Numerical approximation and optimization of the Canham-Helfrich elastic bending energy

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AC2T research GmbH

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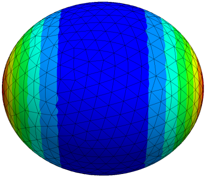
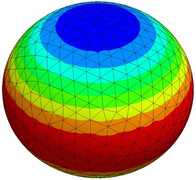
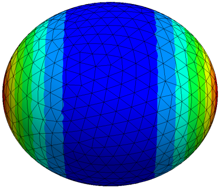
Motivation (cell membranes)







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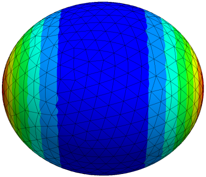

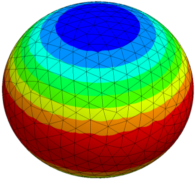

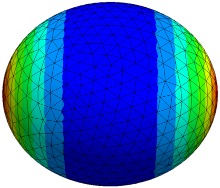

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κ_b bending elastic constant

Problem statement

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Constraints:

$$|\Omega| = V_0, \quad |\mathcal{S}| = A_0, \qquad V_0 \leq \frac{A_0^{\frac{3}{2}}}{6\sqrt{\pi}}$$

$$\mathcal{J}(\mathcal{S}) = \mathcal{W}(\mathcal{S}) + c_A(|\mathcal{S}| - A_0)^2 + c_V(|\Omega| - V_0)^2$$

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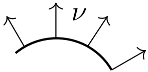
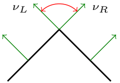
Curvature:

$$H = -\frac{1}{2}\mathrm{tr}(\partial^S \boldsymbol{\nu})$$



Curvature

Shape operator $-\partial^S \boldsymbol{\nu}$ is a distribution



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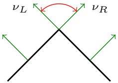
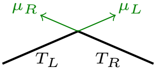
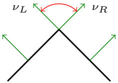


- Duality pairing with $\boldsymbol{\Psi}: \mathcal{S} \to \mathbb{R}^{2\times 2}_{\mathrm{sym}}$,
  $\boldsymbol{\mu}_L^\top \boldsymbol{\Psi} \boldsymbol{\mu}_L = \boldsymbol{\mu}_R^\top \boldsymbol{\Psi} \boldsymbol{\mu}_R$



Distributional curvature

Shape operator $-\partial^S \boldsymbol{\nu}$ is a distribution



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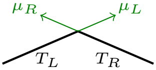

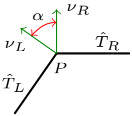

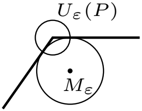

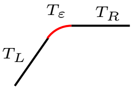

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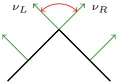
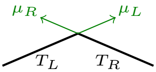
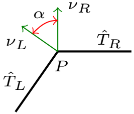
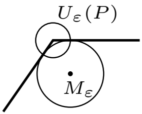
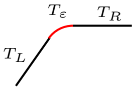


- Duality pairing with $\boldsymbol{\Psi} : \mathcal{S} \to \mathbb{R}^{2\times 2}_{\mathrm{sym}}$, $\boldsymbol{\mu}_L^\top \boldsymbol{\Psi} \boldsymbol{\mu}_L = \boldsymbol{\mu}_R^\top \boldsymbol{\Psi} \boldsymbol{\mu}_R$





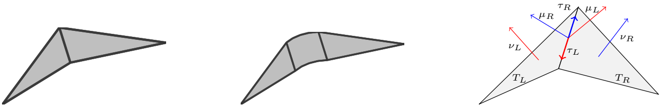




$$\langle -\partial^S \boldsymbol{\nu}, \boldsymbol{\Psi} \rangle_{\mathcal{T}_h} := -\sum_{T\in\mathcal{T}_h} \int_T \partial^S \boldsymbol{\nu}|_T : \boldsymbol{\Psi}\, ds - \sum_{E\in\mathcal{E}_h} \int_E \sphericalangle(\boldsymbol{\nu}_L, \boldsymbol{\nu}_R) \boldsymbol{\Psi}_{\boldsymbol{\mu}\boldsymbol{\mu}}\, d\gamma$$

[1] Grinspun et. al., Computing discrete shape operators on general meshes, *Computer Graphics Forum (2006)*

Distributional curvature



- Direct extension to surfaces
- $\boldsymbol{\Psi}$ is co-normal co-normal continuous HHJ finite element

$$\langle -\partial^S \boldsymbol{\nu}, \boldsymbol{\Psi}\rangle_{\mathcal{T}_h} := -\sum_{T\in\mathcal{T}_h}\int_T \partial^S\boldsymbol{\nu}|_T : \boldsymbol{\Psi}\, ds - \sum_{E\in\mathcal{E}_h}\int_E \sphericalangle(\boldsymbol{\nu}_L,\boldsymbol{\nu}_R)\boldsymbol{\Psi}_{\boldsymbol{\mu}\boldsymbol{\mu}}\, d\gamma.$$

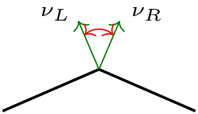
[1] M. Comodi: The Hellan-Herrmann-Johnson method: some new error estimates and postprocessing, *Math. Comp. (1989)*

[2] A. Pechstein and J. Schöberl: The TDNNS method for Reissner-Mindlin plates, *J. Numer. Math. (2017)*

Jump term

Rewrite jump term:

$$\sum_{E\in\mathcal{E}_h}\int_E \sphericalangle(\boldsymbol{\nu}_L,\boldsymbol{\nu}_R)\boldsymbol{\Psi}_{\boldsymbol{\mu}\boldsymbol{\mu}}\,d\gamma$$



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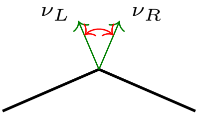
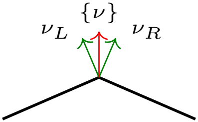


$$\sum_{T \in \mathcal{T}_h} \int_{\partial T} \sphericalangle(\{\boldsymbol{\nu}\}, \boldsymbol{\nu}) \boldsymbol{\Psi}_{\mu\mu} \, d\gamma$$



$$\{\boldsymbol{\nu}\} := \frac{1}{\|\boldsymbol{\nu}_L + \boldsymbol{\nu}_R\|} (\boldsymbol{\nu}_L + \boldsymbol{\nu}_R)$$

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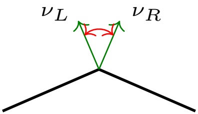

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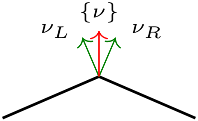

$$\sum_{T\in\mathcal{T}_h}\int_{\partial T} (\frac{\pi}{2}-\sphericalangle(\{\boldsymbol{\nu}\},\boldsymbol{\mu}))\boldsymbol{\Psi}_{\boldsymbol{\mu}\boldsymbol{\mu}}\,d\gamma$$

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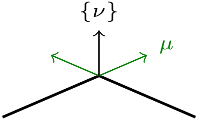

- Lift distributional curvature to more regular $\boldsymbol{\kappa}$

$$\mathcal{L}(\mathcal{T}_h \qquad) = \sum_{T\in\mathcal{T}_h} \Big(\int_T 2\kappa_b(\qquad H - H_0)^2$$

$$\Big)$$

$$+ c_A J_{\mathrm{surf}}(\mathcal{T}_h) + c_V J_{\mathrm{vol}}(\mathcal{T}_h),$$

Three field formulation

- Lift distributional curvature to more regular $\boldsymbol{\kappa}$
- $\boldsymbol{\sigma}$ enforces that $\boldsymbol{\kappa} = -\partial^S \boldsymbol{\nu}$
- $\boldsymbol{\kappa}$, $\boldsymbol{\sigma}$ symmetric, co-normal co-normal continuous

$$\mathcal{L}(\mathcal{T}_h, \boldsymbol{\kappa}, \boldsymbol{\sigma}) = \sum_{T \in \mathcal{T}_h} \Big(\int_T 2\kappa_b\big(\frac{1}{2}\mathrm{tr}(\boldsymbol{\kappa}) - H_0\big)^2 + (\boldsymbol{\kappa} + \partial^S \boldsymbol{\nu}) : \boldsymbol{\sigma} \, ds$$
$$+ \int_{\partial T} \Big(\frac{\pi}{2} - \sphericalangle(\boldsymbol{\mu}, \{\boldsymbol{\nu}\})\Big) \boldsymbol{\sigma}_{\boldsymbol{\mu}\boldsymbol{\mu}} \, d\gamma \Big)$$
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\begin{aligned}
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& + \int_{\partial T} \Big(\frac{\pi}{2} - \sphericalangle(\boldsymbol{\mu}, \{\boldsymbol{\nu}\}) \Big) \boldsymbol{\sigma}_{\boldsymbol{\mu}\boldsymbol{\mu}}\, d\gamma \Big) \\
& + c_A\, J_{\mathrm{surf}}(\mathcal{T}_h) + c_V\, J_{\mathrm{vol}}(\mathcal{T}_h),
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- Fourth order to second order problems

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& + \int_{\partial T} \Big(\frac{\pi}{2} - \sphericalangle(\boldsymbol{\mu}, \{\boldsymbol{\nu}\})\Big)\, \boldsymbol{\sigma}_{\boldsymbol{\mu}\boldsymbol{\mu}}\, d\gamma \Big) \\
& + c_A\, J_{\mathrm{surf}}(\mathcal{T}_h) + c_V\, J_{\mathrm{vol}}(\mathcal{T}_h),
\end{aligned}
$$

- Fourth order to second order problems
- Only $\mathrm{tr}(\boldsymbol{\kappa})$ involved $\rightarrow$ reduction to scalar-valued κ!

Reduction of formulation

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- Additionally $\operatorname{dev}(\boldsymbol{\kappa}) = 0 \Rightarrow \boldsymbol{\kappa} = \kappa\, \boldsymbol{P}_{\mathcal{S}}, \qquad \boldsymbol{P}_{\mathcal{S}} = \boldsymbol{I} - \boldsymbol{\nu} \otimes \boldsymbol{\nu}$

$$\begin{aligned}\mathcal{L}(\mathcal{T}_h, \boldsymbol{\kappa}, \boldsymbol{\sigma}) = \sum_{T \in \mathcal{T}_h} \Big(\int_T 2\kappa_b \big(\frac{1}{2}\operatorname{tr}(\boldsymbol{\kappa}) - H_0\big)^2 + (\boldsymbol{\kappa} + \partial^S \boldsymbol{\nu}) : \boldsymbol{\sigma}\, ds \\ + \int_{\partial T} \Big(\frac{\pi}{2} - \sphericalangle(\boldsymbol{\mu}, \{\boldsymbol{\nu}\})\Big)\, \boldsymbol{\sigma}_{\boldsymbol{\mu}\boldsymbol{\mu}}\, d\gamma \Big) \\ + c_A\, J_{\mathrm{surf}}(\mathcal{T}_h) + c_V\, J_{\mathrm{vol}}(\mathcal{T}_h)\end{aligned}$$

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- $\boldsymbol{\kappa}_{\boldsymbol{\mu}\boldsymbol{\mu}}$ continuous yields κ continuous
- Same for $\boldsymbol{\sigma}$

$$\mathcal{L}(\mathcal{T}_h, \boldsymbol{\kappa}, \boldsymbol{\sigma}) = \sum_{T \in \mathcal{T}_h} \Big(\int_T 2\kappa_b (\frac{1}{2}\mathrm{tr}(\boldsymbol{\kappa}) - H_0)^2 + (\boldsymbol{\kappa} + \partial^S \boldsymbol{\nu}) : \boldsymbol{\sigma}\, ds$$
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- $\kappa,\ \sigma \in H^1(\mathcal{S})$

Shape derivative

Perturbed Lagrangian

$$\mathcal{T}_h^t = \{\boldsymbol{T}_t(T) : \; T \in \mathcal{T}_h\}, \quad \boldsymbol{T}_t(\boldsymbol{x}) = \boldsymbol{x} + t\,\boldsymbol{X}(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathcal{T}_h, t \geq 0 \text{ small}$$

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$$w_t = \det(\partial \boldsymbol{T}_t) \|\partial \boldsymbol{T}_t^{-\top} \boldsymbol{\nu}\|, \quad w_t^E = \|\partial \boldsymbol{T}_t \boldsymbol{\tau}\|,$$

$$\boldsymbol{\nu}^t = \boldsymbol{\nu}_t \circ \boldsymbol{T}_t = \frac{\partial \boldsymbol{T}_t^{-\top} \boldsymbol{\nu}}{\|\partial \boldsymbol{T}_t^{-\top} \boldsymbol{\nu}\|}, \quad \boldsymbol{A}^\top(t) := \partial \boldsymbol{T}_t^{-1}(\boldsymbol{I} - \boldsymbol{\nu}^t \otimes \boldsymbol{\nu}^t)$$

Perturbed Lagrangian

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$$\begin{aligned}\mathcal{L}(\mathcal{T}_h^t, \kappa, \sigma) = \sum_{T \in \mathcal{T}_h} \Big(\int_T & w_t\, 2\kappa_b (\frac{\kappa}{2} - H_0)^2 + w_t\,(\kappa + \mathrm{tr}(\partial^S \boldsymbol{\nu}^t \boldsymbol{A}^\top(t)))\sigma\, ds \\ & + \int_{\partial T} w_t^E \left(\frac{\pi}{2} - \sphericalangle(\boldsymbol{\mu}^t, \{\boldsymbol{\nu}^t\})\right) \sigma\, d\gamma \Big) \\ & + c_A\, J_{\mathrm{surf}}(\mathcal{T}_h^t) + c_V\, J_{\mathrm{vol}}(\mathcal{T}_h^t).\end{aligned}$$

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\end{aligned}
$$

- Shape derivative $D\mathcal{L}(\mathcal{T}_h)(\boldsymbol{X}) = \lim_{t \searrow 0} \frac{\mathcal{L}(\mathcal{T}_h^t) - \mathcal{L}(\mathcal{T}_h)}{t}$

$$\mathcal{L}(\mathcal{T}_h^t, \kappa, \sigma) = \sum_{T \in \mathcal{T}_h} \Big(\int_T w_t\, 2\kappa_b (\frac{\kappa}{2} - H_0)^2 + w_t\, (\kappa + \mathrm{tr}(\partial^S \boldsymbol{\nu}^t \boldsymbol{A}^\top(t)))\sigma\, ds$$
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$$\frac{d}{dt} w_t \big|_{t=0} = \mathrm{div}^S(\boldsymbol{X})$$

Standard shape derivatives

$$\mathcal{L}(\mathcal{T}_h^t,\kappa,\sigma) = \sum_{T\in\mathcal{T}_h}\Big(\int_T w_t\, 2\kappa_b\big(\frac{\kappa}{2}-H_0\big)^2 + w_t\,(\kappa+\mathrm{tr}(\partial^S\boldsymbol{\nu}^t\boldsymbol{A}^\top(t)))\sigma\, ds$$
$$+\int_{\partial T} w_t^E\left(\frac{\pi}{2}-\sphericalangle(\boldsymbol{\mu}^t,\{\boldsymbol{\nu}^t\})\right)\sigma\, d\gamma\Big)$$
$$+\,c_A\, J_{\mathrm{surf}}(\mathcal{T}_h^t)+c_V\, J_{\mathrm{vol}}(\mathcal{T}_h^t).$$

- Shape derivative $D\mathcal{L}(\mathcal{T}_h)(\boldsymbol{X}) = \lim_{t\searrow 0}\frac{\mathcal{L}(\mathcal{T}_h^t)-\mathcal{L}(\mathcal{T}_h)}{t}$

$$\frac{d}{dt}w_t^E|_{t=0} = (\partial^S\boldsymbol{X})_{\boldsymbol{\tau}\boldsymbol{\tau}}$$

Standard shape derivatives

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$$\begin{aligned}\mathcal{L}(\mathcal{T}_h^t, \kappa, \sigma) = \sum_{T \in \mathcal{T}_h} \Big(\int_T & w_t \, 2\kappa_b \big(\frac{\kappa}{2} - H_0\big)^2 + w_t \, (\kappa + \mathrm{tr}(\partial^S \boldsymbol{\nu}^t \boldsymbol{A}^\top(t)))\sigma \, ds \\ & + \int_{\partial T} w_t^E \left(\frac{\pi}{2} - \sphericalangle(\boldsymbol{\mu}^t, \{\boldsymbol{\nu}^t\})\right) \sigma \, d\gamma \Big) \\ & + c_A \, J_{\mathrm{surf}}(\mathcal{T}_h^t) + c_V \, J_{\mathrm{vol}}(\mathcal{T}_h^t).\end{aligned}$$

- Shape derivative $D\mathcal{L}(\mathcal{T}_h)(\boldsymbol{X}) = \lim_{t \searrow 0} \frac{\mathcal{L}(\mathcal{T}_h^t) - \mathcal{L}(\mathcal{T}_h)}{t}$

$$DJ_{\mathrm{surf}}(\mathcal{T}_h)(\boldsymbol{X}) = 2(|\mathcal{T}_h| - A_0) \int_{\mathcal{T}_h} \mathrm{div}^S(\boldsymbol{X}) \, ds$$

$$
\begin{aligned}
\mathcal{L}(\mathcal{T}_h^t, \kappa, \sigma) = \sum_{T \in \mathcal{T}_h} \Big(\int_T w_t \, 2\kappa_b (\frac{\kappa}{2} - H_0)^2 + w_t \, (\kappa + \mathrm{tr}(\partial^S \boldsymbol{\nu}^t \boldsymbol{A}^\top(t)))\sigma \, ds \\
+ \int_{\partial T} w_t^E \left(\frac{\pi}{2} - \sphericalangle(\boldsymbol{\mu}^t, \{\boldsymbol{\nu}^t\}) \right) \sigma \, d\gamma \Big) \\
+ c_A \, J_{\mathrm{surf}}(\mathcal{T}_h^t) + c_V \, J_{\mathrm{vol}}(\mathcal{T}_h^t).
\end{aligned}
$$

- Shape derivative $D\mathcal{L}(\mathcal{T}_h)(\boldsymbol{X}) = \lim_{t \searrow 0} \frac{\mathcal{L}(\mathcal{T}_h^t) - \mathcal{L}(\mathcal{T}_h)}{t}$

$$
DJ_{\mathrm{vol}}(\mathcal{T}_h)(\boldsymbol{X}) = 2(|\Omega_h| - V_0) \int_{\mathcal{T}_h} \boldsymbol{X} \cdot \boldsymbol{\nu} \, ds
$$

$$
\begin{aligned}
\mathcal{L}(\mathcal{T}_h^t,\kappa,\sigma) = \sum_{T\in\mathcal{T}_h} \Big(\int_T & w_t\, 2\kappa_b(\frac{\kappa}{2} - H_0)^2 + w_t\,(\kappa + \mathrm{tr}(\partial^S \boldsymbol{\nu}^t \boldsymbol{A}^\top(t)))\sigma\, ds \\
& + \int_{\partial T} w_t^E \left(\frac{\pi}{2} - \sphericalangle(\boldsymbol{\mu}^t, \{\boldsymbol{\nu}^t\})\right) \sigma\, d\gamma \Big) \\
& + c_A\, J_{\mathrm{surf}}(\mathcal{T}_h^t) + c_V\, J_{\mathrm{vol}}(\mathcal{T}_h^t).
\end{aligned}
$$

- Shape derivative $D\mathcal{L}(\mathcal{T}_h)(\boldsymbol{X}) = \lim_{t\searrow 0} \frac{\mathcal{L}(\mathcal{T}_h^t)-\mathcal{L}(\mathcal{T}_h)}{t}$

Shape operator (mean curvature)

Shape operator

$$\frac{d}{dt}(\partial^{S_t}\boldsymbol{\nu}_t)\circ \boldsymbol{T}_t\big|_{t=0} = \partial^S\boldsymbol{\nu}\left(2\,\mathrm{Sym}(\boldsymbol{\nu}\otimes\boldsymbol{\nu}\partial^S\boldsymbol{X}) - \partial^S\boldsymbol{X}\right) - \mathrm{hess}(\boldsymbol{X})(\boldsymbol{\nu}) - \partial^S\boldsymbol{X}^\top\partial^S\boldsymbol{\nu}$$

Mean curvature

$$\frac{d}{dt}\mathrm{tr}(\partial^{S_t}\boldsymbol{\nu}_t)\circ \boldsymbol{T}_t\big|_{t=0} = -\Delta^S\boldsymbol{X}\cdot\boldsymbol{\nu} - 2\partial^S\boldsymbol{X} : \partial^S\boldsymbol{\nu}$$

Laplace–Beltrami operator $\Delta^S = \mathrm{div}^S(\partial^S)$

Shape operator

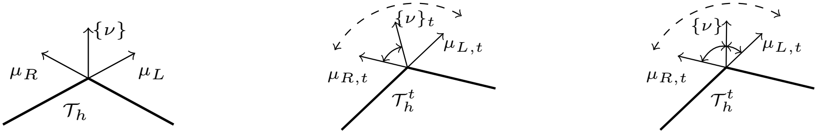
$$\frac{d}{dt}(\partial^{S_t}\boldsymbol{\nu}_t)\circ \boldsymbol{T}_t|_{t=0} = \partial^S\boldsymbol{\nu}\left(2\,\mathrm{Sym}(\boldsymbol{\nu}\otimes\boldsymbol{\nu}\partial^S\boldsymbol{X}) - \partial^S\boldsymbol{X}\right) - \mathrm{hess}(\boldsymbol{X})(\boldsymbol{\nu}) - \partial^S\boldsymbol{X}^\top\partial^S\boldsymbol{\nu}$$

Mean curvature (weak form)

$$\int_T \mathrm{tr}(\partial^{S_t}\boldsymbol{\nu}_t)\circ\boldsymbol{T}_t|_{t=0}\,\sigma\,ds = \int_T \partial^S\boldsymbol{X}\partial^S\sigma\cdot\boldsymbol{\nu} - \partial^S\boldsymbol{X} : \partial^S\boldsymbol{\nu}\sigma\,ds - \int_{\partial T}\partial^S\boldsymbol{X}\boldsymbol{\mu}\cdot\boldsymbol{\nu}\,\sigma\,d\gamma$$

$$\int_{\partial T} \left(\frac{\pi}{2} - \sphericalangle(\boldsymbol{\mu}^t, \{\boldsymbol{\nu}\}^t) \right) \sigma \, d\gamma$$

$$\{\boldsymbol{\nu}\}^t = \frac{1}{\|\boldsymbol{\nu}_L^t + \boldsymbol{\nu}_R^t\|} (\boldsymbol{\nu}_L^t + \boldsymbol{\nu}_R^t)$$

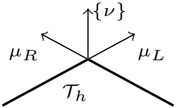


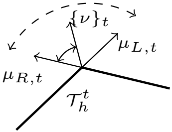
$$\int_{\partial T} \left(\frac{\pi}{2} - \sphericalangle(\boldsymbol{\mu}^t, \{\boldsymbol{\nu}\}^t)\right) \sigma \, d\gamma$$

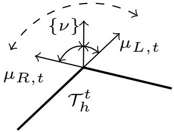
$$\{\boldsymbol{\nu}\}^t = \frac{1}{\|\boldsymbol{\nu}_L^t + \boldsymbol{\nu}_R^t\|}(\boldsymbol{\nu}_L^t + \boldsymbol{\nu}_R^t)$$

$$\int_{\partial T} \left(\frac{\pi}{2} - \sphericalangle(\boldsymbol{\mu}^t, \qquad \{\boldsymbol{\nu}\} \ )\right) \sigma \, d\gamma$$

Jump term



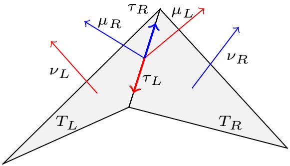




$$\int_{\partial T} \left(\frac{\pi}{2} - \sphericalangle(\boldsymbol{\mu}^t, \{\boldsymbol{\nu}\}^t)\right) \sigma \, d\gamma$$

$$\boldsymbol{P}^{\perp}_{\boldsymbol{\tau}^t}(\{\boldsymbol{\nu}\}) := \frac{\{\boldsymbol{\nu}\} - (\{\boldsymbol{\nu}\} \cdot \boldsymbol{\tau}^t)\boldsymbol{\tau}^t}{\|\{\boldsymbol{\nu}\} - (\{\boldsymbol{\nu}\} \cdot \boldsymbol{\tau}^t)\boldsymbol{\tau}^t\|}$$

$$\int_{\partial T} \left(\frac{\pi}{2} - \sphericalangle(\boldsymbol{\mu}^t, \boldsymbol{P}^{\perp}_{\boldsymbol{\tau}^t}(\{\boldsymbol{\nu}\}))\right) \sigma \, d\gamma$$



Jump term

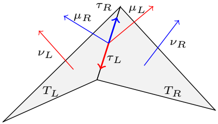
Shape derivative jump term

$$\frac{d}{dt}\sphericalangle(\boldsymbol{\mu}^t, \boldsymbol{P}^{\perp}_{\boldsymbol{\tau}^t}(\{\boldsymbol{\nu}\}))|_{t=0} = -\frac{(\partial^S \boldsymbol{X} - \partial^S \boldsymbol{X}^\top)\boldsymbol{\mu} \cdot \{\boldsymbol{\nu}\}}{\sqrt{1-(\boldsymbol{\mu}\cdot\{\boldsymbol{\nu}\})^2}}$$

Shape derivative jump term

$$\frac{d}{dt}\sphericalangle(\boldsymbol{\mu}^t, \boldsymbol{P}^{\perp}_{\boldsymbol{\tau}^t}(\{\boldsymbol{\nu}\}))|_{t=0} = -\frac{(\partial^S \boldsymbol{X} - \partial^S \boldsymbol{X}^\top)\boldsymbol{\mu}\cdot\{\boldsymbol{\nu}\}}{\sqrt{1-(\boldsymbol{\mu}\cdot\{\boldsymbol{\nu}\})^2}}$$

- Same first shape derivative as for $\sphericalangle(\boldsymbol{\mu}^t, \{\boldsymbol{\nu}\})$
- $\frac{d}{dt}\boldsymbol{\mu}^t|_{t=0} = ((\boldsymbol{I} - \boldsymbol{\tau}\otimes\boldsymbol{\tau})\partial^S \boldsymbol{X} - \partial^S \boldsymbol{X}^\top)\boldsymbol{\mu}$



Total shape derivative

- For fixed $\mathcal{T}_h$, κ, and σ

$$
\begin{aligned}
D\mathcal{L}(\mathcal{T}_h)(\boldsymbol{X}) = \sum_{T\in\mathcal{T}_h} \Big(\int_T & \mathrm{div}^S(\boldsymbol{X}) \Big(2\kappa_b(\frac{\kappa}{2} - H_0)^2 + (\kappa + \mathrm{tr}(\partial^S \boldsymbol{\nu}))\sigma\Big) \\
& + \partial^S \boldsymbol{X} \partial^S \sigma \cdot \boldsymbol{\nu} - \partial^S \boldsymbol{X} : \partial^S \boldsymbol{\nu}\sigma\, ds - \int_{\partial T} \partial^S \boldsymbol{X} \boldsymbol{\mu} \cdot \boldsymbol{\nu}\, \sigma\, d\gamma \\
& + \int_{\partial T} (\partial^S \boldsymbol{X}_{\boldsymbol{\tau}\boldsymbol{\tau}} \Big(\frac{\pi}{2} - \sphericalangle(\boldsymbol{\mu}, \{\boldsymbol{\nu}\})\Big) + \frac{(\partial^S \boldsymbol{X} - \partial^S \boldsymbol{X}^\top)\boldsymbol{\mu} \cdot \{\boldsymbol{\nu}\}}{\sqrt{1 - (\boldsymbol{\mu} \cdot \{\boldsymbol{\nu}\})^2}})\sigma\, d\gamma\Big) \\
& + c_A DJ_{\mathrm{surf}}(\mathcal{T}_h)(\boldsymbol{X}) + c_V DJ_{\mathrm{vol}}(\mathcal{T}_h)(\boldsymbol{X})
\end{aligned}
$$

Total shape derivative

- For fixed $\mathcal{T}_h$, κ, and σ
- lowest-order: lifting only via jump term

$$D\mathcal{L}(\mathcal{T}_h)(\boldsymbol{X}) = \sum_{T\in\mathcal{T}_h}\Big(\int_T \mathrm{div}^S(\boldsymbol{X})\Big(2\kappa_b(\frac{\kappa}{2}-H_0)^2+(\kappa \qquad\qquad)\sigma\Big)$$

$$+\int_{\partial T}(\partial^S\boldsymbol{X}_{\boldsymbol{\tau}\boldsymbol{\tau}}\Big(\frac{\pi}{2}-\sphericalangle(\boldsymbol{\mu},\{\boldsymbol{\nu}\})\Big)+\frac{(\partial^S\boldsymbol{X}-\partial^S\boldsymbol{X}^\top)\boldsymbol{\mu}\cdot\{\boldsymbol{\nu}\}}{\sqrt{1-(\boldsymbol{\mu}\cdot\{\boldsymbol{\nu}\})^2}})\sigma\,d\gamma\Big)$$

$$+c_A DJ_{\mathrm{surf}}(\mathcal{T}_h)(\boldsymbol{X})+c_V DJ_{\mathrm{vol}}(\mathcal{T}_h)(\boldsymbol{X})$$

Total shape derivative

- For fixed $\mathcal{T}_h$, κ, and σ
- lowest-order: lifting only via jump term

$$D\mathcal{L}(\mathcal{T}_h)(\boldsymbol{X}) = \sum_{T\in\mathcal{T}_h} \Big(\int_T \mathrm{div}^S(\boldsymbol{X}) \Big(2\kappa_b(\frac{\kappa}{2} - H_0)^2 + (\kappa \qquad\qquad)\sigma \Big)$$

$$+ \int_{\partial T} \Big(\partial^S \boldsymbol{X}_{\boldsymbol{\tau}\boldsymbol{\tau}} \Big(\frac{\pi}{2} - \sphericalangle(\boldsymbol{\mu}, \{\boldsymbol{\nu}\}) \Big) + \frac{(\partial^S \boldsymbol{X} - \partial^S \boldsymbol{X}^\top)\boldsymbol{\mu} \cdot \{\boldsymbol{\nu}\}}{\sqrt{1 - (\boldsymbol{\mu} \cdot \{\boldsymbol{\nu}\})^2}} \Big)\sigma \, d\gamma \Big)$$

$$+ c_A DJ_{\mathrm{surf}}(\mathcal{T}_h)(\boldsymbol{X}) + c_V DJ_{\mathrm{vol}}(\mathcal{T}_h)(\boldsymbol{X})$$

Solving algorithm

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For fixed $\mathcal{T}_h$

$$\begin{aligned} &\text{find } \kappa, \text{ such that } \partial_\sigma \mathcal{L}(\mathcal{T}_h, \kappa, \sigma)(\delta\sigma) = 0 \quad \text{for all } \delta\sigma \in V_h(\mathcal{T}_h), \\ &\text{find } \sigma, \text{ such that } \partial_\kappa \mathcal{L}(\mathcal{T}_h, \kappa, \sigma)(\delta\kappa) = 0 \quad \text{for all } \delta\kappa \in V_h(\mathcal{T}_h), \end{aligned}$$

$$\begin{aligned} \partial_\sigma \mathcal{L}(\mathcal{T}_h, \kappa, \sigma)(\delta\sigma) &= \sum_{T \in \mathcal{T}_h} \Big(\int_T \kappa\, \delta\sigma + \mathrm{tr}(\partial^S \boldsymbol{\nu}) \delta\sigma \, ds \\ &\qquad + \int_{\partial T} \left(\frac{\pi}{2} - \sphericalangle(\boldsymbol{\mu}, \boldsymbol{P}_{\boldsymbol{\tau}}^{\perp}(\{\boldsymbol{\nu}\})) \right) \delta\sigma \, d\gamma \Big) \\ \partial_\kappa \mathcal{L}(\mathcal{T}_h, \kappa, \sigma)(\delta\kappa) &= \int_{\mathcal{T}_h} 2\kappa_b \left(\frac{\kappa}{2} - H_0\right) \delta\kappa + \delta\kappa\, \sigma \, ds \end{aligned}$$

Solving algorithm

Input: surface $\mathcal{T}_h^0$, $n = 0$, $N_{\max} > 0$, $\epsilon > 0$, $\alpha > 0$
Output: optimal shape $\mathcal{T}_h^*$
while $n \leq N_{\max}$ and $|\nabla \mathcal{J}(\mathcal{T}_h^n)| > \epsilon$ **do**
    if $\mathcal{J}((\mathrm{id} - \alpha \nabla \mathcal{J}(\mathcal{T}_h^n))(\mathcal{T}_h^n)) \leq \mathcal{J}(\mathcal{T}_h^n)$ **then**
        $\mathcal{T}_h^{n+1} \leftarrow (\mathrm{id} - \alpha \nabla \mathcal{J}(\mathcal{T}_h^n))(\mathcal{T}_h^n)$
        $n \leftarrow n + 1$, increase α
    else
        reduce α
    end if
end while

One iteration on $\mathcal{T}_h^n$ involves

1. Average normal vector and solve (adjoint) state problem
2. With new κ and σ compute shape gradient

Solving algorithm

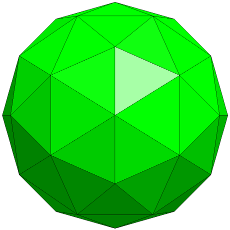
NGSolve [1]

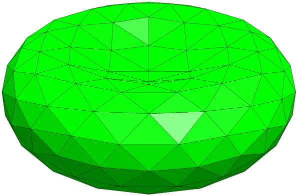
- Fully automated shape differentiation
- Deform mesh via ALE without remeshing

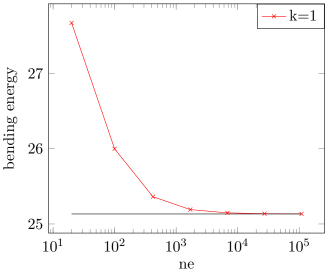
[1] GANGL, STURM, N., SCHÖBERL, Fully and Semi-Automated Shape Differentiation in NGSolve, *Structural and Multidisciplinary Optimization (2021)*

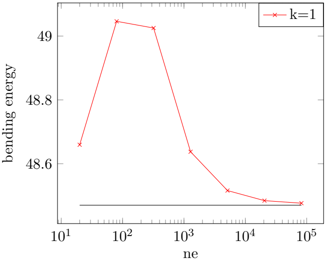
[1] www.ngsolve.org

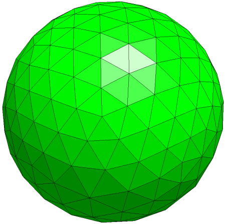
Numerical examples

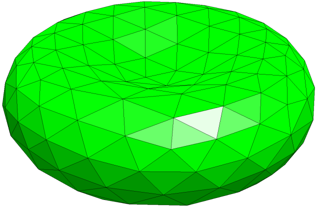


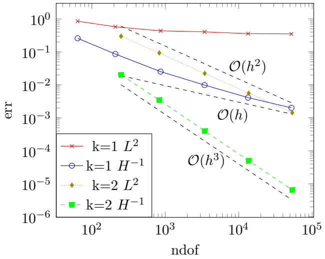


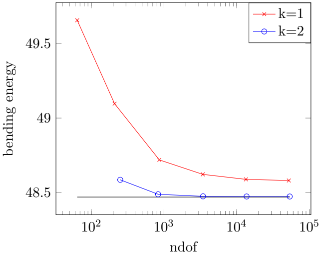

k=1
27
26
25
bending energy
10^1
10^2
10^3
10^4
10^5
ne


k=1
49
48.8
48.6
bending energy
10^1
10^2
10^3
10^4
10^5
ne

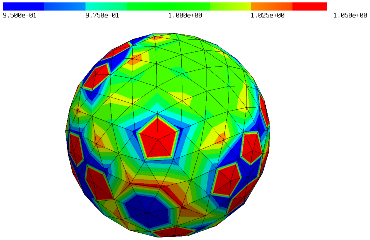


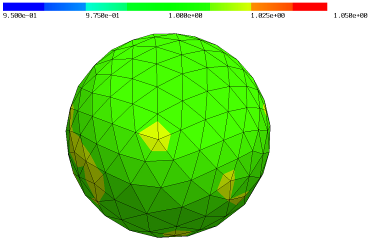


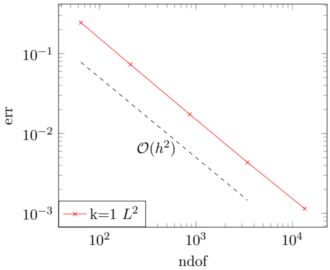

err
ndof
$\mathcal{O}(h^2)$
$\mathcal{O}(h)$
$\mathcal{O}(h^3)$
k=1 L^2
k=1 H^{-1}
k=2 L^2
k=2 H^{-1}

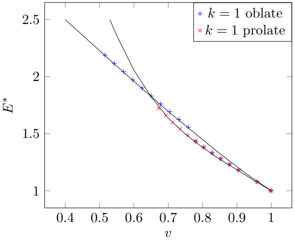

bending energy
ndof
k=1
k=2

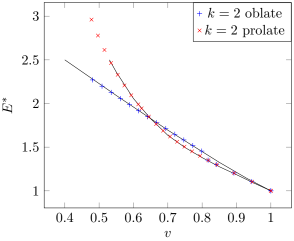
Curvature computation

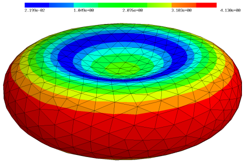


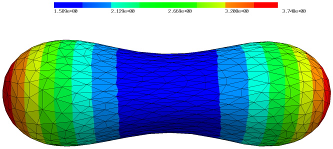












[1] Seifert, Berndl, Lipowsky, Shape transformations of vesicles: Phase diagram for spontaneous- curvature and bilayer-coupling models, *Phys. Rev. A (1991)*

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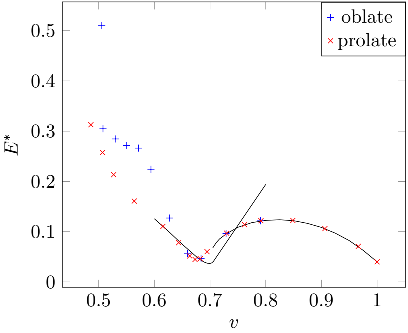
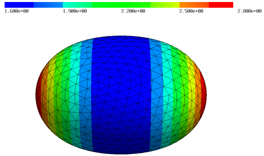
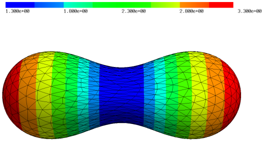
- $\mathcal{W}(\mathcal{S}) = 2\kappa_b \int_{\mathcal{S}} (H - H_0)^2 \, ds, \; H_0 = 1.2$

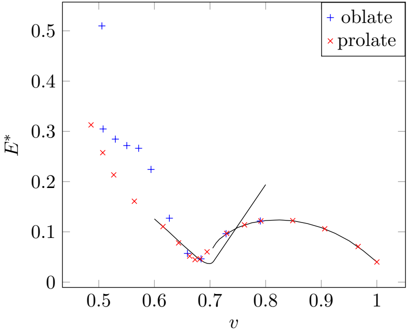


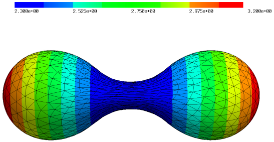




Spontaneous curvature

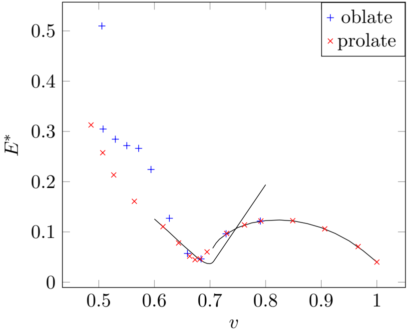
- $\mathcal{W}(\mathcal{S}) = 2\kappa_b \int_{\mathcal{S}} (H - H_0)^2 \, ds, \; H_0 = 1.2$

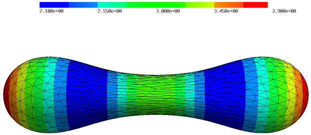


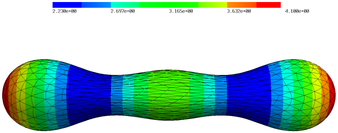


Spontaneous curvature

- $\mathcal{W}(\mathcal{S}) = 2\kappa_b \int_{\mathcal{S}} (H - H_0)^2 \, ds, \; H_0 = 1.2$

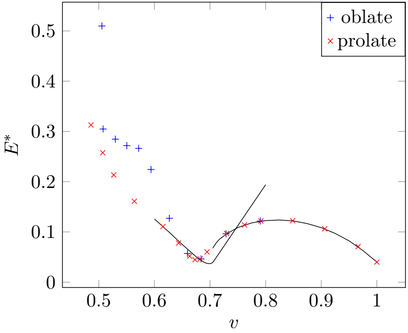


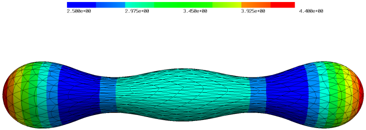


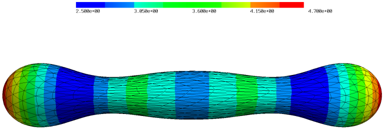


Spontaneous curvature

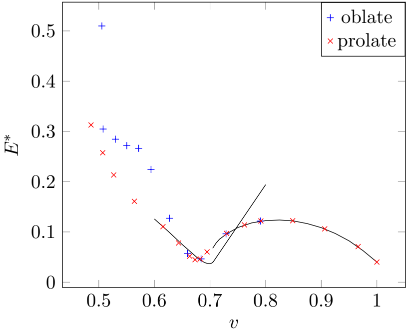
- $\mathcal{W}(\mathcal{S}) = 2\kappa_b \int_{\mathcal{S}} (H - H_0)^2 \, ds, \; H_0 = 1.2$

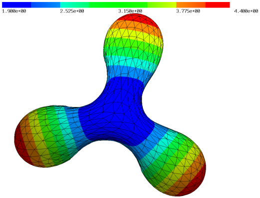


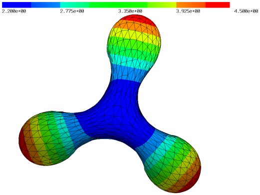




- $\mathcal{W}(\mathcal{S}) = 2\kappa_b \int_{\mathcal{S}} (H - H_0)^2 \, ds, \; H_0 = 1.2$







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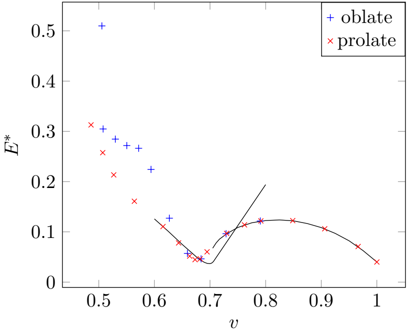

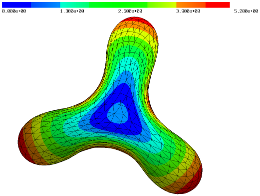

Spontaneous curvature

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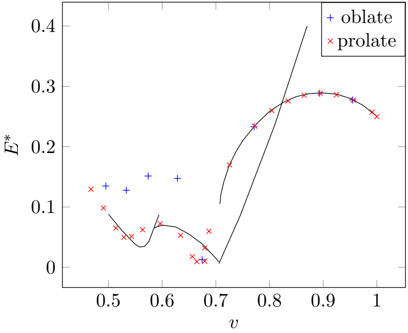

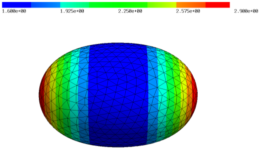

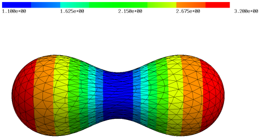

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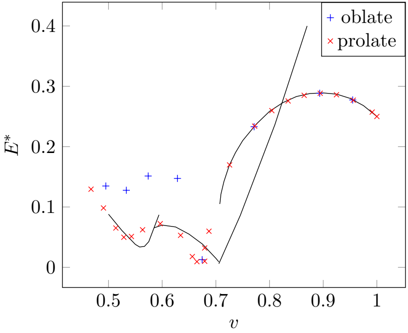

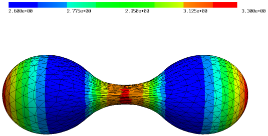

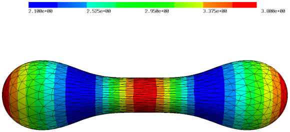

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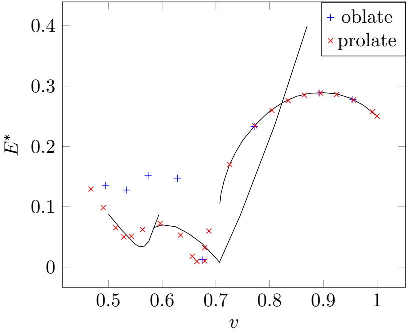

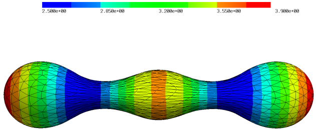

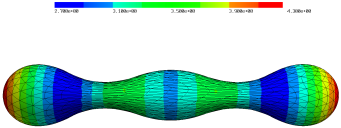

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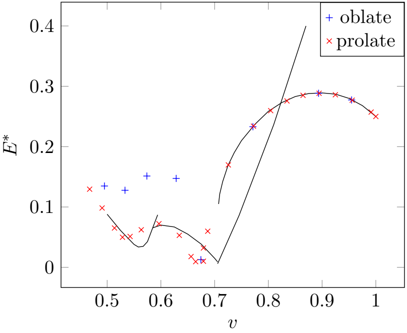

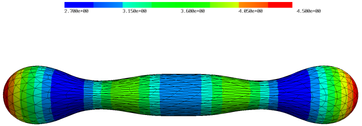

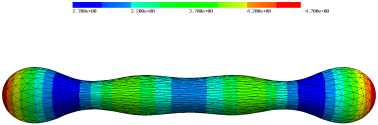

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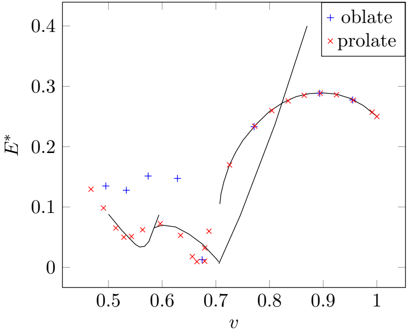

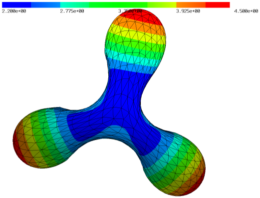

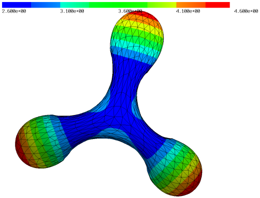

Summary

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- General shape derivative

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[1] N., SCHÖBERL, STURM, Numerical shape optimization of Canham-Helfrich-Evans bending energy, *in preparation*

[2] GANGL, STURM, N., SCHÖBERL, Fully and Semi-Automated Shape Differentiation in NGSolve, *Structural and Multidisciplinary Optimization (2021)*

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Thank You for Your attention!

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