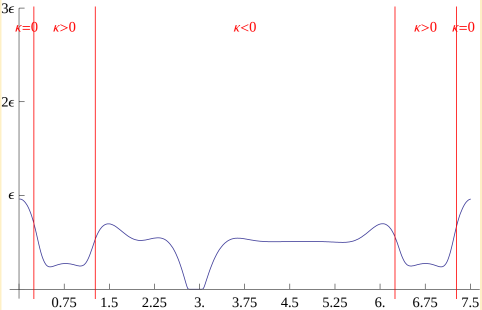


Evolution of a film with rupture

liquid lining ($\epsilon = .03$) of alveolus-like shape with a rupture on the top left

$$t = 25\tau$$

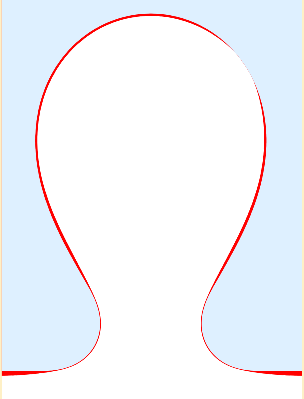


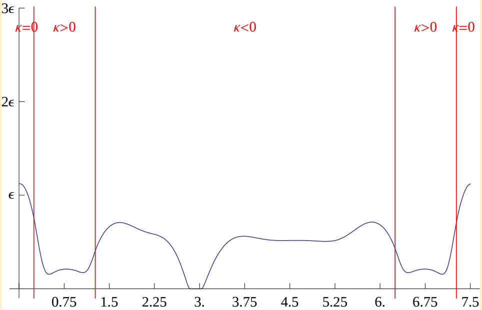


Evolution of a film with rupture

liquid lining ($\epsilon = .03$) of alveolus-like shape with a rupture on the top left

$$t = 50\tau$$

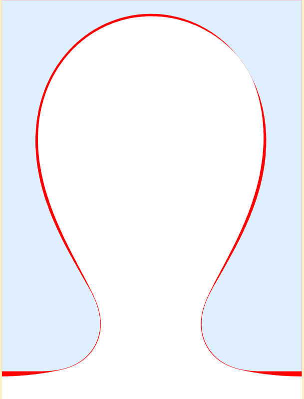


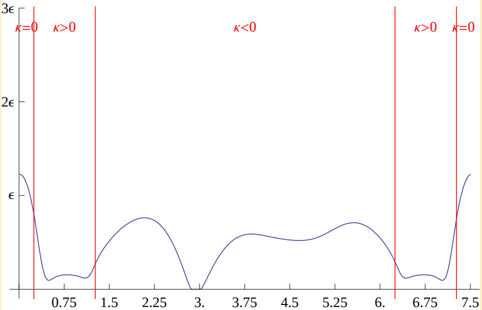


Evolution of a film with rupture

liquid lining ($\epsilon = .03$) of alveolus-like shape with a rupture on the top left

$$t = 100\tau$$

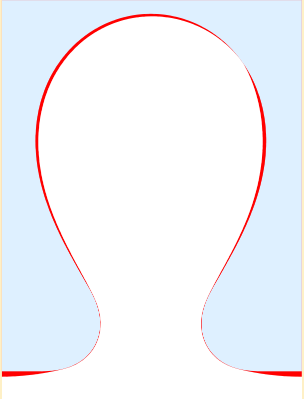


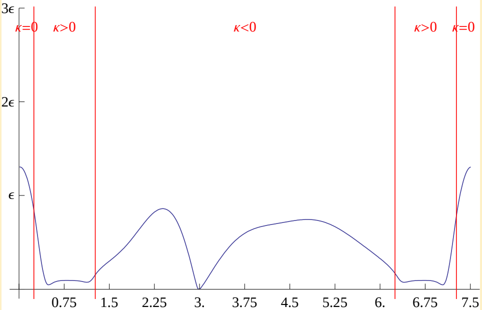


Evolution of a film with rupture

liquid lining ($\epsilon = .03$) of alveolus-like shape with a rupture on the top left

$$t = 250\tau$$





Evolution of a film with rupture

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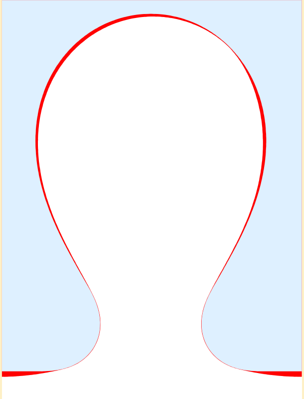
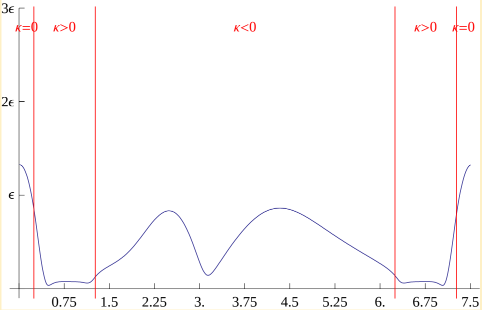
liquid lining ($\epsilon = .03$) of alveolus-like shape with a rupture on the top left

$$t = 350\tau$$





Evolution of a film with rupture

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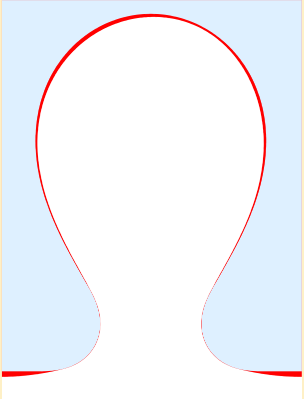
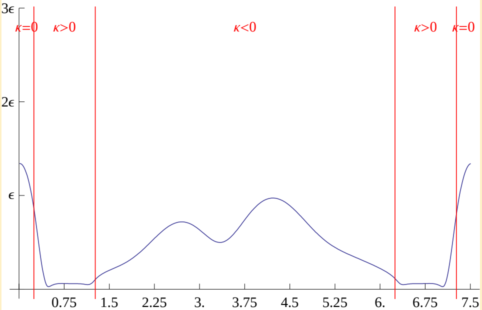
liquid lining ($\epsilon = .03$) of alveolus-like shape with a rupture on the top left

$$t = 500\tau$$

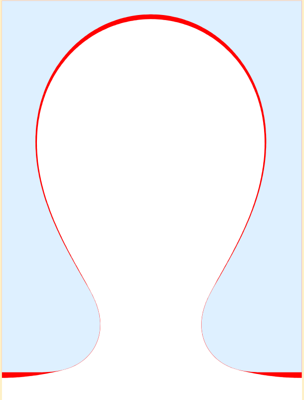


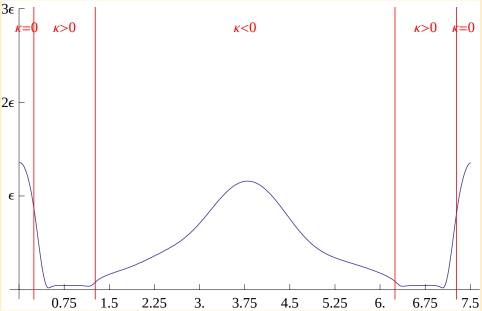


Evolution of a film with rupture

liquid lining ($\epsilon = .03$) of alveolus-like shape with a rupture on the top left

$$t = 7500\tau$$

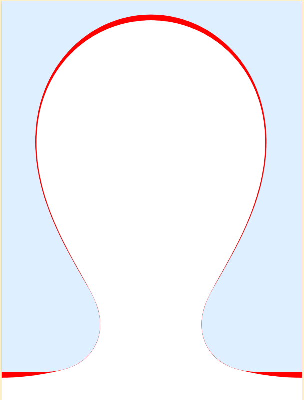


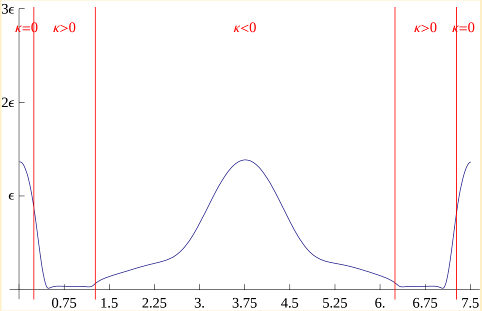


Evolution of a film with rupture

liquid lining ($\epsilon = .03$) of alveolus-like shape with a rupture on the top left

$$t = 1000\tau$$

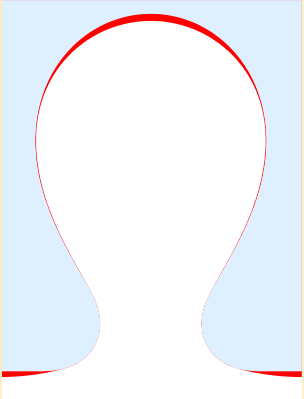


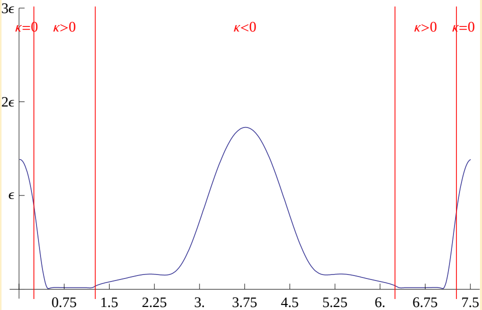


Evolution of a film with rupture

liquid lining ($\epsilon = .03$) of alveolus-like shape with a rupture on the top left

$$t = 2500\tau$$

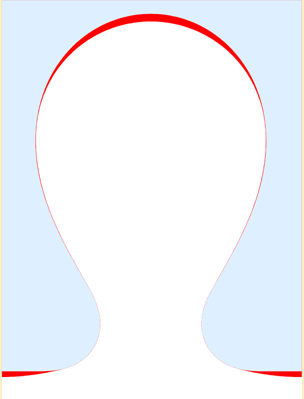


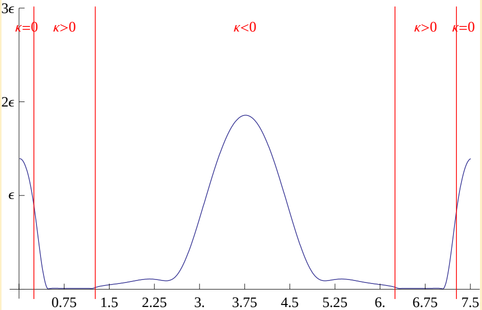


Evolution of a film with rupture

liquid lining ($\epsilon = .03$) of alveolus-like shape with a rupture on the top left

$$t = 5000\tau$$

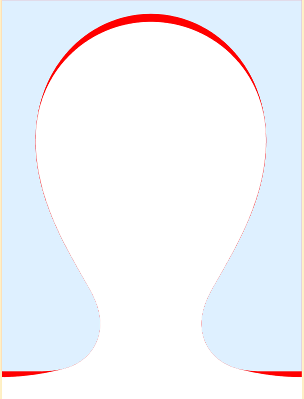


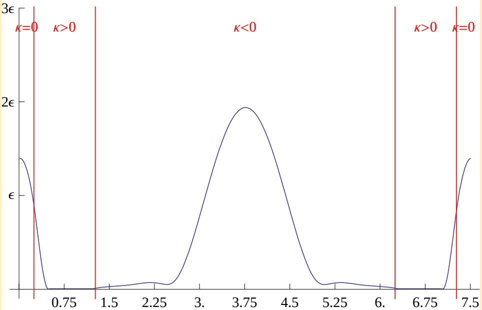


Evolution of a film with rupture

liquid lining ($\epsilon = .03$) of alveolus-like shape with a rupture on the top left

$$t = 10000\tau$$

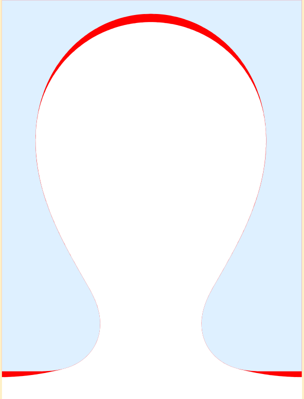


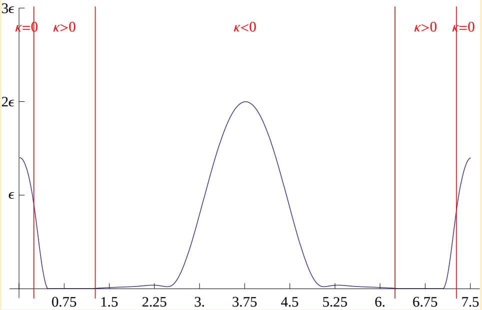


Evolution of a film with rupture

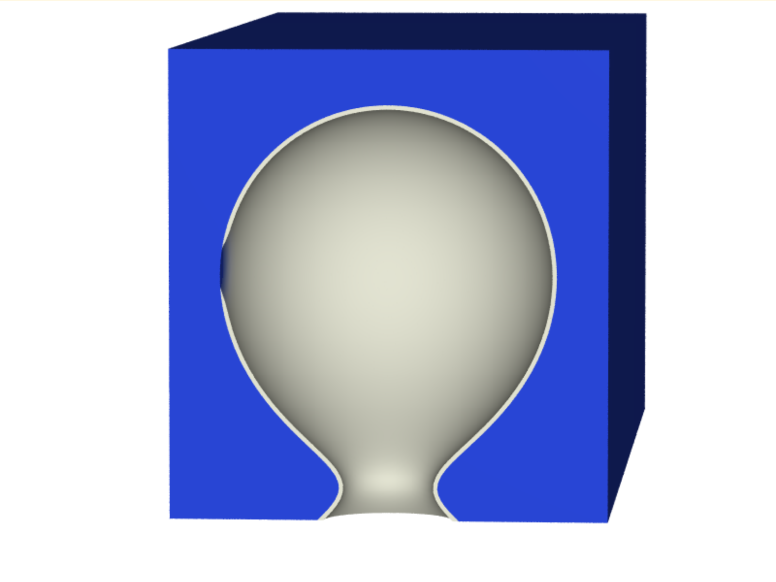
liquid lining ($\epsilon = .03$) of alveolus-like shape with a rupture on the top left

$$t = 25000\tau$$



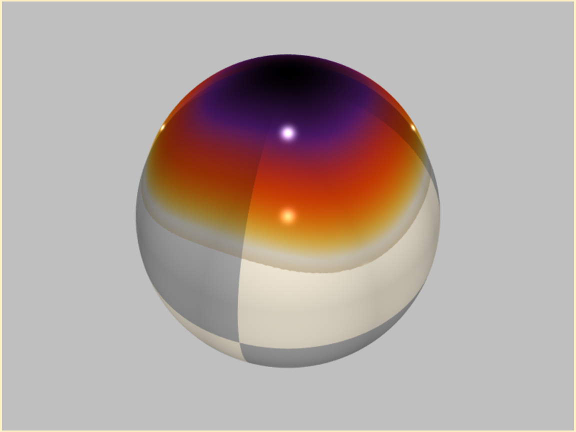


Evolution of a film with rupture



Droplet on a sphere

Four-fold symmetry perturbed droplet sliding down a sphere:



cf. [Bertozzi, Greer, Sapiro ´06]

Two step discretization of Willmore flow

Recall mean curvature motion:

$$y[x] = x^{k+1}, \quad x = x^k$$

$$y[x] = \arg\min_y \frac{1}{2\tau}\,\mathrm{dist}(\mathcal{S}[y], \mathcal{S}[x])^2 + \int_{\mathcal{S}[y]} \mathrm{d}a$$

(natural gradient descent scheme)

Two step discretization of Willmore flow

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Recall mean curvature motion:

$$\begin{aligned} y[x] &= x^{k+1}, \quad x = x^k \\ y[x] &= \arg\min_y \frac{1}{2\tau}\,\mathrm{dist}(\mathcal{S}[y],\mathcal{S}[x])^2 + \int_{\mathcal{S}[y]} \mathrm{d}a \end{aligned}$$

(natural gradient descent scheme)

approximation

$$y[x] = \arg\min_y \int_{\mathcal{S}[x]} \frac{1}{2\tau}|y-x|^2 + \frac{1}{2}|\nabla_{\mathcal{S}[x]} y|^2 \,\mathrm{d}a$$

cf. [Dziuk '89]

Two step discretization of Willmore flow

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Recall mean curvature motion:

$$y[x] = x^{k+1}, \quad x = x^k$$

$$y[x] = \arg\min_y \frac{1}{2\tau}\,\mathrm{dist}(\mathcal{S}[y],\mathcal{S}[x])^2 + \int_{\mathcal{S}[y]} \mathrm{d}a$$

(natural gradient descent scheme)

approximation

$$y[x] = \arg\min_y \int_{\mathcal{S}[x]} \frac{1}{2\tau}|y-x|^2 + \frac{1}{2}|\nabla_{\mathcal{S}[x]} y|^2 \,\mathrm{d}a$$

cf. [Dziuk '89]

approximation of curvature vector and Willmore energy

$$h[x]\,n[x] \approx \frac{y[x]-x}{\tau}$$

Two step discretization of Willmore flow

Recall mean curvature motion:

$$
\begin{aligned}
y[x] &= x^{k+1}, \quad x = x^k \\
y[x] &= \arg\min_y \frac{1}{2\tau} \operatorname{dist}(\mathcal{S}[y], \mathcal{S}[x])^2 + \int_{\mathcal{S}[y]} \mathrm{d}a
\end{aligned}
$$

(natural gradient descent scheme)

approximation

$$
y[x] = \arg\min_y \int_{\mathcal{S}[x]} \frac{1}{2\tau} |y - x|^2 + \frac{1}{2} |\nabla_{\mathcal{S}[x]} y|^2 \, \mathrm{d}a
$$

cf. [Dziuk '89]

approximation of curvature vector and Willmore energy

$$
h[x]\, n[x] \approx \frac{y[x] - x}{\tau}, \quad w[x] \approx \frac{1}{2} \int_{\mathcal{S}[x]} \frac{|y[x] - x|^2}{\tau^2} \, \mathrm{d}a
$$

Two step discretization of Willmore flow (cont.)

Abstract Willmore flow time step:

$$x^{k+1} = \arg\min_x \frac{1}{2\tau} \operatorname{dist}(\mathcal{S}[x], \mathcal{S}[x^k])^2 + w[x]$$

Two step discretization of Willmore flow (cont.)

Abstract Willmore flow time step:

$$x^{k+1} = \arg\min_x \frac{1}{2\tau}\,\mathrm{dist}(\mathcal{S}[x], \mathcal{S}[x^k])^2 + w[x]$$

Based on the approximation $w[x] \approx \frac{1}{2}\int_{\mathcal{S}[x]} \frac{|y[x]-x|^2}{\tau^2}\,\mathrm{d}a$ we obtain:

two step time discretization

$$x^{k+1} \;=\; \arg\min_x \int_{\mathcal{S}[x^k]} |x - x^k|^2\,\mathrm{d}a + \frac{1}{\tau}\int_{\mathcal{S}[x]} |y[x] - x|^2\,\mathrm{d}a$$

Two step discretization of Willmore flow (cont.)

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Abstract Willmore flow time step:

$$x^{k+1} = \arg\min_x \frac{1}{2\tau}\operatorname{dist}(\mathcal{S}[x], \mathcal{S}[x^k])^2 + w[x]$$

Based on the approximation $w[x] \approx \frac{1}{2}\int_{\mathcal{S}[x]} \frac{|y[x]-x|^2}{\tau^2}\,\mathrm{d}a$ we obtain:

two step time discretization

$$\begin{aligned} x^{k+1} &= \arg\min_x \int_{\mathcal{S}[x^k]} |x - x^k|^2\,\mathrm{d}a + \frac{1}{\tau}\int_{\mathcal{S}[x]} |y[x] - x|^2\,\mathrm{d}a \\ \text{where } y[x] &= \arg\min_y \int_{\mathcal{S}[x]} \frac{1}{2\tau}|y - x|^2 + \frac{1}{2}|\nabla_{\mathcal{S}[x]} y|^2\,\mathrm{d}a \end{aligned}$$

Two step discretization of Willmore flow (cont.)

$$x^{k+1} = \arg\min_x \int_{\mathcal{S}[x^k]} |x - x^k|^2 \, \mathrm{d}a + \frac{1}{\tau} \int_{\mathcal{S}[x]} |y[x] - x|^2 \, \mathrm{d}a$$

Two step discretization of Willmore flow (cont.)

$$x^{k+1} = \arg\min_x \int_{\mathcal{S}[x^k]} |x - x^k|^2 \, \mathrm{d}a + \frac{1}{\tau} \int_{\mathcal{S}[x]} |y[x] - x|^2 \, \mathrm{d}a$$

finite element space discretization:

X	nodal vector	
$\mathbf{M}[X]$	mass matrix	$\mathbf{M}[X]\Phi \cdot \Psi = \int_{\mathcal{S}[X]} \Phi\Psi \, \mathrm{d}a$
$\mathbf{L}[X]$	stiffness matrix	$\mathbf{L}[X]\Phi \cdot \Psi = \int_{\mathcal{S}[X]} \nabla_{\mathcal{S}[x]}\Phi \nabla_{\mathcal{S}[x]}\Psi \, \mathrm{d}a$

Two step discretization of Willmore flow (cont.)

$$x^{k+1} = \arg\min_x \int_{\mathcal{S}[x^k]} |x - x^k|^2 \, \mathrm{d}a + \frac{1}{\tau} \int_{\mathcal{S}[x]} |y[x] - x|^2 \, \mathrm{d}a$$

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inner problem (time discrete mean curvature)

$Y[X]$ solves $(\mathbf{M}[X] + \tau\mathbf{L}[X])Y = \mathbf{M}[X]X$ (constraint)

Two step discretization of Willmore flow (cont.)

$$x^{k+1} = \arg\min_x \int_{\mathcal{S}[x^k]} |x - x^k|^2 \, \mathrm{d}a + \frac{1}{\tau} \int_{\mathcal{S}[x]} |y[x] - x|^2 \, \mathrm{d}a$$

finite element space discretization:

X	nodal vector	
$\mathbf{M}[X]$	mass matrix	$\mathbf{M}[X]\Phi \cdot \Psi = \int_{\mathcal{S}[X]} \Phi\Psi \, \mathrm{d}a$
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inner problem (time discrete mean curvature)

$Y[X]$ solves $(\mathbf{M}[X] + \tau \mathbf{L}[X])Y = \mathbf{M}[X]X$ (constraint)

outer problem (time discrete Willmore flow)

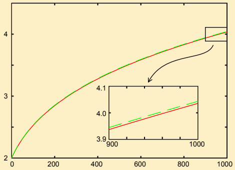
$$X^{k+1} = \arg\min_X \big(\mathbf{M}[X^k](X - X^k)\cdot(X - X^k) + \tau^{-1}\mathbf{M}[X](Y[X] - X)\cdot(Y[X] - X)\big)$$

Comparison to exact solutions

- Circles expand according the ODE

$$\dot{R}(t) = \frac{1}{2} R(t)^{-3}$$

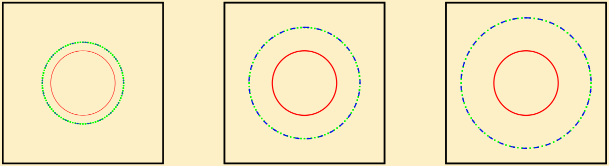
for the radius $R(t)$.



- Discrete two step radii $R^{k+1} \approx R((k+1)\tau)$ are solutions of

$$\frac{R - R_k}{\tau} = \frac{1}{2} \, \frac{R^4 - 3R^2\tau}{(R^2+\tau)^3 \, R_k} \, ,$$

Fully discrete numerical simulation ($\tau = \Delta x$):

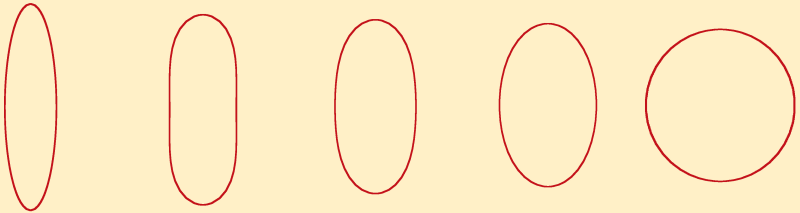


$t = 100\tau$ $\quad t = 500\tau$ $\quad t = 1000\tau$

Evolution of an ellipse under elastic flow

$x_0(s) = (\cos(s), 4\sin(s))$ for $s \in [0, 2\pi]$ as initial parametrization.

modified functional: $w[x] + \lambda a[x]$

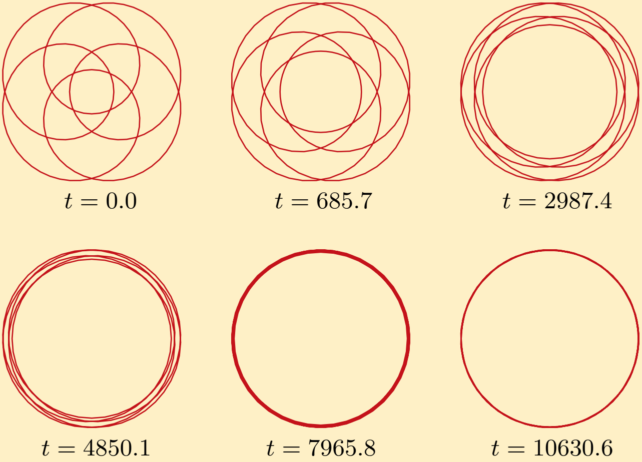


$t = 0.0$ $t = 2.25$ $t = 4.75$ $t = 9.75$ $t = 24.75$

$[n = 2,\ N = 100,\ \tau = \Delta x = 0.0632847,\ \lambda = 0.025.]$

Evolution of a planar hypocycloid

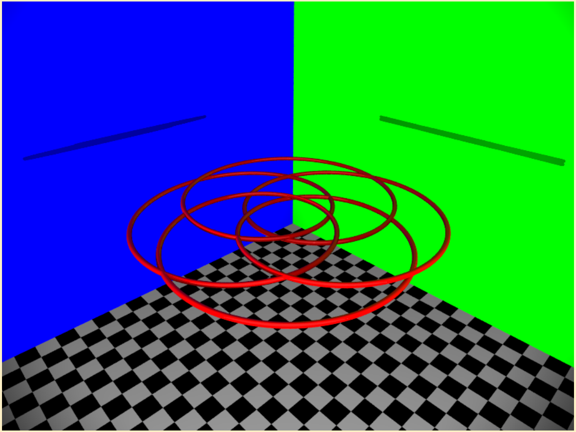
$$x_0(s) = \left(-\tfrac{5}{2}\cos(s) + 4\cos(5s), -\tfrac{5}{2}\sin(s) + 4\sin(5s), \delta\sin(3s)\right),\ \delta = 0.0$$



$[\ n = 3,\ N = 200,\ \tau = \Delta x = 0.5493,\ \lambda = 0.025]$

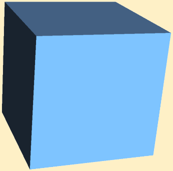
cf. [Dziuk et al. '06]

Evolution of a vertically perturbed hypocycloid



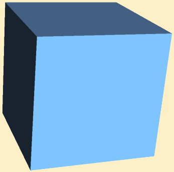
cf. [Dziuk et al. '06]

Willmore flow for surfaces

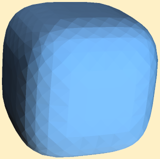


$t = 0$

Willmore flow for surfaces

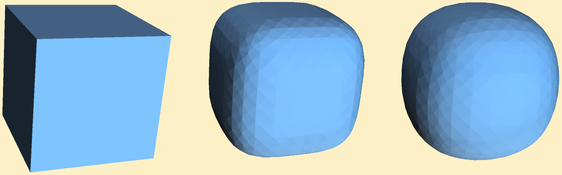


$t = 0$



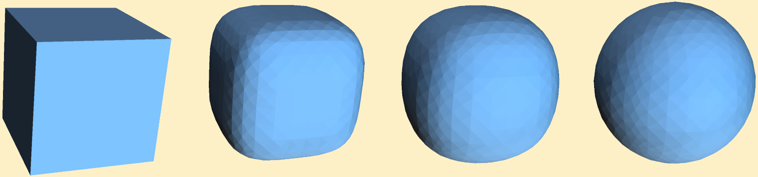
$t = \tau \; (\tau = h)$

Willmore flow for surfaces



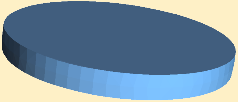
$t = 0$ $\quad$ $t = \tau \ (\tau = h)$ $\quad$ $t = 2\tau$

Willmore flow for surfaces



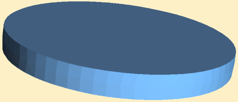
$t = 0$ $t = \tau \ (\tau = h)$ $t = 2\tau$ $t = 8\tau$

Willmore flow of surfaces (cont.)

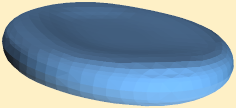


$t = 0$

Willmore flow of surfaces (cont.)

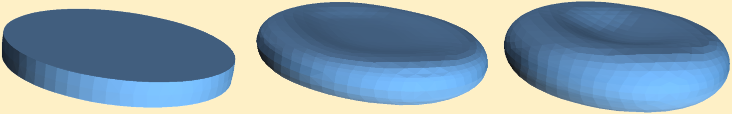


$t = 0$



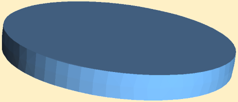
$t = \tau \ (\tau = h)$

Willmore flow of surfaces (cont.)

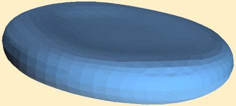


$t = 0$ $\quad$ $t = \tau \ (\tau = h)$ $\quad$ $t = 6\tau$

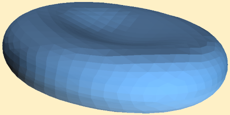
Willmore flow of surfaces (cont.)



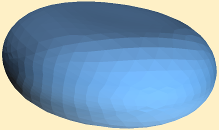
$t = 0$



$t = \tau \ (\tau = h)$

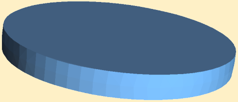


$t = 6\tau$

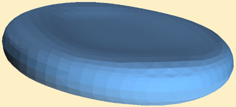


$t = 30\tau$

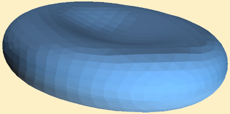
Willmore flow of surfaces (cont.)



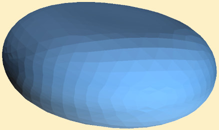
$t = 0$



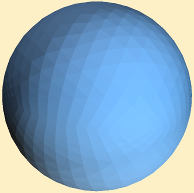
$t = \tau \ (\tau = h)$



$t = 6\tau$

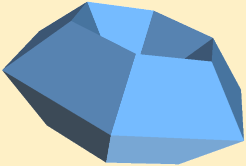


$t = 30\tau$



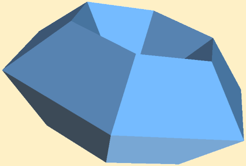
$t = 430\tau$

Willmore flow of surfaces (cont.)

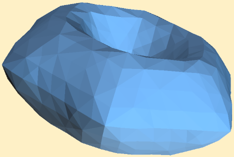


$t = 0$

Willmore flow of surfaces (cont.)

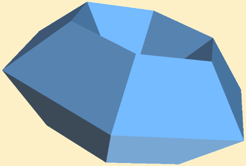


$t = 0$

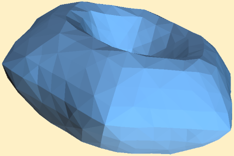


$t = \tau \; (\tau = h^2)$

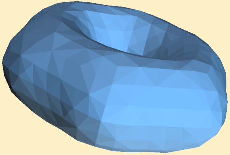
Willmore flow of surfaces (cont.)



$t = 0$

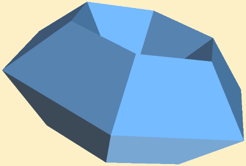


$t = \tau \ (\tau = h^2)$

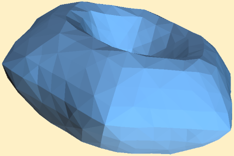


$t = 2\tau$

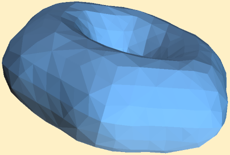
Willmore flow of surfaces (cont.)



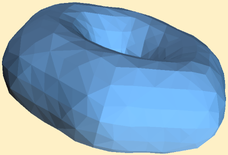
$t = 0$



$t = \tau \ (\tau = h^2)$

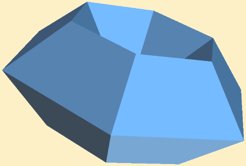


$t = 2\tau$

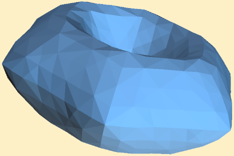


$t = 3\tau$

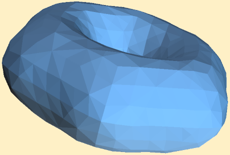
Willmore flow of surfaces (cont.)



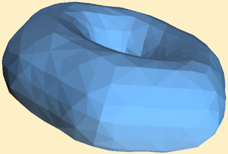
$t = 0$



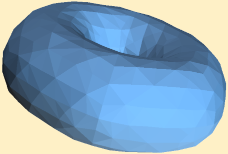
$t = \tau \ (\tau = h^2)$



$t = 2\tau$

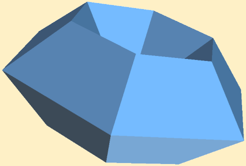


$t = 3\tau$

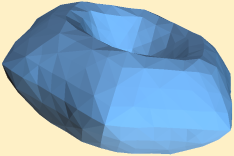


$t = 10\tau$

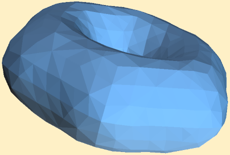
Willmore flow of surfaces (cont.)



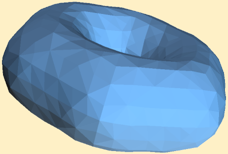
$t = 0$



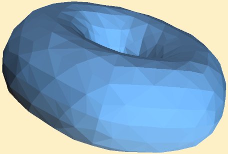
$t = \tau \ (\tau = h^2)$



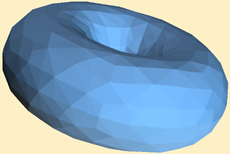
$t = 2\tau$



$t = 3\tau$

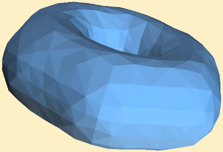


$t = 10\tau$



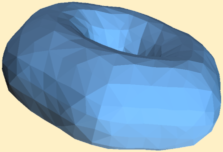
$t = 54\tau$

Willmore flow of surfaces (cont.)

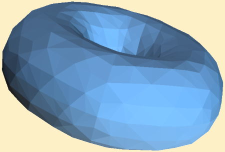


$$t = 2197\,\tau \approx 0.04$$
$$\tau = h^4$$

Willmore flow of surfaces (cont.)

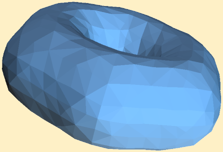


$t = 2197\,\tau \approx 0.04$
$\tau = h^4$

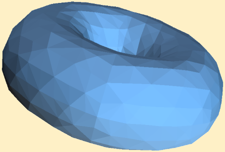


$t = 13\,\tau \approx 0.04$
$\tau = h^2$

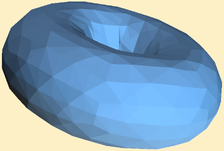
Willmore flow of surfaces (cont.)



$t = 2197\,\tau \approx 0.04$
$\tau = h^4$



$t = 13\,\tau \approx 0.04$
$\tau = h^2$



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Conclusions and Outlook

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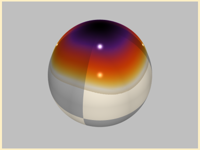
Droplet on a sphere

Four-fold symmetry perturbed droplet sliding down a sphere:



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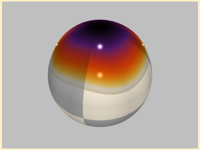
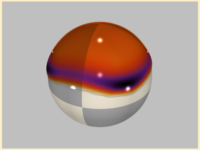

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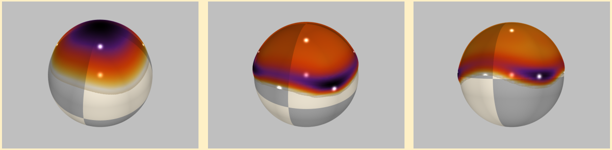

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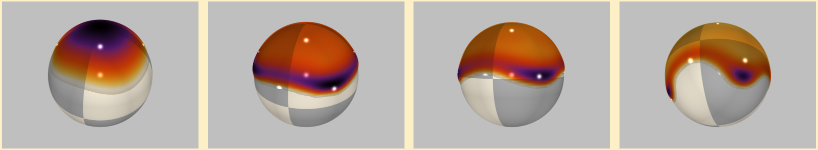

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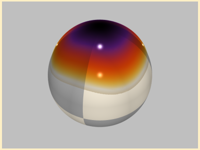
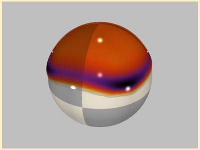
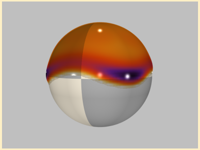
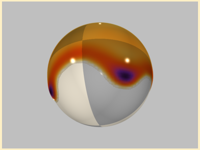
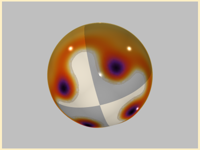

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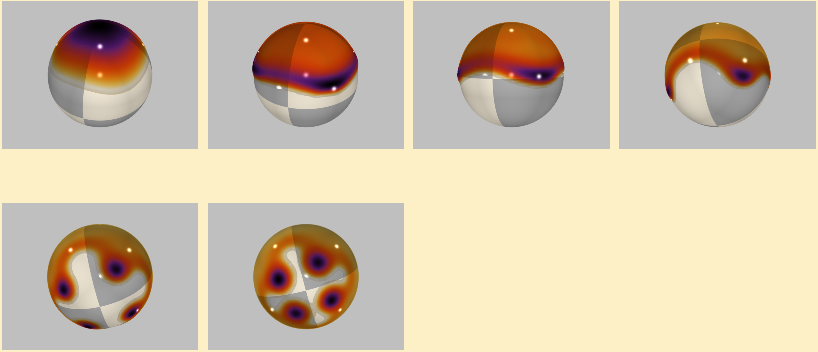

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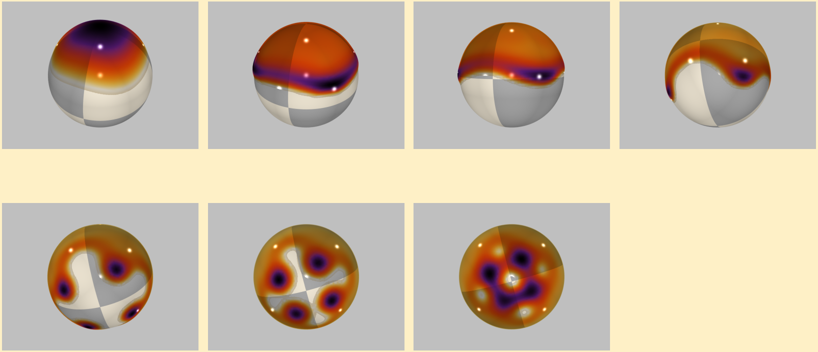

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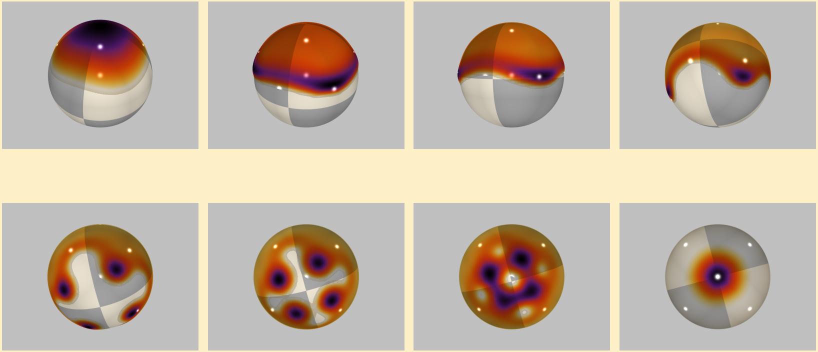

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$$\begin{aligned}\frac{\partial}{\partial X} W(X, Y(X))(\Theta) \quad = \quad & \frac{1}{\tau}\partial_X \mathbf{M}(\Theta)(Y-X)\cdot(Y-X) \\ & + \frac{2}{\tau}\mathbf{M}(X-Y)\cdot\Theta - (\partial_X \mathbf{M}(\Theta))X\cdot P \\ & + ((\partial_X \mathbf{M} + \tau \partial_X \mathbf{L})(\Theta))Y\cdot P\end{aligned}$$

Details: algorithm for Willmore flow (cont.)

$$\begin{aligned}\frac{\partial}{\partial X} W(X, Y(X))(\Theta) &= \frac{1}{\tau}\partial_X \mathbf{M}(\Theta)(Y-X)\cdot(Y-X) + \frac{2}{\tau}\mathbf{M}(X-Y)\cdot\Theta \\ &\quad + ((\partial_X \mathbf{M} + \tau\partial_X \mathbf{L})(\Theta))Y \cdot P \\ (\mathbf{M}[X] + \tau\mathbf{L}[X])P &= -\partial_Y W \quad \text{(dual problem)}\end{aligned}$$

Pf.:

$$(\mathbf{M} + \tau\mathbf{L})Y = \mathbf{M}X$$

Details: algorithm for Willmore flow (cont.)

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(\mathbf{M}[X] + \tau\mathbf{L}[X])P &= -\partial_Y W \quad \text{(dual problem)}
\end{aligned}$$

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$$(\partial_X \mathbf{M}(\Theta))X = ((\partial_X \mathbf{M} + \tau\partial_X \mathbf{L})(\Theta))Y + (\mathbf{M} + \tau\mathbf{L})(\partial_X Y(\Theta)) \Rightarrow$$

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&\quad = \partial_X W(\Theta) - (\mathbf{M}+\tau\mathbf{L})P \cdot \partial_X Y(\Theta)
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&\quad = \frac{1}{\tau}\partial_X \mathbf{M}(\Theta)(Y-X)\cdot(Y-X) + \frac{2}{\tau}\mathbf{M}(X-Y)\cdot\Theta \\
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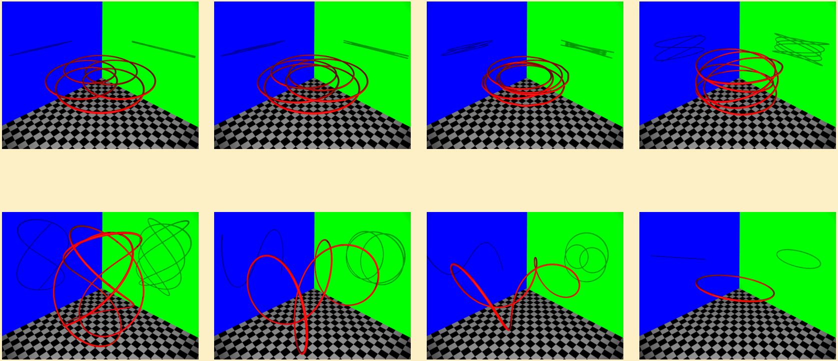
&\quad = \frac{1}{\tau}\partial_X \mathbf{M}(\Theta)(Y-X)\cdot(Y-X) + \frac{2}{\tau}\mathbf{M}(X-Y)\cdot\Theta \\
&\qquad +(((\partial_X \mathbf{M} + \tau\partial_X \mathbf{L})(\Theta))Y - (\partial_X \mathbf{M}(\Theta))X)\cdot P
\end{aligned}$$

Evolution of a vertically perturbed hypocycloid

$$x_0(s) = \left(-\tfrac{5}{2}\cos(s) + 4\cos(5s), -\tfrac{5}{2}\sin(s) + 4\sin(5s), \delta\sin(3s)\right),\ \delta = 0.1$$

$t = 0.0$ $t = 1348.9$ $t = 4264.1$ $t = 4670.2$



$t = 6555.7$ $t = 9108.4.9$ $t = 9297.0$ $t = 9489.1$

cf. [Dziuk et al. '06]