AFEM for Geometric Biomembranes and Fluid-Membrane Interaction

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University of Maryland
Department of Mathematics, Texas A&M (3)

New Directions in Computational PDEs

Outline

Basic Models

Refs: Helfrich (73), Jenkins (77), Seifert (97)

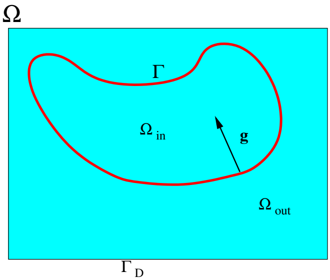
Assumptions

Membrane:

- Layer of Incompressible Fluid
- Bending Rigidity
- Non Permeable

Surrounding Fluid:

- Newtonian, Incompressible.



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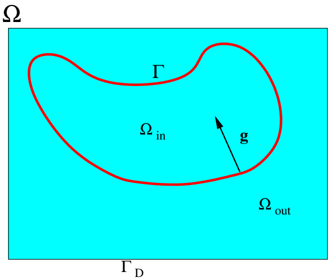

Gradient Flow

- Decreasing Energy
- Area and Volume Constraint
- Non Physical Dynamics

Fluid-Membrane Interaction

- Fluid Equations of Motion
- Immerse and Exerts Forces
- Membrane moves with Fluid

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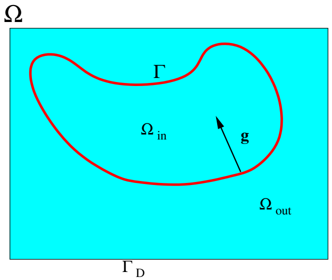

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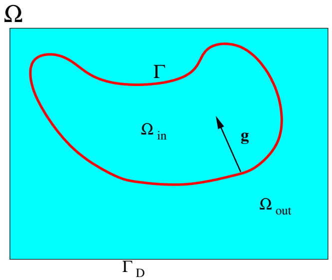

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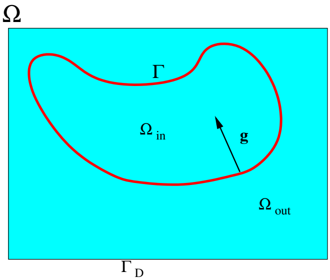

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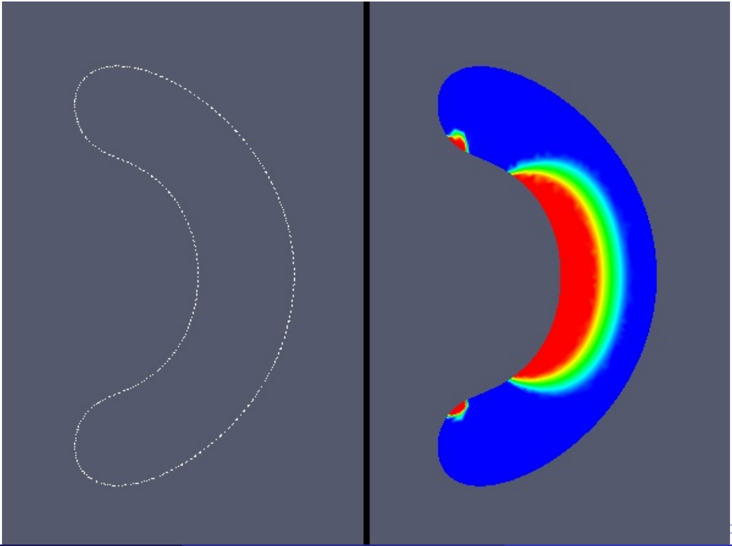
Geometric Model vs. Fluid-Membrane Model

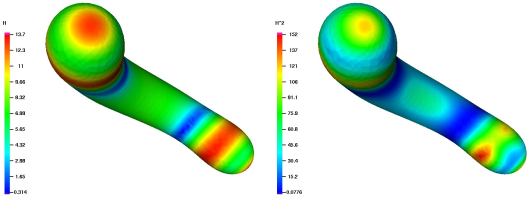
play



Bending energy (Refs: Kuwert, Schätzle, Simonett, Willmore)

$$W(\Gamma) = \int_\Gamma h^2$$

$$\delta W = \left(\Delta_\Gamma h + \frac{1}{2} h^3 - 2kh \right) \nu$$



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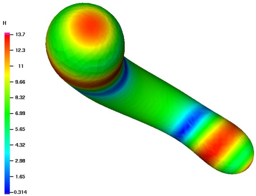

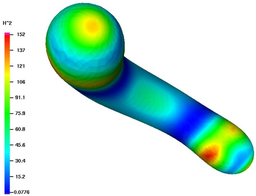

Constraints

Augmented Energy J, Lagrange Multipliers λ (area) and p (volume)

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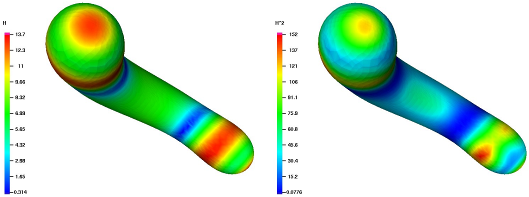

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Gradient Flow for Biomembrane Modeling

Trajectory

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Weak Helfrich flow

Given Γ^0 and $T > 0$, find $\mathrm{rx} : G_T \to \mathbb{R}^{d+1}$, $\lambda : [0, T] \to \mathbb{R}$ and $p : [0, T] \to \mathbb{R}$ such that $\Gamma(0) = \Gamma^0$ and for all $t \in (0, T]$

$$\int_{\Gamma(t)} \dot{\mathrm{x}} \cdot \phi = \; - \delta J(\Gamma(t); \phi)$$

for all smooth $\phi : \Gamma(t) \to \mathbb{R}^{d+1}$ and

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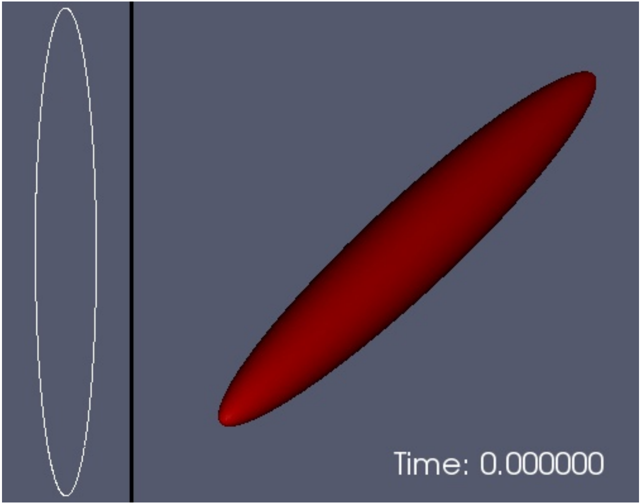
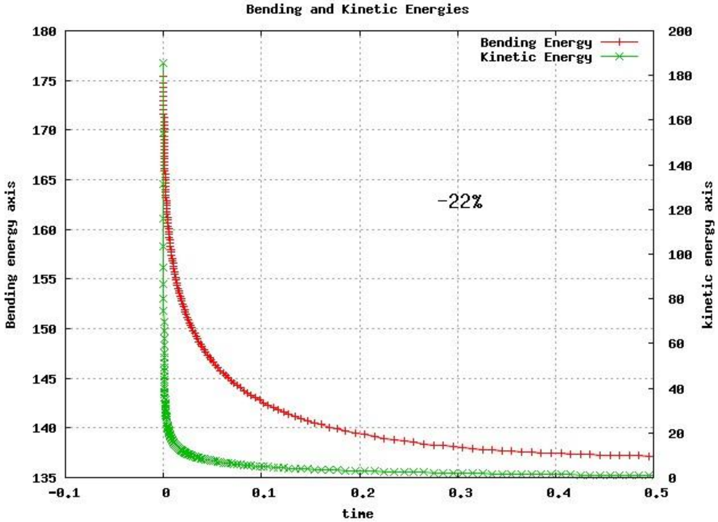
Dumbbell Bar Shaped Family

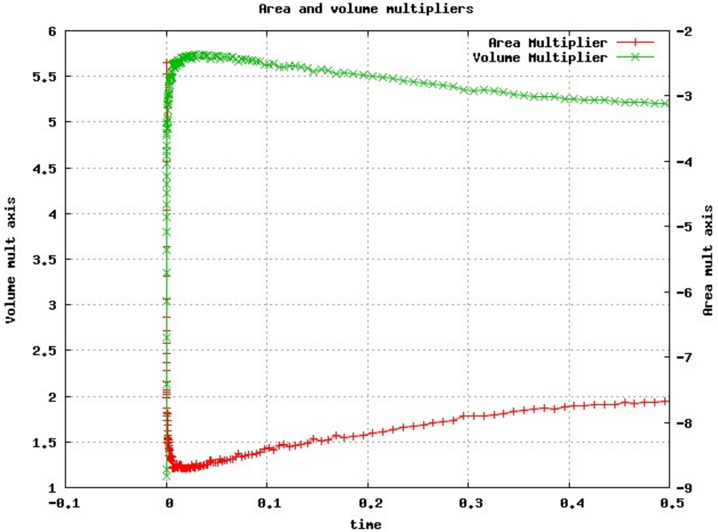
Ellipsoid 8x1x1



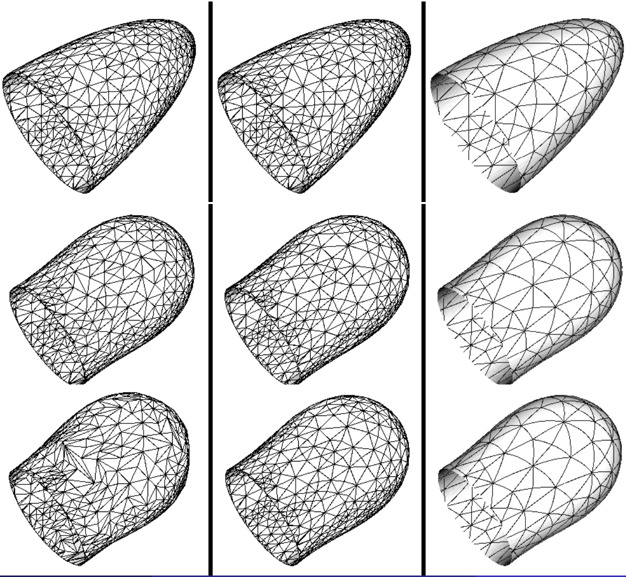
Dumbbell Bar Shaped Family - Ellipsoid 8x1x1: Energies



Dumbbell Bar Shaped Family - Ellipsoid 8x1x1: Multipliers

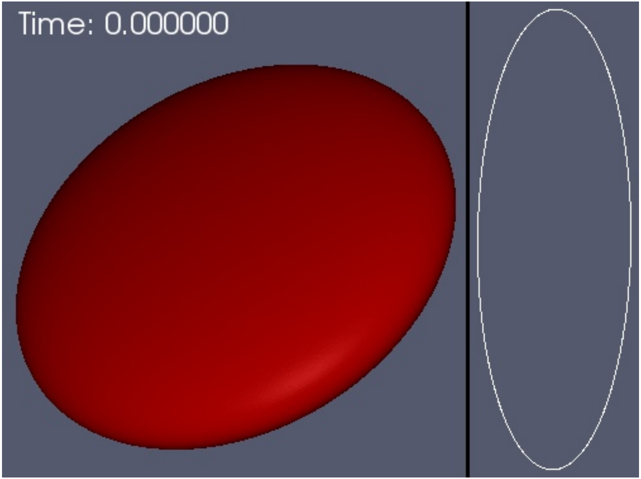


Mesh Smoothing: Comparison between P^1 and P^2



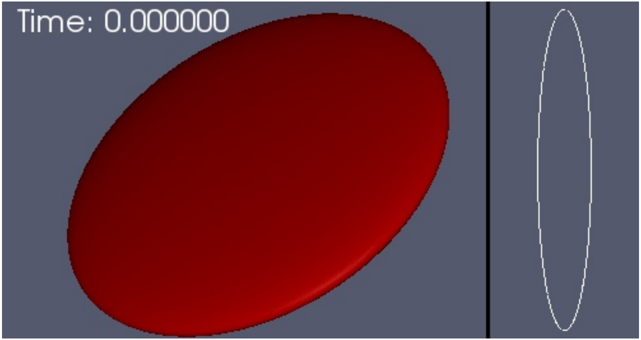
Red Bood Cell Family

Ellipsoid 3x3x1



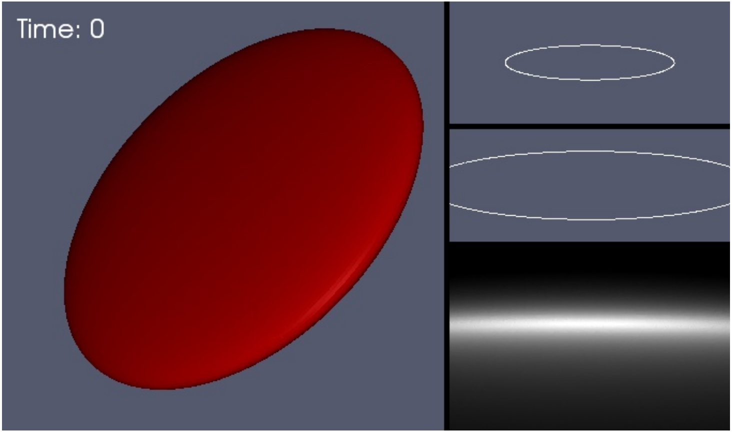
Red Bood Cell Family (Continued)

Ellipsoid 6x6x1



Red Bood Cell Family (Continued)

Ellipsoid 5x5x1



Shape Derivative of Willmore Energy δW: Vector Form

Refs: Rusu (2005), Dziuk (2008), Barrett-Garcke-Nürnberg (2008)

Shape Calculus: $\boldsymbol{\nu}'(\Gamma, \boldsymbol{\phi}) = -\nabla_\Gamma \phi, \quad h'(\Gamma, \boldsymbol{\phi}) = -\Delta_\Gamma \phi, \quad \partial_\nu h = -|\nabla_\Gamma \boldsymbol{\nu}|^2$

$$\delta W(\Gamma, \phi) = \int_\Gamma \nabla_\Gamma \phi \cdot \nabla_\Gamma h - \int_\Gamma h |\nabla_\Gamma \boldsymbol{\nu}|^2 \phi + \frac{1}{2} \int_\Gamma h^3 \phi; \qquad \phi = \boldsymbol{\phi} \cdot \boldsymbol{\nu}$$

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$$\int_\Gamma \nabla_\Gamma \phi \cdot \nabla_\Gamma h = \int_\Gamma \nabla_\Gamma \boldsymbol{\phi} : \nabla_\Gamma \mathbf{h} - \int_\Gamma (\nabla_\Gamma \mathbf{x} + \nabla_\Gamma \mathbf{x}^T) \nabla_\Gamma \boldsymbol{\phi} : \nabla_\Gamma \mathbf{h} - \int_\Gamma h \Delta_\Gamma \boldsymbol{\nu} \cdot \boldsymbol{\phi}$$

$$-\int_\Gamma h \Delta_\Gamma \boldsymbol{\nu} \cdot \boldsymbol{\phi} = \int_\Gamma h |\nabla_\Gamma \boldsymbol{\nu}|^2 - \frac{1}{2} \int_\Gamma \nabla_\Gamma h^2 \cdot \boldsymbol{\phi}$$

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$$dW(\Gamma;\phi) = \int_\Gamma \nabla_\Gamma \boldsymbol{\phi} : \nabla_\Gamma \mathbf{h} - \int_\Gamma (\nabla_\Gamma \mathbf{x} + \nabla_\Gamma \mathbf{x}^T)\nabla_\Gamma \boldsymbol{\phi} : \nabla_\Gamma \mathbf{h} + \frac{1}{2}\int_\Gamma \nabla_\Gamma \cdot \mathbf{h} \nabla_\Gamma \cdot \boldsymbol{\phi}$$

Discrete Geometric Scheme: Ingredients

- Curvature: $\mathbf{h} = -\Delta_\Gamma \mathbf{x}, \quad \mathbf{x} = \text{identity on } \Gamma$ (Dziuk' 91)
- Semi-implicit Time Discretization $(t_n \to t_{n+1})$: explicit geometry $(\Gamma = \Gamma_n, \quad \nabla_\Gamma = \nabla_{\Gamma^n}, \quad \boldsymbol{\nu} = \boldsymbol{\nu}^n)$ (Dziuk' 91)

$$\int_{\Gamma^n} \mathbf{h}^{n+1} \cdot \boldsymbol{\psi} = \int_{\Gamma^n} \nabla_{\Gamma^n} \mathbf{x}^{n+1} : \nabla_{\Gamma^n} \boldsymbol{\psi}, \qquad \mathbf{x}^{n+1} = \mathbf{x}^n + \tau^n \mathbf{v}^{n+1}$$

$$\Rightarrow \quad \int_{\Gamma^n} \mathbf{h}^{n+1} \cdot \boldsymbol{\psi} - \tau^n \int_{\Gamma^n} \nabla_{\Gamma^n} \mathbf{v}^{n+1} : \nabla_{\Gamma^n} \boldsymbol{\psi} = \int_{\Gamma^n} \nabla_{\Gamma^n} \mathbf{x}^n : \nabla_{\Gamma^n} \boldsymbol{\psi}$$

- Mixed Method: operator splitting
  1. Velocity: $\int_{\Gamma^n} \mathbf{v}^{n+1} \cdot \boldsymbol{\phi} = -\delta J^{n+1}(\Gamma^n; \boldsymbol{\phi})$
  2. Curvature: $\int_{\Gamma^n} \mathbf{h}^{n+1} \cdot \boldsymbol{\psi} - \tau^n \int_{\Gamma^n} \nabla_{\Gamma^n} \mathbf{v}^{n+1} : \nabla_{\Gamma^n} \boldsymbol{\psi} = \int_{\Gamma^n} \nabla_{\Gamma^n} \mathbf{x}^n : \nabla_{\Gamma^n} \boldsymbol{\psi}$
- Space discretization: linears or quadratics

Fully Discrete Geometric Scheme

$$\int_{\Gamma_h^n} \mathbf{V}^{n+1} \cdot \mathbf{\Phi} = -dW_h^{n+1}(\Gamma_h^n; \mathbf{\Phi}) - \lambda^{n+1} dA_h^n(\Gamma_h^n; \mathbf{\Phi}) - p^{n+1} dV_h^n(\Gamma_h^n; \mathbf{\Phi})$$

$$\int_{\Gamma_h^n} \mathbf{H}^{n+1} \cdot \mathbf{\Psi} - \tau_n \int_{\Gamma_h^n} \nabla_{\Gamma_h^n} \mathbf{V}^{n+1} : \nabla_{\Gamma_h^n} \mathbf{\Psi} = \int_{\Gamma_h^n} \nabla_{\Gamma_h^n} \mathbf{x}^n : \nabla_{\Gamma_h^n} \mathbf{\Psi},$$

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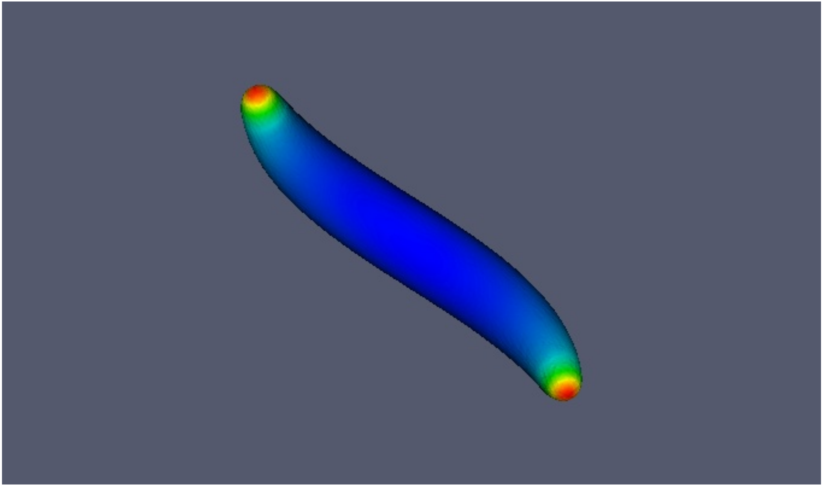
for all $\mathbf{\Phi}, \mathbf{\Psi} \in \mathbb{S}_h^{n+1}$, where

$$dW_h^{n+1}(\Gamma_h^n; \mathbf{\Phi}) = \int_{\Gamma_h^n} \nabla_{\Gamma_h^n} \mathbf{H}^{n+1} : \nabla_{\Gamma_h^n} \mathbf{\Phi} + \frac{1}{2} \int_{\Gamma_h^n} \nabla_{\Gamma_h^n} \cdot \mathbf{H}^{n+1} \nabla_{\Gamma_h^n} \cdot \mathbf{\Phi}$$
$$- \int_{\Gamma_h^n} (\nabla_{\Gamma_h^n} \mathbf{x}^n + \nabla_{\Gamma_h^n} \mathbf{x}^{n\mathsf{T}}) \nabla_{\Gamma_h^n} \mathbf{\Phi} : \nabla_{\Gamma_h^n} \mathbf{H}^{n+1},$$

$$dA_h^n(\Gamma_h^n; \mathbf{\Phi}) = \int_{\Gamma_h^n} \mathbf{H}^n \cdot \mathbf{\Phi}, \qquad dV_h^n(\Gamma_h^n; \mathbf{\Phi}) = \int_{\Gamma_h^n} \mathbf{\Phi} \cdot \nu.$$

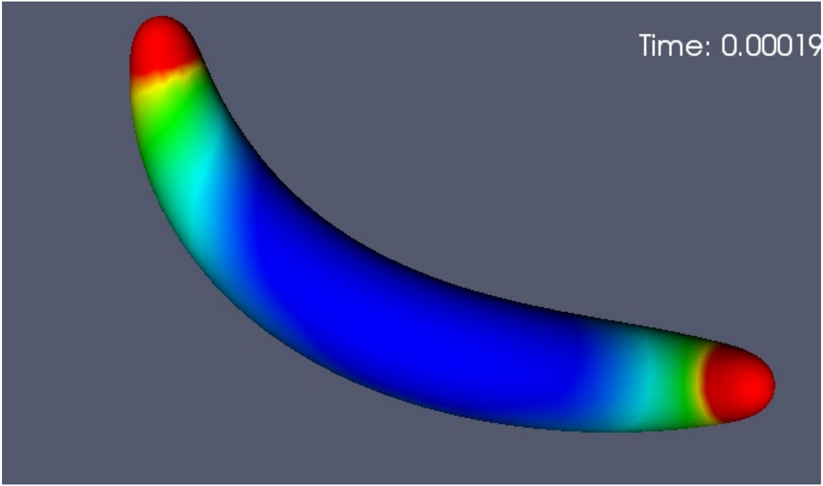
Boomerang Shape

Twisted Banana



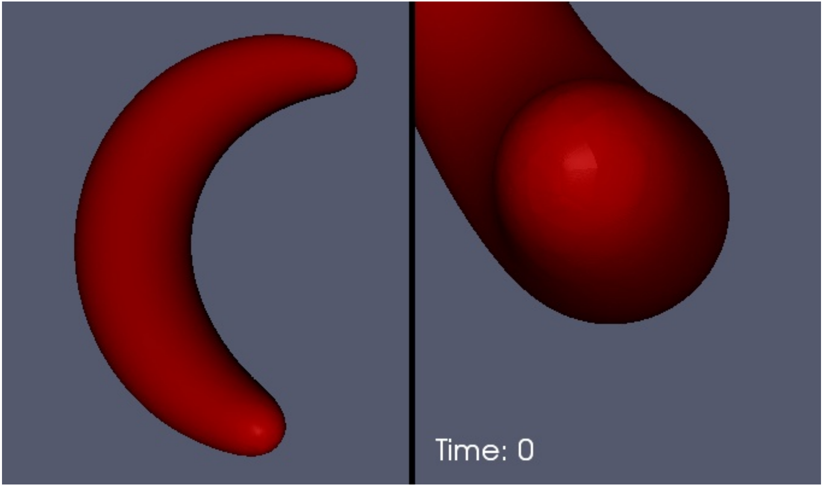
Boomerang Shape: Full Simulation

Full Simulation



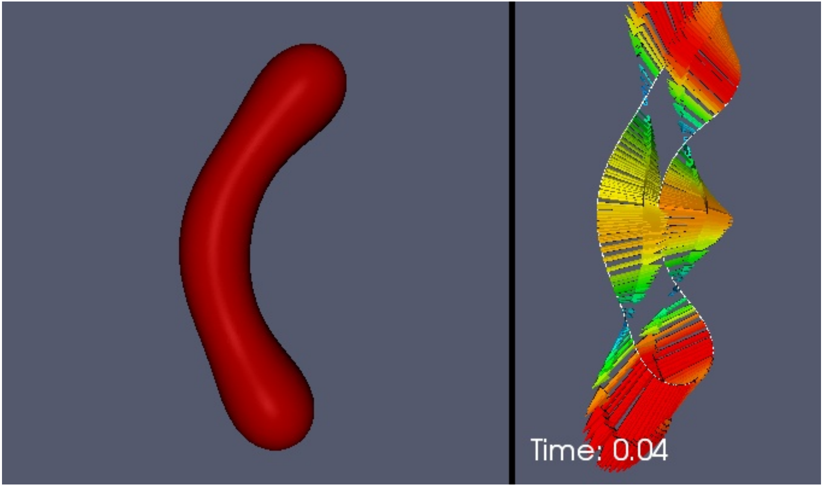
Boomerang Shape: Fast Time Scale

Fast time scale

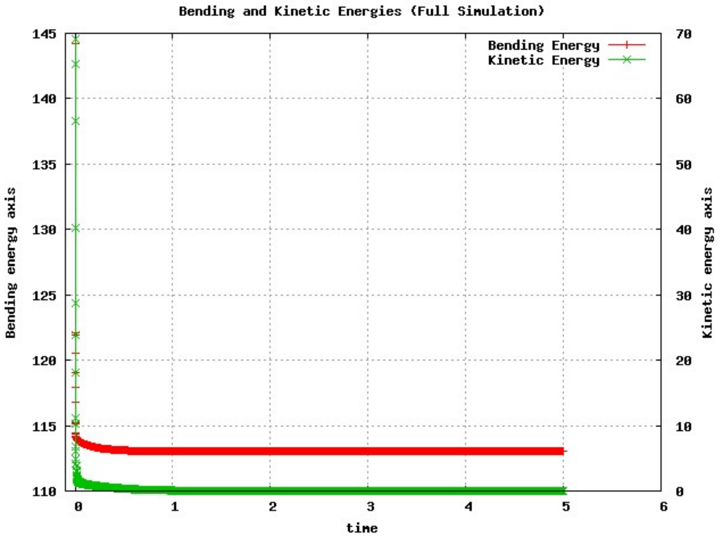


Boomerang Shape: Slow Time Scale

Slow time scale



Boomerang Shape - Energy Graphs: Full



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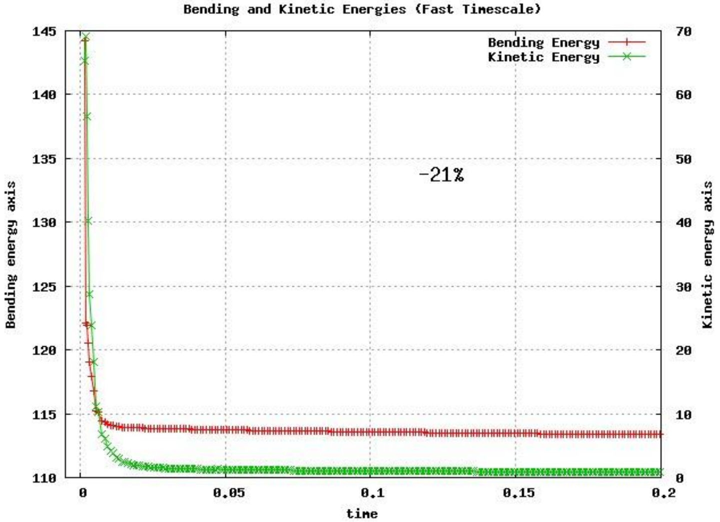
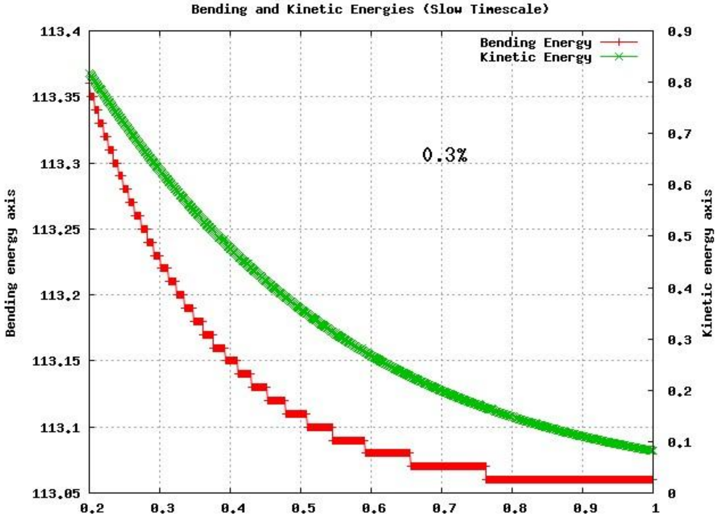
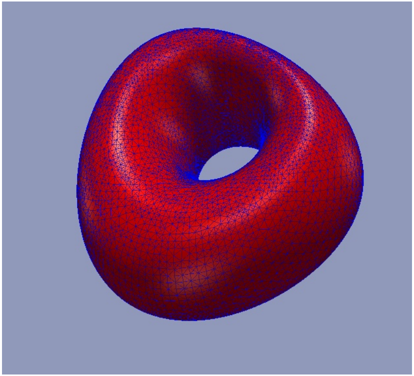
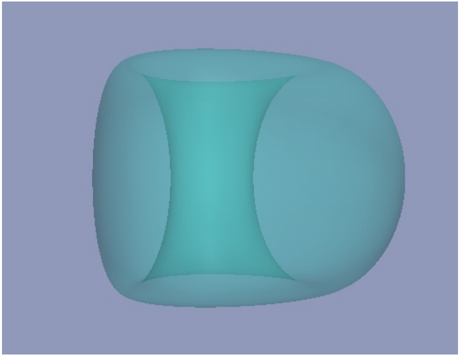


Boomerang Shape - Energy Graphs: Slow Time



Non-axisymmetric Torus





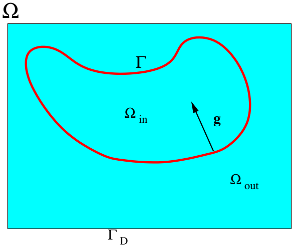
Coupled Fluid-Membrane Model

Refs: Coutand-Shkoller

(Incompressible) Navier-Stokes Equations

$$\rho\dot{\mathbf{v}} - \nabla\cdot\underbrace{(-p\mathbf{I} + \mu D(\mathbf{v}))}_{\Sigma} = \mathbf{b} \qquad \text{in } \Omega_t,$$

$$\nabla\cdot\mathbf{v} = 0 \qquad \text{in } \Omega_t,$$



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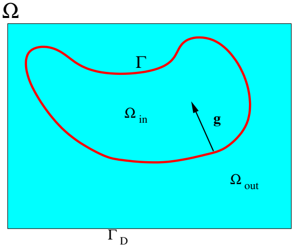

Membrane Force: Bending

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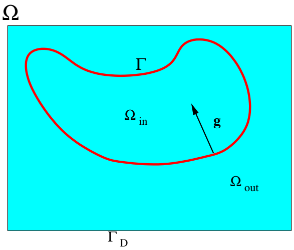
$$\mathbf{v}(\cdot,0) = \mathbf{v}_0 \qquad \text{in } \Omega_0.$$



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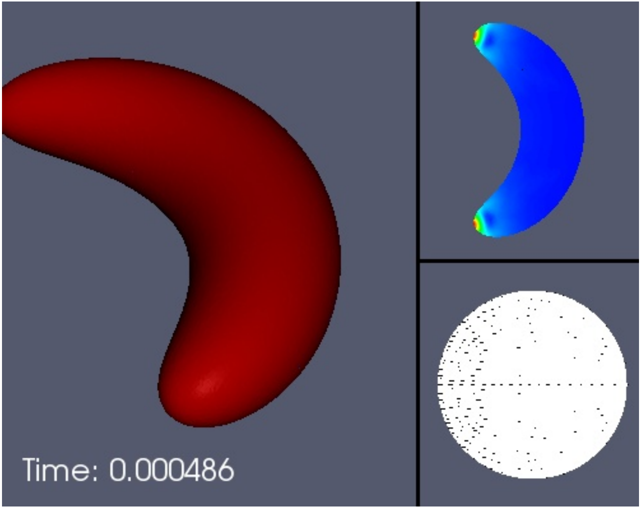
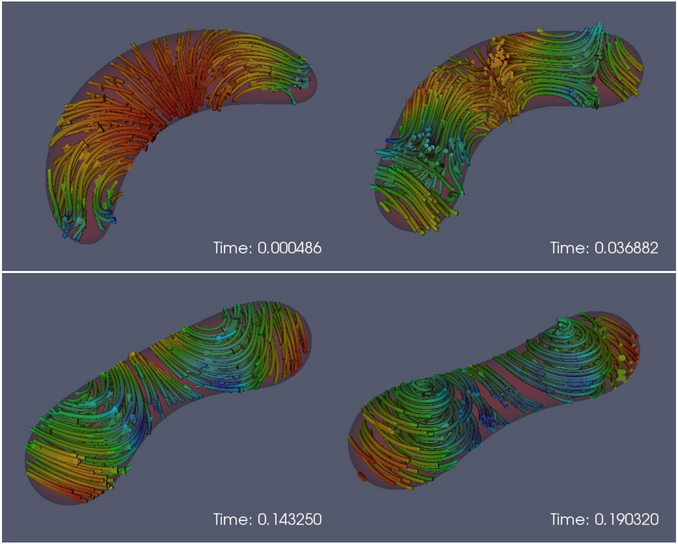
Fluid Biomembrane: 3D Boomerang

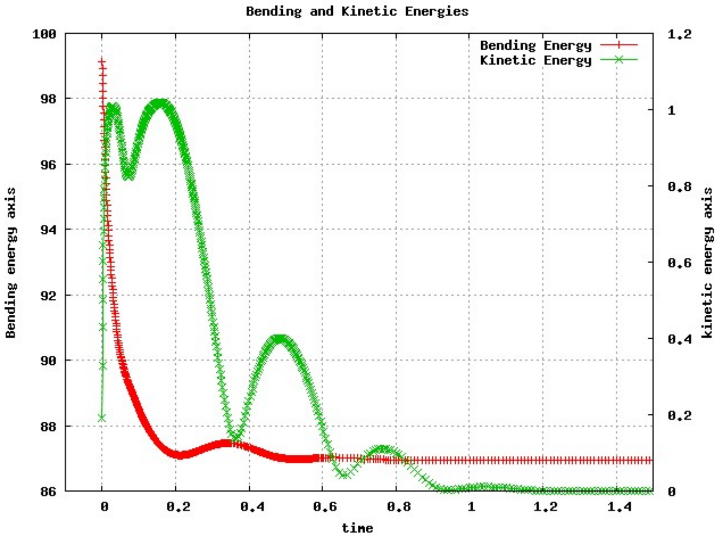
3D Banana



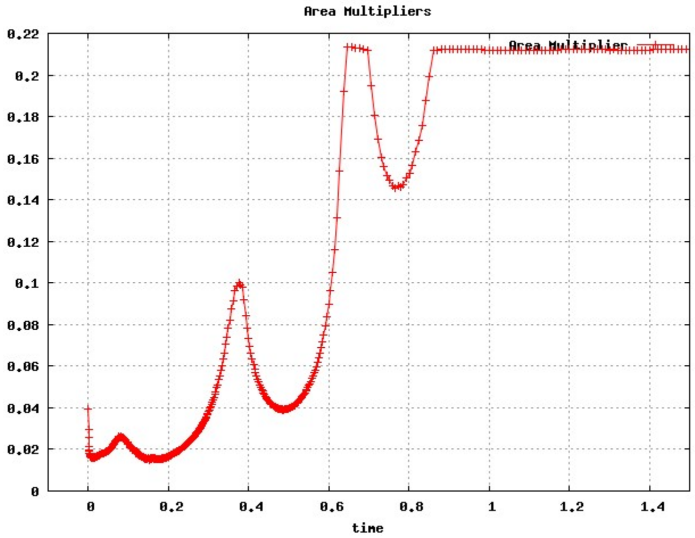
Fluid Biomembrane: 3D Boomerang Streamlines



Fluid Biomembrane: 3D Boomerang Energies

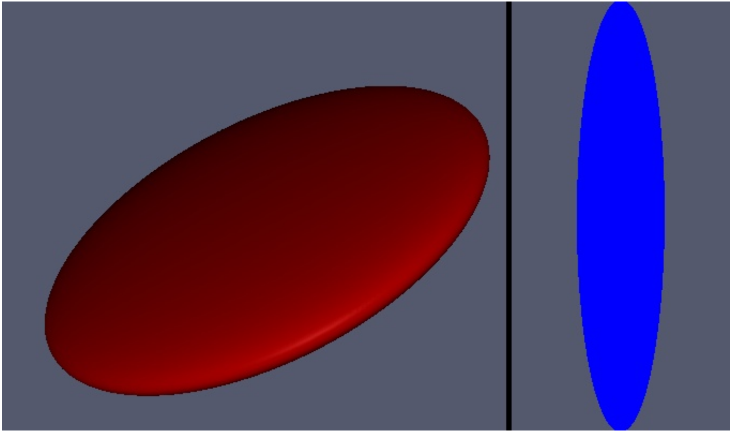


Fluid Biomembrane: 3D Boomerang Multiplier

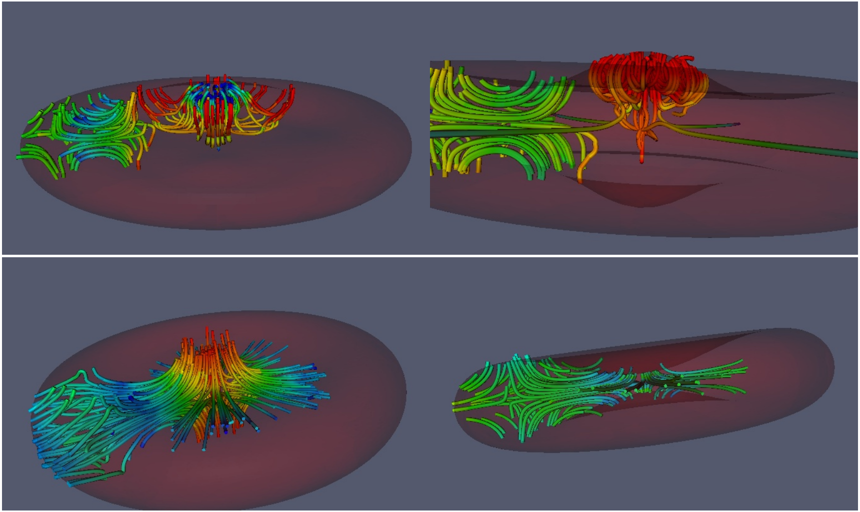


Fluid Red Blood Cell: Ellipsoid 5x5x1

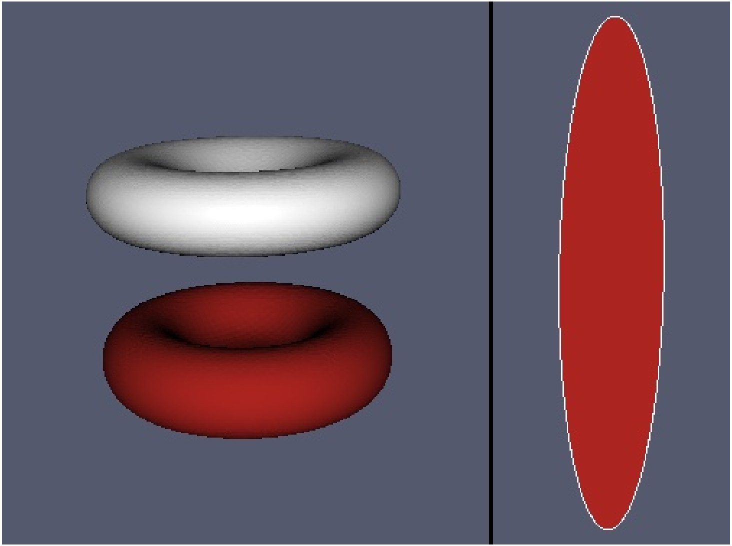
Ellipsoid 5x5x1



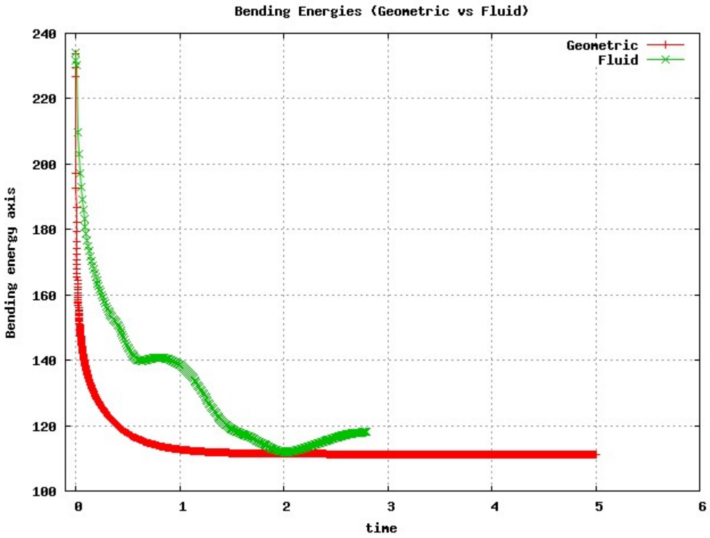
Fluid Red Blood Cell: Ellipsoid 5x5x1 Streamlines



Geometric vs Fluid Red Cell: 5x5x1 Ellipsoid

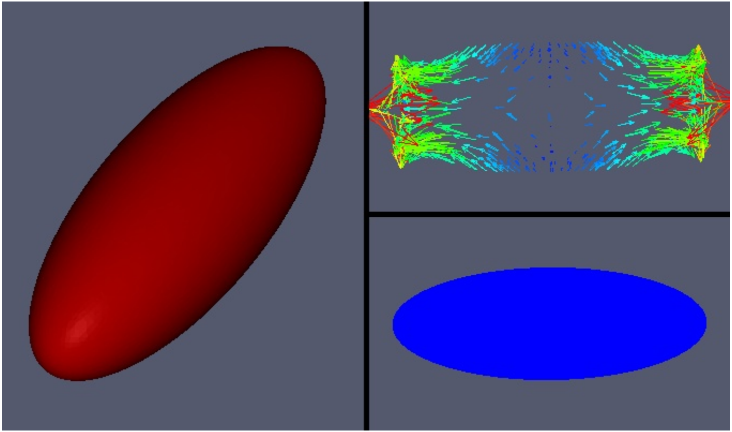


Geometric vs Fluid Red Cell - 5x5x1 Ellipsoid: Energies

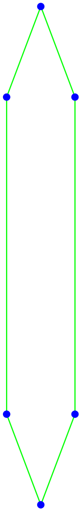


Fluid Biomembrane: Ellipsoid 4x1x1

Ellipsoid 4x1x1



Refinement Consistent Refinement



Problem

- Free boundary problem
- Γ is major unknown
- Increase local resolution

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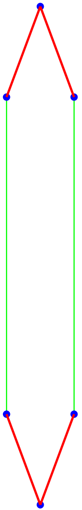

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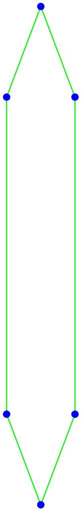

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How to add local resolution with incomplete geometric information of Γ?

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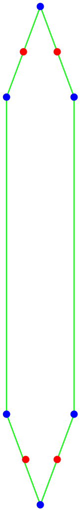

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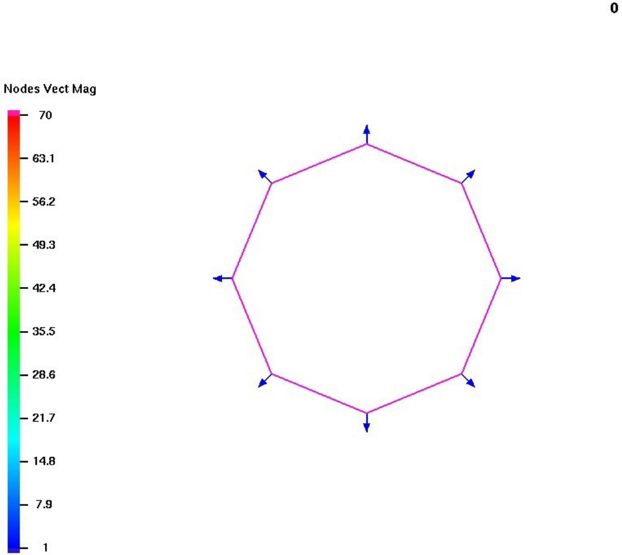
Answer 1

Linear interpolation

Counterxample to Answer 1



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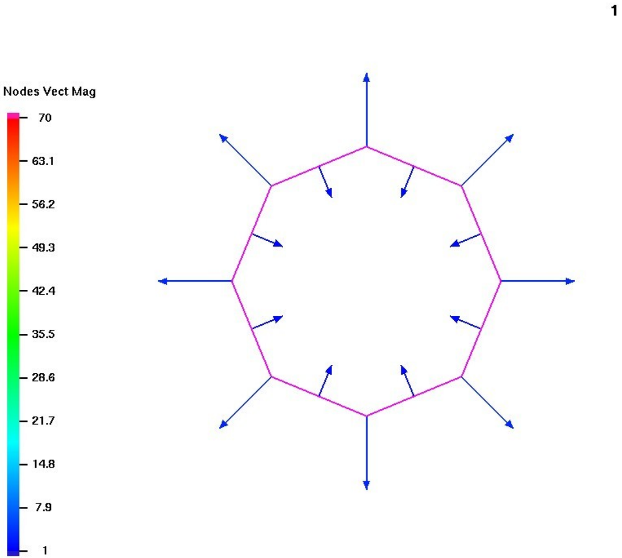

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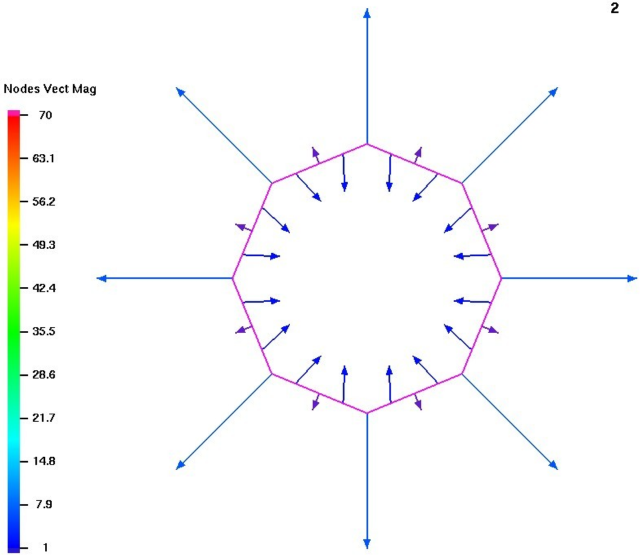
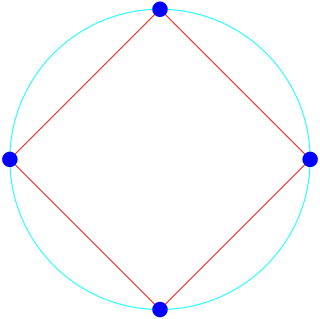


Understanding the Counterexample



Perform linear interpolation:

- Smooth curve γ and polygonal approximation Γ
- Refine by linear interpolation
- Pass a smooth curve $\tilde{\gamma}$ through all interpolation points

For 1D curves the FEM theory in flat domain extends:

$$\int_\Gamma \mathbf{H}\cdot\phi = \int_\Gamma \partial_s \mathbf{X}\cdot\partial_s\phi = -\int_\Gamma \partial_s^2\tilde{\mathbf{x}}\cdot\phi \quad \forall\phi\in\mathbb{S}_h \quad \Rightarrow \quad \mathbf{H} = P_h(\partial_s^2\tilde{\mathbf{x}})$$

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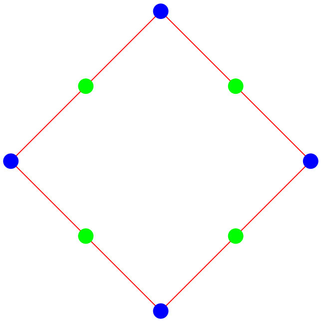

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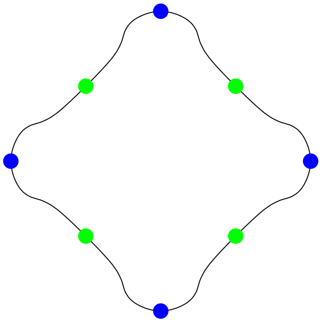

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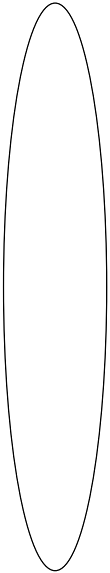
Exact Interpolation in 2D



Assume we know γ and interpolate it exactly

- γ smooth curve (surface)
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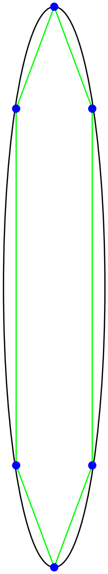

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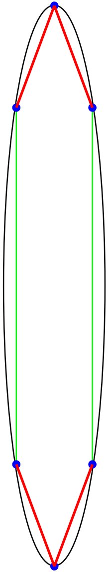

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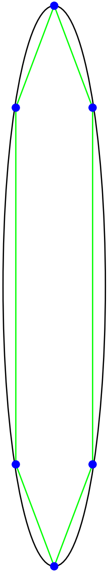

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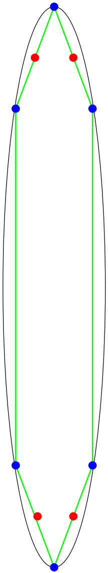

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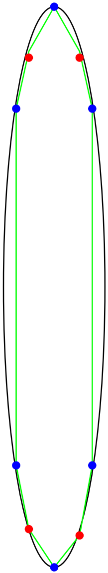

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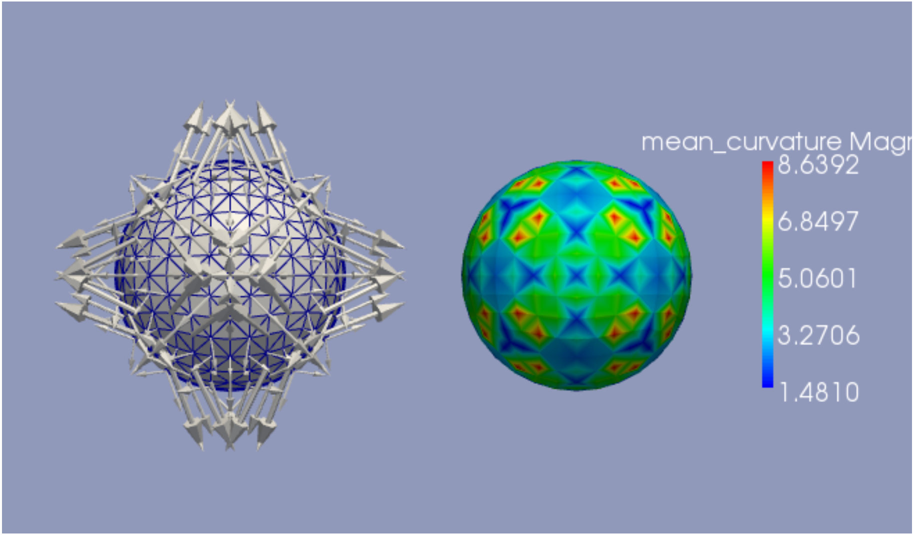
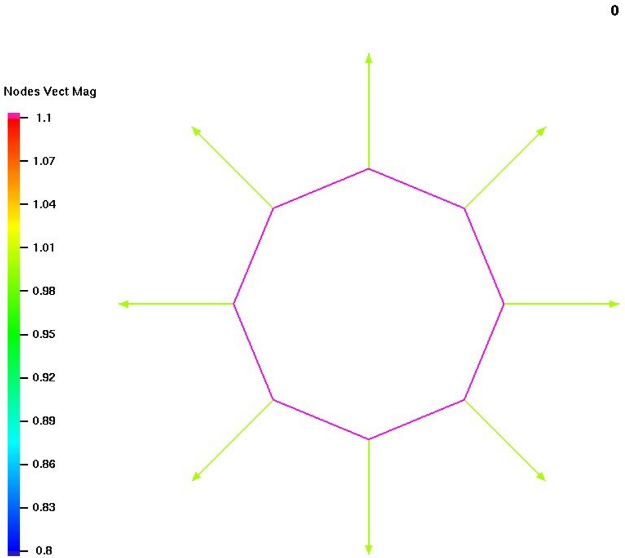
Exact Interpolation in 3D



Geometrically Consistent Algorithm



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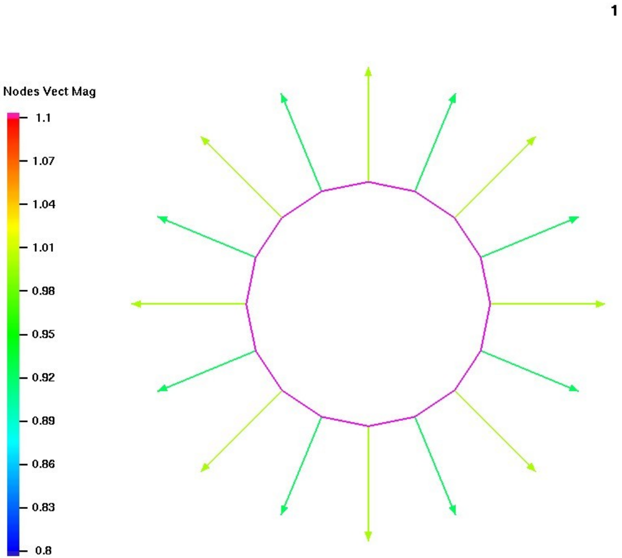

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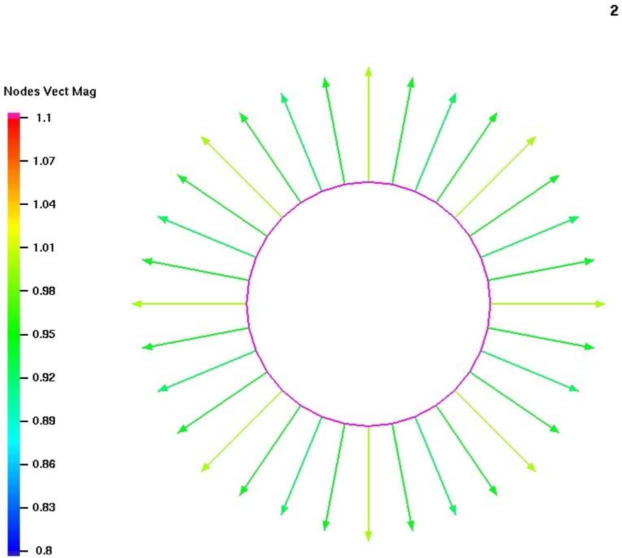

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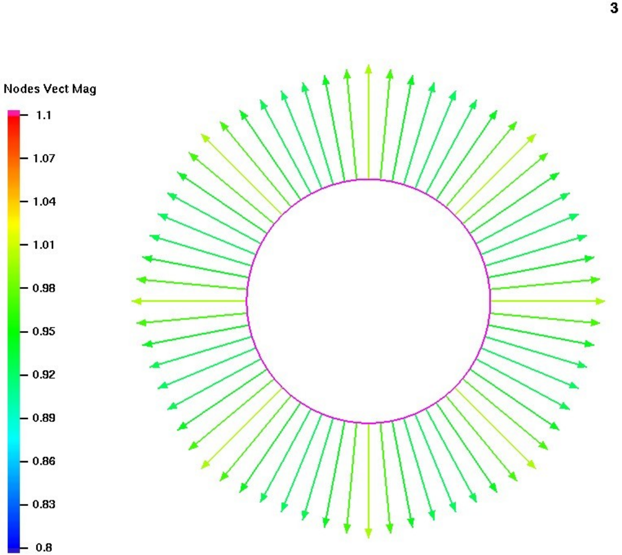

Geometric Consistency

- Geometric identity $\mathbf{h} = -\Delta_\gamma \mathbf{x}$
- Discrete geometric identity $\mathbf{H} = -\Delta_\Gamma \mathbf{X}$
- Assume $\Gamma, \mathbf{X}, \mathbf{H}$ approximate $\gamma, \mathbf{x}, \mathbf{h}$
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Geometric Consistency

A finite element triple $(\Gamma, \mathbf{X}, \mathbf{H})$ is *GC* if

$$\mathbf{X}, \mathbf{H} \in \mathbb{V} : \qquad \int_\Gamma \mathbf{H} \cdot \Phi = \int_\Gamma \nabla_\Gamma \mathbf{X} : \nabla_\Gamma \Phi, \qquad \forall \Phi \in \mathbb{V},$$

and it is an approximation of the exact triplet $(\gamma, \mathbf{x}, \mathbf{h})$

Geometrically Consistency Refinement

Refinement Algorithm

$(\Gamma^*, \mathbf{X}^*, \mathbf{H}^*) = \text{Surf Ref}(\Gamma, \mathbf{H}, \mathbf{X}, \mathcal{M})$

1. $\Gamma^* = \text{Isoparametric Refinement}(\Gamma)$
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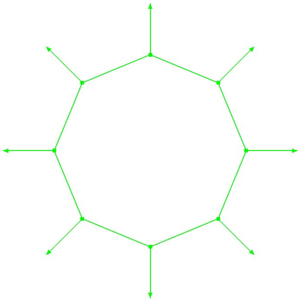

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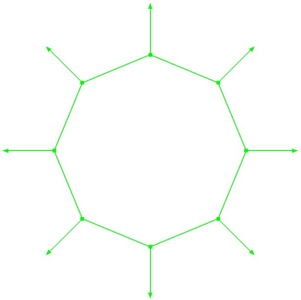

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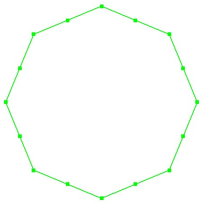

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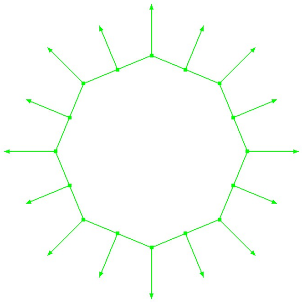

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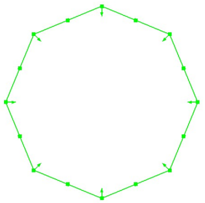

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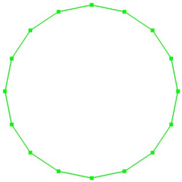

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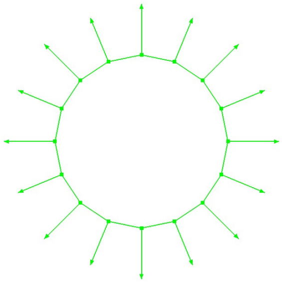

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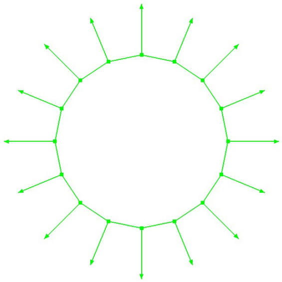

Remarks

- Procedure independent of polynomial degree and dimension
- Refinement can be replaced by coarsening and mesh smoothing

Mathematical Statement

In heuristic terms

1. This refinement guarantees that the errors for position and mean curvature are of the same order as they were before.
2. Unstable numerical differentiation is replaced by stable interpolation plus inversion of $-\Delta_\Gamma$.

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Theorem (Geometrically Consistent Refinement)

If the triple $(\Gamma, \mathbf{X}, \mathbf{H})$ *is GC and* $\mathcal{E}$ *is a Strang-type upper bound for the error* $|\mathbf{x} - \mathbf{X}|_{H^1(\Gamma)}$, *then the following statements are valid*

1. $\|\mathbf{h} - \mathbf{H}^*\|_{L^2(\Gamma)} = \|\mathbf{h} - \mathbf{H}\|_{L^2(\Gamma)}$;
2. $|\mathbf{x} - \mathbf{X}^*|_{H^1(\Gamma)} \leq \mathcal{E}$;
3. *the triple* $(\Gamma^*, \mathbf{X}^*, \mathbf{H}^*)$ *is GC.*

Conclusions

- Spherical caps: for shapes with distinctive ends, spherical caps seem to be most effective to reduce the bending energy
- Red cells: for disk-like shapes, there is a thickening of the outer edge and depression in the center. The fluid membrane dynamics is quite different from the gradient flow.
- Kinetic energy: is decays exponentially for gradient flows (with a nonobvious dependence of the equilibrium shape), but it oscillates for fluid membranes due to inertia.
- Geometric consistency: this is important for refinement, coarsening and mesh smoothing to avoid numerical artifacts.
- Mesh smoothing: control of mesh distortion due large domain deformations in a Lagrangian approach.
- Time-step control: this accounts for geometry and highly varying time scales.

Large Deformation: Willmore Flow of Helix

Large Simulation