

Solution Techniques for Constrained Shape Optimization Problems in Shape Spaces

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Seminar No. 125 on
"Piecewise smooth system and
optimization with piecewise
linearization via algorithmic
differentiation"

Shonan Village Center, Japan

June 25-28, 2018



- 1 Optimization in the manifold of smooth shapes
- 2 PDE constrained interface problem
- 3 Optimization based on Steklov-Poincaré metrics
- 4 Diffeological space of $H^{1/2}$ -shapes
- 5 VI constrained optimization in shape spaces
- 6 Conclusion



$$\min_{\Omega} J(\Omega)$$

PDE or VI constraints

- J shape functional depending on a solution of a partial differential equation (PDE) or a variational inequality (VI)

(Definition: Let $D \subset \mathbb{R}^d$ be non-empty and let $\mathcal{A} \subset \{\Omega: \Omega \subset D\}$ denote a set of subsets. A function $J: \mathcal{A} \rightarrow \mathbb{R}$, $\Omega \mapsto J(\Omega)$ is called a *shape functional*.)

- Ω shape
 - \rightsquigarrow *2D shape*: Simply connected, compact subset Ω of \mathbb{R}^2 with $\Omega \neq \emptyset$ and C^∞ boundary $\partial\Omega$
 - \rightsquigarrow *How is the set of all shapes defined?*



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- B_e is a manifold (cf. [1])
- *Generalization to higher dimensions*: $B_e(M, N) := \text{Emb}(M, N) / \text{Diff}(M)$, where M is a compact manifold and N denotes a Riemannian manifold with $\dim(M) < \dim(N)$

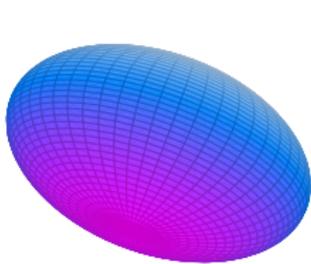
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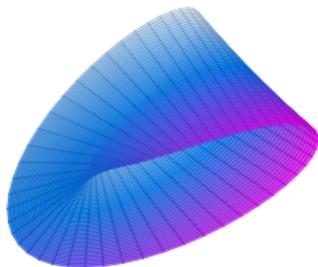
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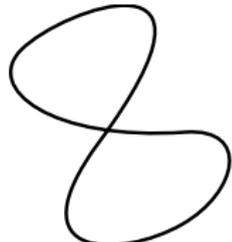
$b_1 \in B_e(S^2, \mathbb{R}^3)$



$b_2 \notin B_e(S^2, \mathbb{R}^3)$



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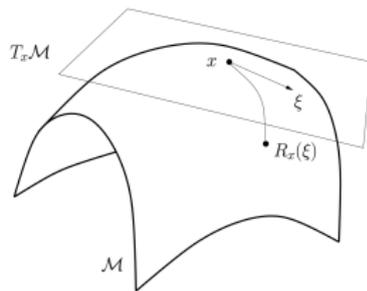
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- Line-search methods in \mathbb{R}^n : $x_{k+1} = x_k + t_k \xi_k$
- Manifolds are not necessarily linear spaces
 - ⇒ Select ξ_k as a tangent vector to \mathcal{M} at x_k
 - ⇒ Points from the tangent space have to be mapped to the manifold

[2] P.-A. Absil, R. Mahony and R. Sepulchre. *Optimization Algorithms on Matrix Manifolds*. Princeton University Press, 2008.

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Example: Steepest descent method on B_e

Goal: Find a solution of $\min_{x \in B_e} J(x)$

Input: $x_0 \in B_e$

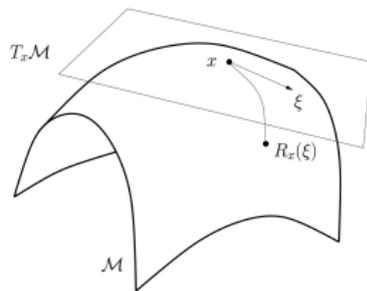
for $k = 0, 1, \dots$ **do**

[1] Compute the increment $\xi_k := -\text{grad}J(x^k) \in T_{x^k} B_e$

[2] Set $x_{k+1} := \mathcal{R}_{x^k}(t_k \xi_k)$ for some steplength t_k and a retraction \mathcal{R}

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A *Riemannian metric* on a manifold M is a collection $g = (g_p)_{p \in M}$ of inner products

$$g_p: T_p M \times T_p M \rightarrow \mathbb{R}, (v, w) \mapsto g_p(v, w),$$

one for every $p \in M$, such that the map $M \rightarrow \mathbb{R}, p \mapsto g_p(X(p), Y(p))$ is smooth for every pair of vector fields X, Y on M .



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Sobolev metric (cf. [3])

$$g^1: T_c B_e \times T_c B_e \rightarrow \mathbb{R}, (h, k) \mapsto \langle (I - A\Delta_c)\alpha, \beta \rangle_{L^2(c)} \text{ with } A > 0$$

Here $h = \alpha n$ and $k = \beta n$ denote two elements of the tangent space

$$T_c B_e \cong \{\psi \mid \psi = \alpha n, \alpha \in C^\infty(S^1, \mathbb{R})\}.$$

[3] M. Bauer, P. Harms, and P. Michor. Sobolev metrics on shape space of surfaces. *JGM*, 3(4):389–438, 2011.



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Riemannian shape gradient w.r.t. g^1

Representation of $DJ(x)$ such that $g^1(\text{grad}J(x), h) = DJ(x)[h] \quad \forall h \in T_x B_e$

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Definition

Let $D \subset \mathbb{R}^d$ be non-empty and open and let $\Omega \subset D$ be measurable. The *shape derivative* of a shape functional J at Ω in direction $V \in C_0^k(D, \mathbb{R}^d)$, $k \in \mathbb{N} \cup \{\infty\}$, is defined by the *Eulerian derivative*

$$DJ(\Omega)[V] = \lim_{t \rightarrow 0^+} \frac{J(\Omega_t) - J(\Omega)}{t} \quad (\Omega_t = \{x + t \cdot V(x) : x \in \Omega\}).$$

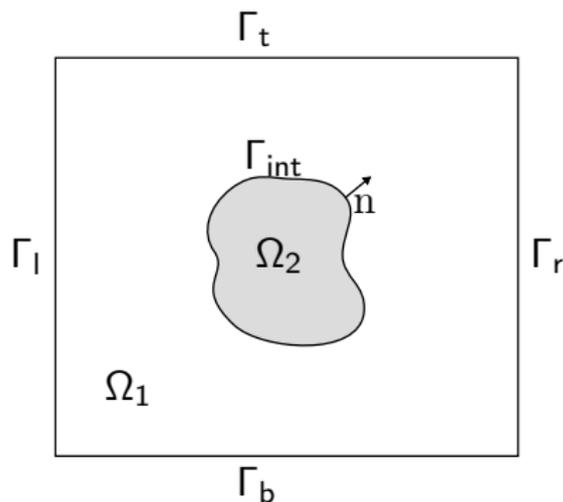
- Shape derivative of a shape differentiable functional is a directional derivative in the direction of a differentiable vector field
- **Hadamard Structure Theorem** (cf. Theorem 2.17 in [4]):
 - Only the normal part of a vector field on the boundary Γ of a domain Ω has an impact on the value of the shape derivative
 - Existence of a scalar distribution r on Γ
 - If $r \in L^1(\Gamma)$, then $DJ(\Omega)[V] = \int_{\Gamma} r \langle V, n \rangle ds$
- r is often called the *shape gradient* but gradients depend on chosen scalar products defined on the space under consideration

[4] J. Sokolowski and J.-P. Zolésio. *Introduction to Shape Optimization*, volume 16 of *Computational Mathematics* Springer, 1992.



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- Diffusion process
- $\Omega \subset \mathbb{R}^2$ bounded Lipschitz domain
- Two materials $\Omega_1, \Omega_2 \subset \Omega$ with different permeability
- Fixed outer boundary
 $\partial\Omega = \Gamma_b \cup \Gamma_l \cup \Gamma_r \cup \Gamma_t$
- Variable boundary $\Gamma_{\text{int}} \in \mathcal{B}_e(S^1, \mathbb{R}^2)$
 \Rightarrow Fit to measured concentration
- Homogeneous concentration in Ω for $t = 0$
- Higher concentration on the top in the beginning



For concentration y and diffusion coefficient k :

$$\begin{aligned} \min_{\Gamma_{\text{int}}} J(y, \Omega) &= j(y, \Omega) + j^{\text{reg}}(\Omega) := \frac{1}{2} \int_0^T \int_{\Omega} (y - \bar{y})^2 dx dt + \mu \int_{\Gamma_{\text{int}}} 1 ds \\ \text{s.t. } \frac{\partial y}{\partial t} - \text{div}(k \nabla y) &= f \quad \text{in } \Omega \times (0, T] \\ y &= 1 \quad \text{on } \Gamma_t \times (0, T] \\ \frac{\partial y}{\partial n} &= 0 \quad \text{on } (\Gamma_b \cup \Gamma_l \cup \Gamma_r) \times (0, T] \\ y &= y_0 \quad \text{in } \Omega \times \{0\} \end{aligned}$$

- Data measurements: $\bar{y} \in L^2(0, T; L^2(\Omega))$
- Right hand-side: $f = \text{const.} \quad \text{in } \Omega \times (0, T]$
- Jumping coefficient: $k = \begin{cases} k_1 = \text{const.} & \text{in } \Omega_1 \\ k_2 = \text{const.} & \text{in } \Omega_2 \end{cases}$
- Transmission conditions: $\llbracket y \rrbracket = 0, \quad \left[\left[k \frac{\partial y}{\partial n} \right] \right] = 0 \quad \text{on } \Gamma_{\text{int}} \times (0, T]$



Shape derivative of the regularization term j^{reg}

$$Dj^{\text{reg}}(\Omega)[V] = \mu \int_{\Gamma_{\text{int}}} \langle V, n \rangle \kappa \, ds$$



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$$Dj_{\Omega}(y, \Omega)[V] = Dj(y, \Omega)[V] = Dj_{\Gamma_{\text{int}}}(y, \Omega)[V]$$

- $$Dj_{\Omega}(y, \Omega)[V] = \int_0^T \int_{\Omega} -k \nabla y^{\top} (\nabla V + \nabla V^{\top}) \nabla p - p \nabla f^{\top} V + \text{div}(V) \left(\frac{1}{2} (y - \bar{y})^2 + \frac{\partial y}{\partial t} p + k \nabla y^{\top} \nabla p - fp \right) dx \, dt$$
- $$Dj_{\Gamma_{\text{int}}}(y, \Omega)[V] = \int_0^T \int_{\Gamma_{\text{int}}} \llbracket k \rrbracket \nabla y_1^{\top} \nabla p_2 \langle V, n \rangle \, ds \, dt$$

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 - Volume formulation: $y \in L^2(0, T; H^1(\Omega))$, $p \in W(0, T; H^1(\Omega))$
 - Surface formulation: H^2 -regularity in space is necessary

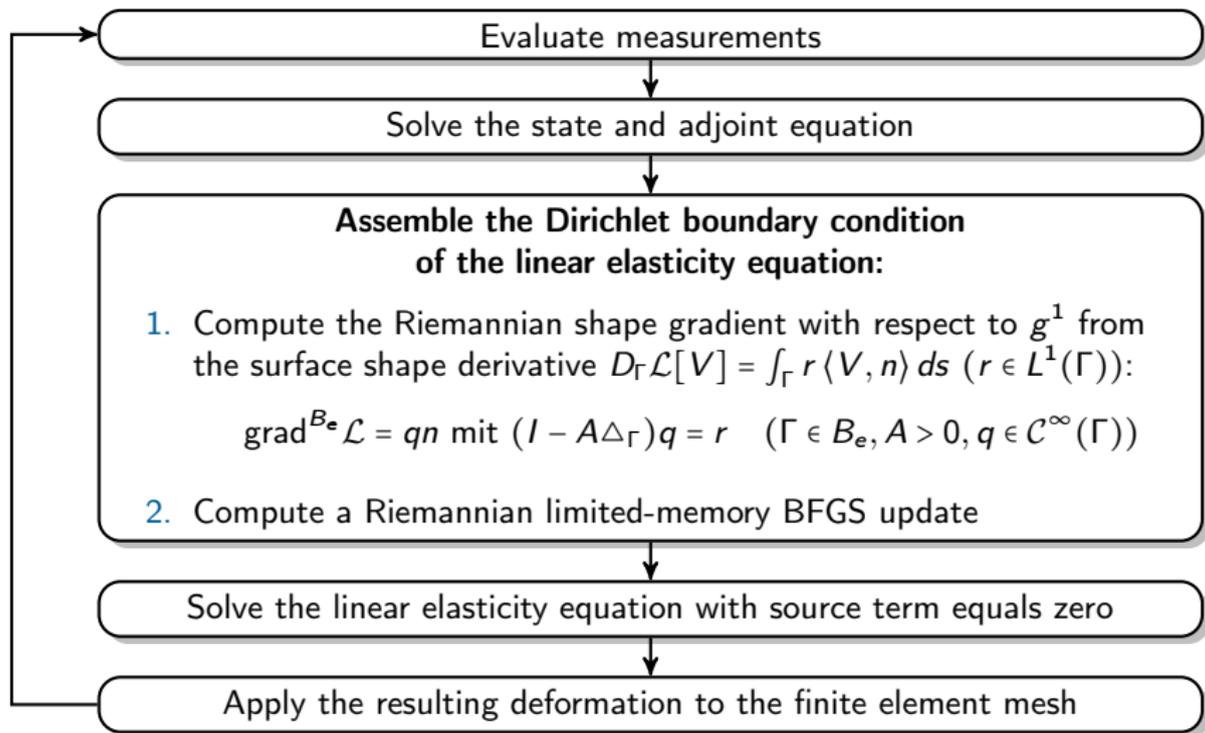
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[5] V. Schulz, M. Siebenborn and K. W. Structured inverse modeling in parabolic diffusion problems. *SICON*, 53(6):3319–3338, 2015.



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- Derivation of surface shape derivative formulations is a time-consuming process
⇒ **Aim:** *Usage of volume shape derivative expressions*
- Gradient representation and afterwards mesh deformation
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Definition of an inner product based on volume formulations

- Inner product should be derived from the second shape derivative
 - Second shape derivative can be related to the Steklov-Poincaré operator (cf. [6])
- ⇒ Definition of a *Steklov-Poincaré type metric*

[6] S. Schmidt and V. Schulz. Impulse response approximations of discrete shape Hessians with application in CFD. *SICON*, 48(4):2562–2580, 2009.



Definition

$$g^S: H^{1/2}(\Gamma) \times H^{1/2}(\Gamma) \rightarrow \mathbb{R}, (\alpha, \beta) \mapsto \int_{\Gamma} \alpha \cdot (S^{\text{pr}})^{-1} \beta \, ds$$

Here S^{pr} denotes the projected Poincaré-Steklov operator and is given by

$$S^{\text{pr}}: H^{-1/2}(\Gamma) \rightarrow H^{1/2}(\Gamma), \xi \mapsto (\gamma_0 U)^{\top} n,$$

where $U \in H_0^1(\Omega, \mathbb{R}^d)$ solves $a(U, V) = \int_{\Gamma} \xi \cdot (\gamma_0 V)^{\top} n \, ds \quad \forall V \in H_0^1(\Omega, \mathbb{R}^d)$.



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Shape derivative in surface formulation $DJ_{\Gamma}[V] = \int_{\Gamma} r \langle V, n \rangle \, ds$

\leadsto **Shape gradient with respect to g^S** is given by $h \in T_{\Gamma} B_e \cong C^{\infty}(\Gamma)$ s.t.

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Construction of the g^S -metric yields

$$g^S(u, v) = DJ_\Gamma[V] = DJ_\Omega[V] = a(U, V) \quad \forall V \in H_0^1(\Omega, \mathbb{R}^d) \text{ and } v = (\gamma_0 V)^\top n$$

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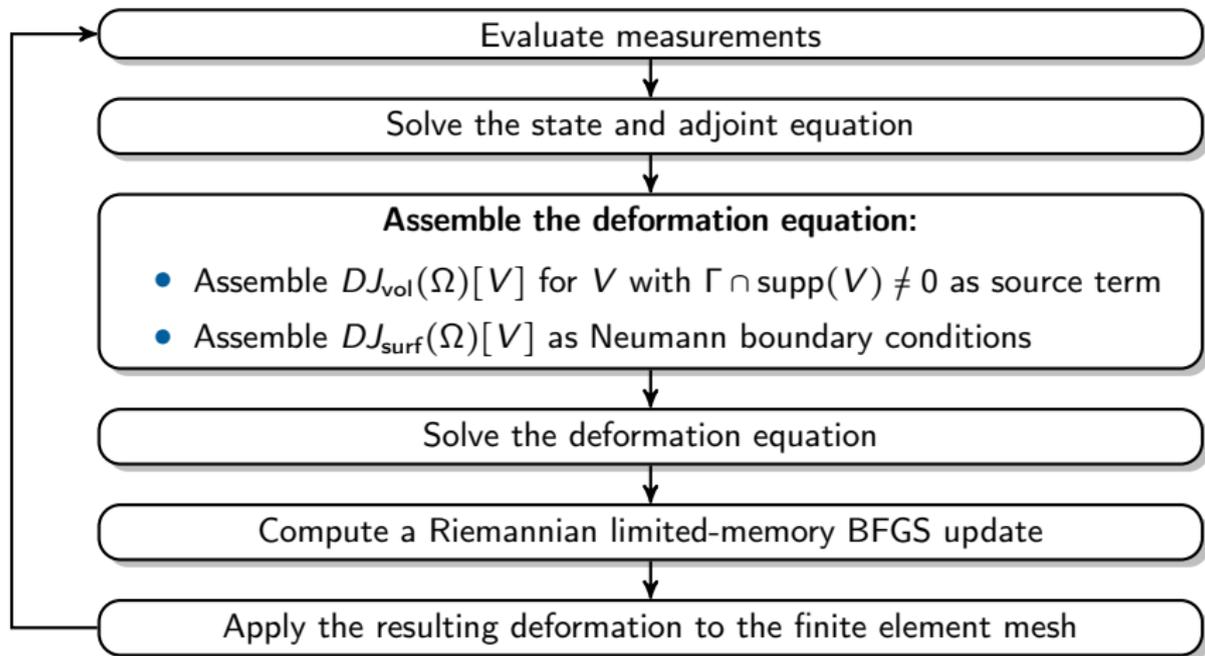
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We have to solve the *deformation equation*:

$$a(U, V) = b(V) \quad \forall V \in H_0^1(\Omega, \mathbb{R}^d)$$

- $a(\cdot, \cdot)$ symmetric and coercive bilinearform
- $b(V) := DJ_{\text{vol}}(\Omega)[V] + DJ_{\text{surf}}(\Omega)[V]$
 - $J_{\text{vol}}(\Omega)$ parts of J leading to volume shape derivative expressions
 - $J_{\text{surf}}(\Omega)$ parts of J leading to surface shape derivative expressions

\Rightarrow Combination of surface and volume formulation of shape derivatives



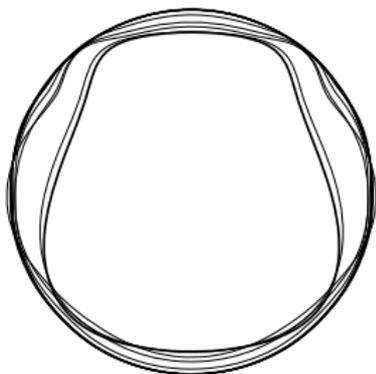
[7] V. Schulz, M. Siebenborn and K. W. Efficient PDE constrained optimization based on Steklov-Poincaré type metrics. *SIOPT*, 26(4):2800-2819, 2016.



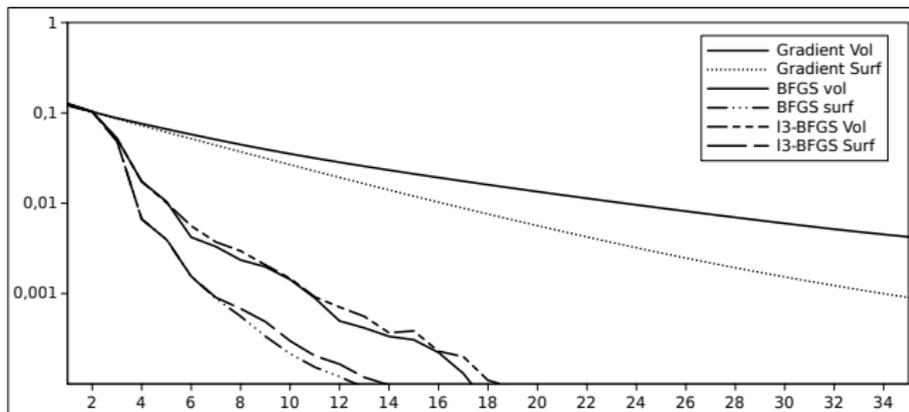
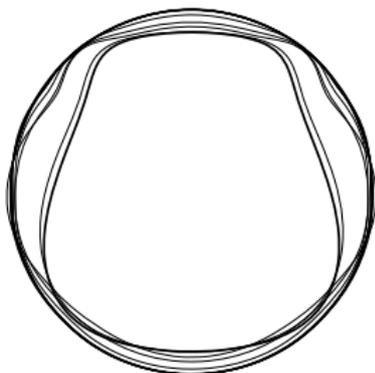
- Diffusion problem with $T = 20$, $k = \begin{cases} k_1 = 1 & \text{in } \Omega_1 \\ k_2 = 0.001 & \text{in } \Omega_2 \end{cases}$
- $A = 0.001$
- Data \bar{y} are generated from a solution of the state equation for the setting $\Omega_2 = \{x: \|x\|_2 < 0.5\}$



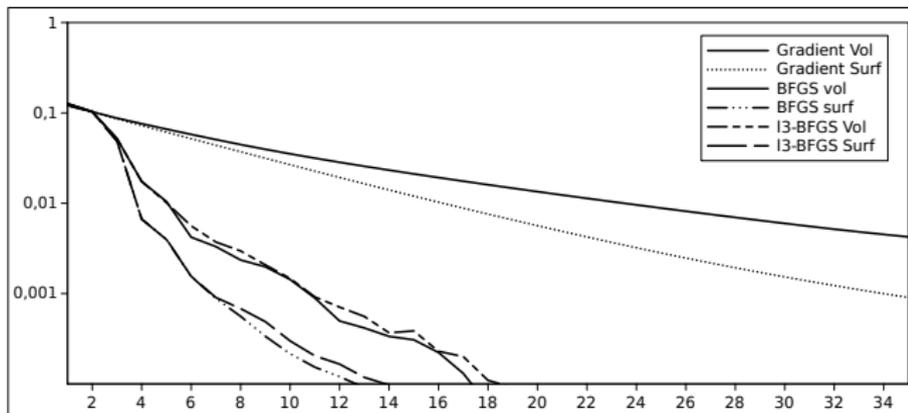
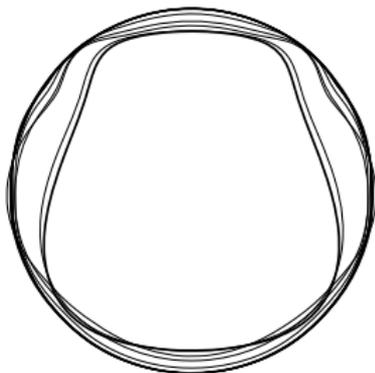
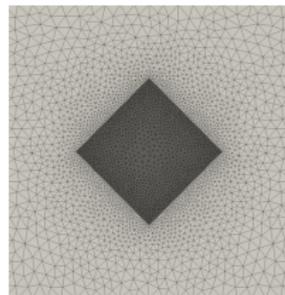
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$$\mathcal{B}^{1/2}(\Gamma_0, \mathbb{R}^d) := \mathcal{H}^{1/2}(\Gamma_0, \mathbb{R}^d) / \sim$$

- $\Gamma_0 \subset \mathbb{R}^d$ d -dimensional Lipschitz shape
(Definition: A d -dimensional *Lipschitz shape* is defined as the boundary $\Gamma_0 = \partial\mathcal{X}_0$ of a compact Lipschitz domain $\mathcal{X}_0 \subset \mathbb{R}^d$ with $\mathcal{X}_0 \neq \emptyset$.)
- $\mathcal{H}^{1/2}(\Gamma_0, \mathbb{R}^d)$
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Challenges

- Properties of $w \in H^{1/2}(\Gamma_0, \mathbb{R}^d)$ such that $w(\Gamma_0)$ Lipschitz shape
- Independence of the definition of $\mathcal{B}^{1/2}(\Gamma_0, \mathbb{R}^d)$ from the Lipschitz shape Γ_0
- Structure of $\mathcal{B}^{1/2}(\Gamma_0, \mathbb{R}^d)$



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- $\mathcal{H}^{1/2}(\Gamma_0, \mathbb{R}^d)$ is obviously a subset of $H^{1/2}(\Gamma_0, \mathbb{R}^d)$
- $H^{1/2}(\Gamma_0, \mathbb{R}^d)$ is a Banach space and, thus, a manifold
 \Rightarrow We can view $H^{1/2}(\Gamma_0, \mathbb{R}^d)$ with the corresponding diffeology

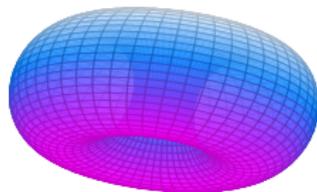
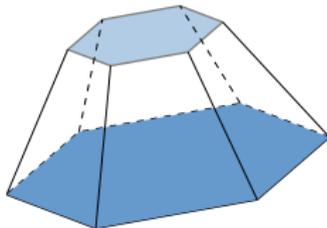
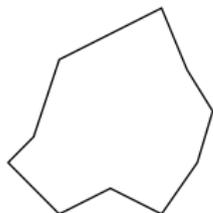
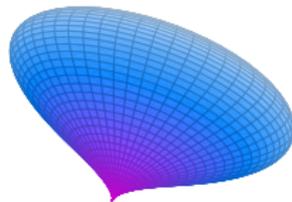
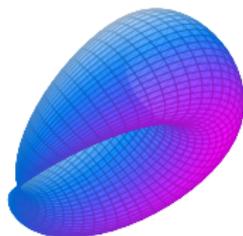
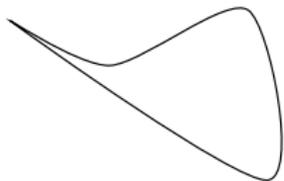
Results in [9]:

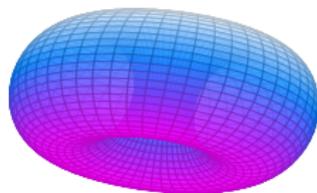
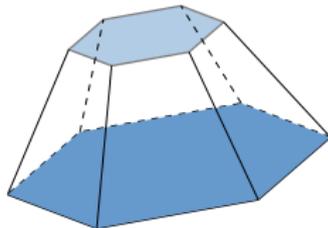
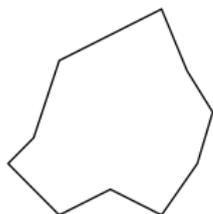
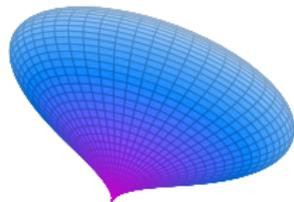
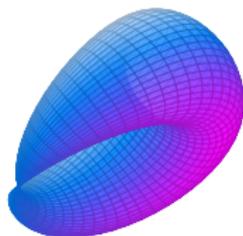
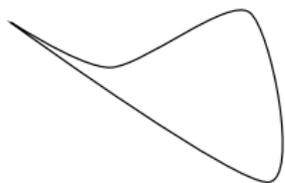
- Every subset of a diffeological space carries a natural *subset diffeology*, which is defined by the *pullback* of the ambient diffeology by the *natural inclusion*
- Every quotient of a diffeological space carries a natural *quotient diffeology* defined by the *pushforward* of the diffeology of the source space to the quotient by the *canonical projection*

\Rightarrow We can construct diffeologies on $\mathcal{H}^{1/2}(\Gamma_0, \mathbb{R}^d)$ and $\mathcal{B}^{1/2}(\Gamma_0, \mathbb{R}^d)$ □

[8] K. W. Suitable spaces for shape optimization, 2017. (arXiv:1702.07579)

[9] P. Iglesias-Zemmour. *Diffeology*. Volume 185, American Mathematical Society, 2013.





- No theory for shape optimization on diffeological spaces so far
- Diffeological structure suffices for many differential-geometric tools used in shape optimization techniques
- Riemannian structures can be used to measure shape distances and state convergence properties



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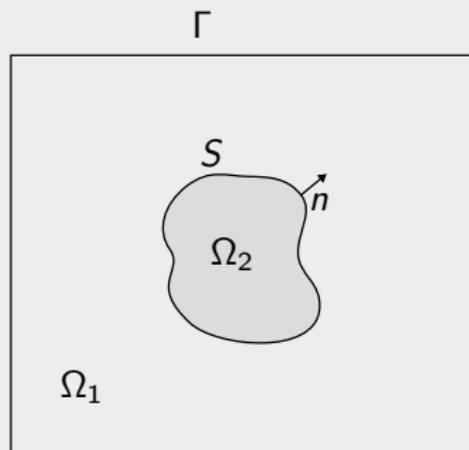


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Setting

- $\Omega \subset \mathbb{R}^2$ bounded Lipschitz domain
- Two subdomains $\Omega_1, \Omega_2 \subset \Omega$
- Fixed outer boundary
 $\partial\Omega = \Gamma_b \cup \Gamma_l \cup \Gamma_r \cup \Gamma_t$
- Variable boundary $S \in \mathcal{B}_e(S^1, \mathbb{R}^2)$
or $S \in \mathcal{B}^{1/2}(\Gamma_0, \mathbb{R}^2)$
- Outer normal vector n to Ω_2





$$\min_S J(y, S) = j(y, S) + j^{\text{reg}}(S) := \frac{1}{2} \int_{\Omega(S)} (y - \bar{y})^2 dx + \mu \int_S 1 ds$$

$$\text{s.t. } -\Delta y + \lambda = f \quad \text{in } \Omega$$

$$y \leq \psi \quad \text{in } \Omega$$

$$\lambda \geq 0 \quad \text{in } \Omega$$

$$\lambda(y - \psi) = 0 \quad \text{in } \Omega$$

$$y = 0 \quad \text{on } \Gamma$$

- Obstacle: $\psi \in H^4(\Omega)$ with $0 < \psi \leq M$ for $M > 0$

- Jumping coefficient: $f = \begin{cases} f_{\text{int}} = \text{const.} & \text{in } \Omega_{\text{int}} \\ f_{\text{out}} = \text{const.} & \text{in } \Omega_{\text{out}} \end{cases}$

- Transmission conditions: $\llbracket y \rrbracket = 0, \quad \left[\left[\frac{\partial y}{\partial n} \right] \right] = 0 \quad \text{on } S$



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$$\left. \begin{array}{l} \text{s.t. } -\Delta y + \lambda = f \quad \text{in } \Omega \\ y \leq \psi \quad \text{in } \Omega \\ \lambda \geq 0 \quad \text{in } \Omega \\ \lambda(y - \psi) = 0 \quad \text{in } \Omega \\ y = 0 \quad \text{on } \Gamma \end{array} \right\} \begin{array}{l} \text{Regularized version [10]: } \boxed{-\Delta y + \lambda_c = f \quad \text{in } \Omega} \\ \bullet \lambda_c = \max\{0, \bar{\lambda} + c(y - \psi)\}^2 \\ \bullet c > 0, 0 \geq \bar{\lambda} \in L^4(\Omega) \end{array}$$

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[10] M. Hintermüller and A. Laurain. Optimal shape design subject to elliptic variational inequalities. *SICON*, 49(3):1015-1047, 2011.



Idea: Adapt the primal-dual active set (PDAS) algorithm in [11] to our problem

Modified PDAS (mPDAS) algorithm

1. Choose y_0 , $k = 0$ and $\lambda_0 = 0$
2. $\mathcal{A}_{k+1} := \{x: [\lambda_k + c(y - \psi)](x) > 0\}$ and $\mathcal{I}_{k+1} := \Omega \setminus \mathcal{A}_{k+1}$
3. Compute $y_{k+1} \in H_0^1(\Omega)$ as solution of

$$a(y_{k+1}, v) + \left([\lambda_k + c(y_{k+1} - \psi)]^2, \mathcal{X}_{\mathcal{A}_{k+1}} v \right) = (f, v) \quad \forall v \in H_0^1(\Omega) \quad (*)$$

4. $\lambda_{k+1} := \begin{cases} 0 & \text{if } x \in \mathcal{I}_{k+1} \\ \lambda_k + c(y_{k+1} - \psi) & \text{if } x \in \mathcal{A}_{k+1} \end{cases}$
5. Stop or $k := k + 1$ and go to 2.

[11] K. Ito and K. Kunisch. Semi-smooth Newton methods for variational inequalities of the first kind. *ESAIM: Mathematical Modelling and Numerical Analysis*, 37(1):41-62, 2003.



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Step 3 in mPDAS algorithm

Compute $y_{k+1} \in H_0^1(\Omega)$ as solution of

$$a(y_{k+1}, v) + ([\lambda_k + c(y_{k+1} - \psi)]^2, \mathcal{X}_{A_{k+1}} v) = (f, v) \quad \forall v \in H_0^1(\Omega) \quad (*)$$

Problem: (*) is not linear

\leadsto **Idea:** Compute $\Delta y := y_{k+1} - y_k$ instead of y_{k+1} and use the linearization

$$(\lambda_k + c(y_k + \Delta y - \psi))^2 \doteq (\lambda_k + c(y_k - \psi))^2 + 2c\Delta y(\lambda_k + c(y_k - \psi))$$

Step 3 in linear mPDAS algorithm

a) Compute Δy as solution of

$$\begin{aligned} & a(\Delta y, v) + (2c\Delta y [\lambda_k + c(y_k - \psi)], \mathcal{X}_{A_{k+1}} v) \\ & = (f, v) - a(y_k, v) - ([\lambda_k + c(y_k - \psi)]^2, \mathcal{X}_{A_{k+1}} v) \quad \forall v \in H_0^1(\Omega) \end{aligned}$$

b) $y_{k+1} := y_k + \Delta y$

[12] B. Führ, V. Schulz and K. W. Shape optimization for interface identification with obstacle problems. Appears in: *Vietnam Journal of Mathematics*, 2018.

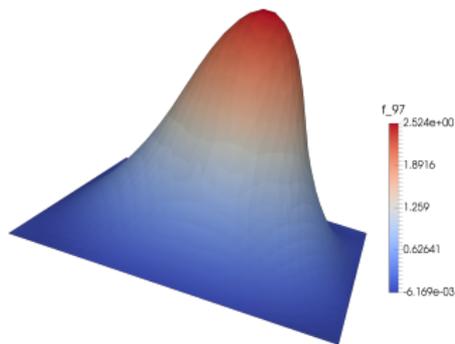


$$-\Delta y + \lambda_c = f \quad \text{in } \Omega$$

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- $0 \geq \bar{\lambda} \in L^4(\Omega)$, $c = 5$, $f = \begin{cases} f_1 = -10 & \text{in } \Omega_1 \\ f_2 = 100 & \text{in } \Omega_2 \end{cases}$

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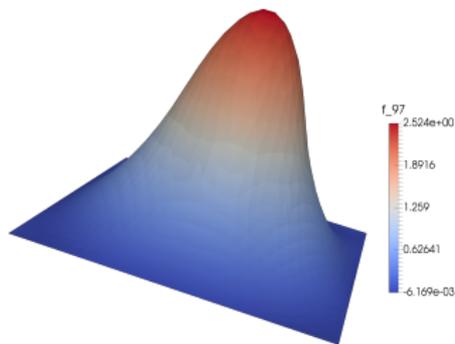
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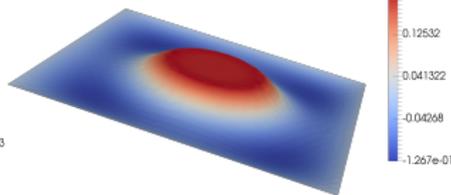
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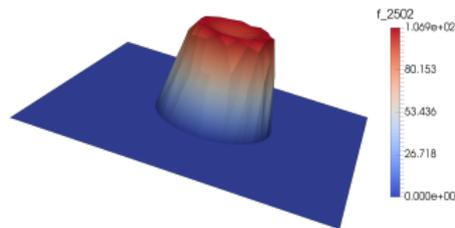
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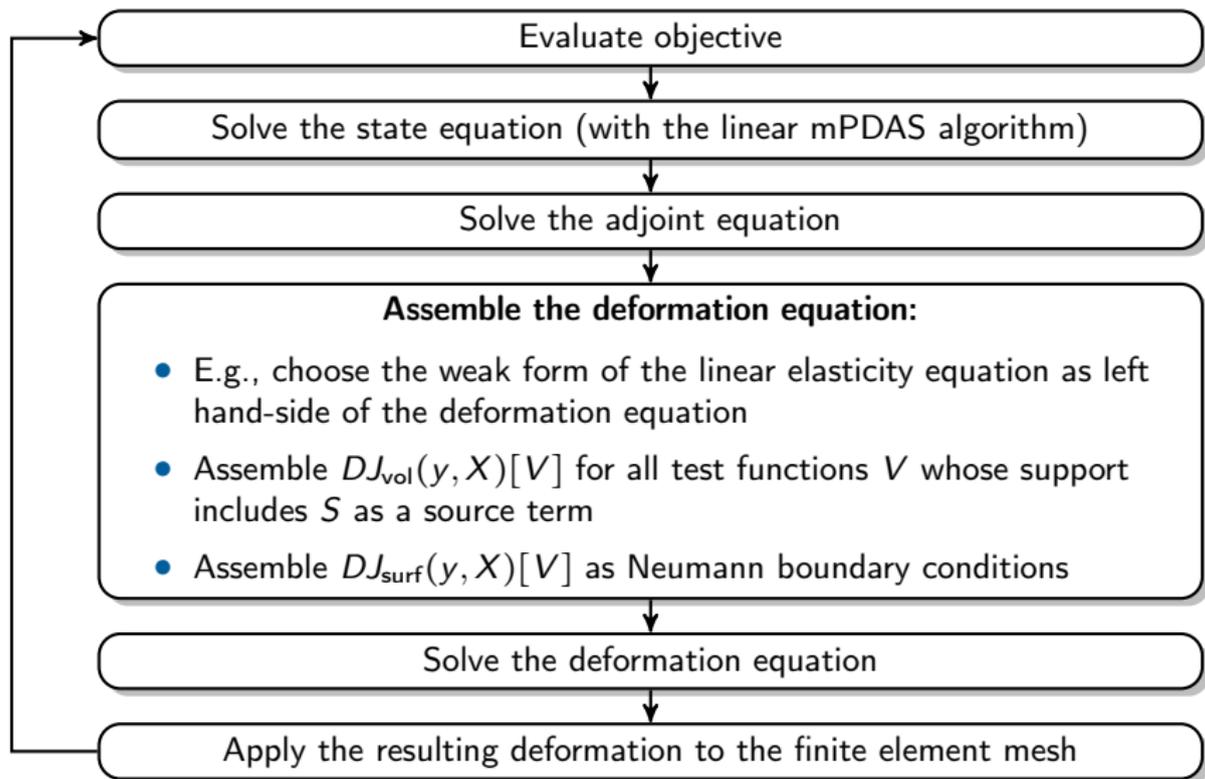
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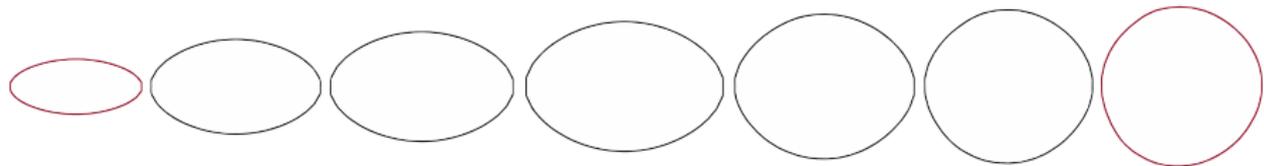


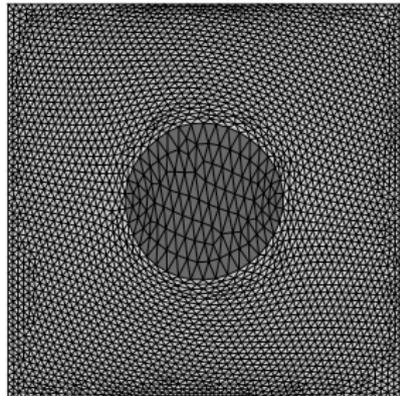
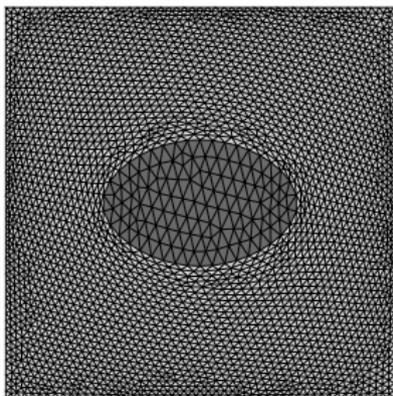
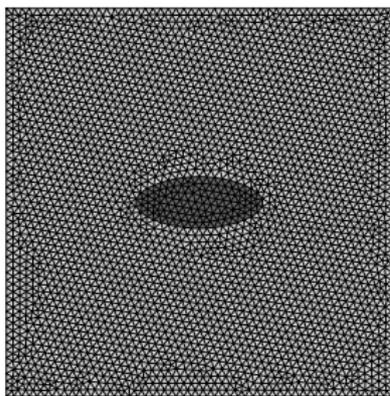
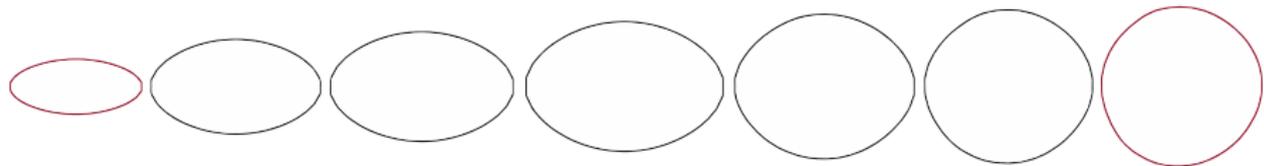
y with $\psi = 0.2$



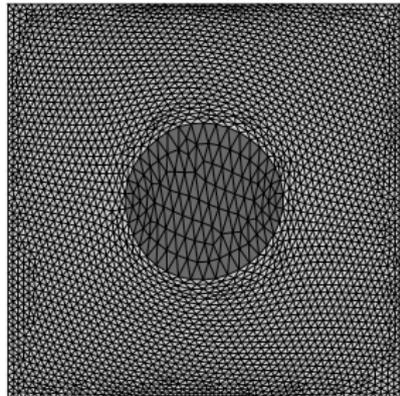
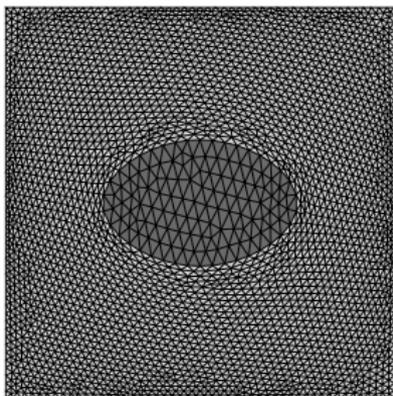
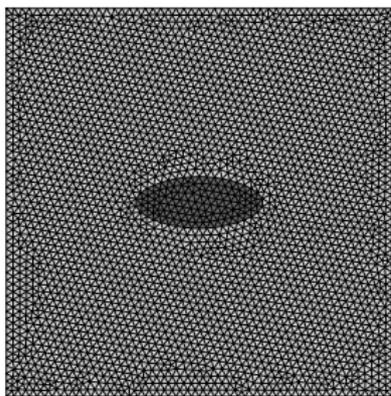
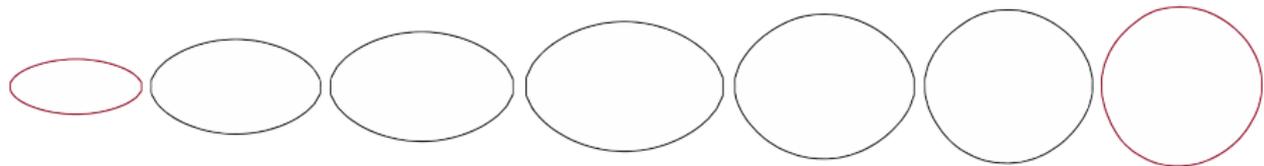
Corresponding λ_c



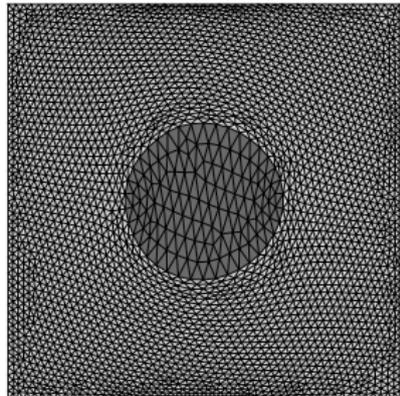
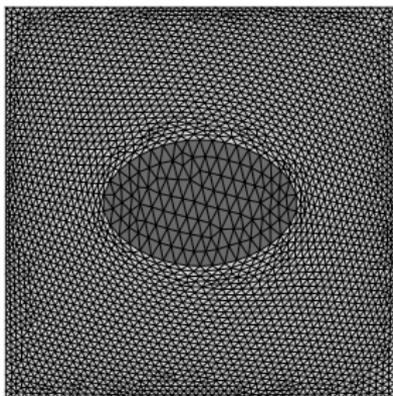
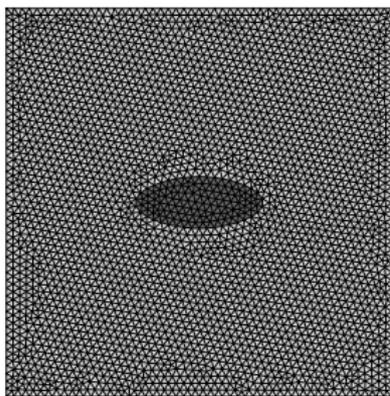
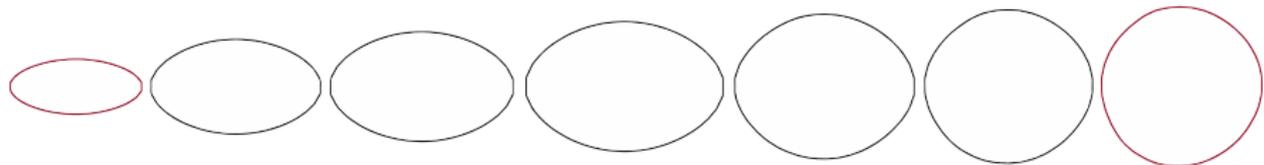




- Computations on unstructured grids with about 1 500 up to 6 000 triangles



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 \leadsto Choose locally adapted meshes or re-mesh after a few iterations
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- In the interior domain, elements are magnified by the mesh deformations
 \leadsto Choose locally adapted meshes or re-mesh after a few iterations
- Largest deformations at the beginning of the iteration process
- Algorithmic performance deteriorates if the obstacle problem is strongly binding
- More iterations for tighter obstacles, i.e., small values of ψ (494 iterations for $\psi = 0.5$ vs. 22 iterations for $\psi = 10$)



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Thank you for your attention!