Seminar for Applied Mathematics SAM

ETH Eidgenössische Technische Hochschule Zürich
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Shape optimization by pursuing diffeomorphisms

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Outline

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- Introduction to Shape Optimization.
- Shape Optimization by pursuing diffeomorphisms.
- Test on a benchmark problem.
- Conclusion and further issues.

Let $\mathcal{U}_{\mathrm{ad}}$ be a collection of admissible shapes.

A shape functional is

$$\mathcal{J} : \mathcal{U}_{\mathrm{ad}} \to \mathbb{R}\,, \quad \Omega \mapsto \mathcal{J}(\Omega)\,.$$

Goal: find

$$\Omega^* := \operatorname*{argmin}_{\Omega \in \mathcal{U}_{\mathrm{ad}}} \mathcal{J}(\Omega)\,.$$

EXAMPLES:

- Dido's Problem: maximal area for a fixed perimeter.
- $\mathcal{J}(\Omega) = \int_\Omega j(u)\,\mathrm{d}\mathbf{x}\,, \quad \mathcal{A}(u) = f \quad \text{in } \Omega\,.$

Space of Shapes

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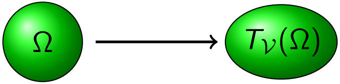
Transformation $T_{\mathcal{V}}$:



given by

$$T_{\mathcal{V}} := \mathcal{I} + \mathcal{V},$$

for a vectorfield $\mathcal{V} \in C^1(\mathbb{R}^N; \mathbb{R}^N)$.

Lemma 6.13[1]: $\|\mathcal{V}\|_{C^1} < 1 \Rightarrow T_{\mathcal{V}}$ is a diffeomorphism.

Family of admissible domains: shapes $\leftrightarrow$ vectorfields, that is,

$$\mathcal{U}_{\mathrm{ad}}(\Omega_0) := \{\, T_{\mathcal{V}}(\Omega_0); \|\mathcal{V}\|_{C^1} < 1\}\text{“}\subset\text{”}\, C^1(\mathbb{R}^N; \mathbb{R}^N).$$

[1] Allaire, *Conception optimale de structures*, 2007.

1^{st} derivative: Fréchet derivative of $\mathcal{V} \mapsto \mathcal{J}(T_{\mathcal{V}}(\Omega))$,

$$d\mathcal{J}(\Omega;\cdot) : \mathcal{V} \mapsto d\mathcal{J}(\Omega;\mathcal{V}) := \lim_{s \searrow 0} \frac{\mathcal{J}\left(T_{s \cdot \mathcal{V}}(\Omega)\right) - \mathcal{J}(\Omega)}{s}$$

is linear and continuous on $C^1(\mathbb{R}^N;\mathbb{R}^N)$.

2^{nd} derivative[2]: for $T_{\mathcal{V}} := \mathcal{I} + \mathcal{V} + \frac{1}{2}[D\mathcal{V}]\mathcal{V}$,

$$d^2\mathcal{J}(\Omega;\mathcal{V};\mathcal{W}) := \lim_{s \searrow 0} \frac{d\mathcal{J}\left(T_{s \cdot \mathcal{W}}(\Omega);\mathcal{V}\right)) - d\mathcal{J}(\Omega;\mathcal{V})}{s}$$

is linear and continuous on $C^2(\mathbb{R}^N;\mathbb{R}^N) \otimes C^2(\mathbb{R}^N;\mathbb{R}^N)$.

[2] Delfour-Zolésio, *Velocity method and Lagrangian formulation for the computation of the Shape Hessian*, SIAM J. Control Optim. 29 (1991).

Uniqueness

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Reference: Eppler, Harbrecht, and Schneider, *On convergence in elliptic shape optimization*, SIAM J. Control Optim. 46 (2007).

Abstract framework: $\mathcal{J} : X \to \mathbb{R}$, X Banach Space, with

- $d\mathcal{J}(\cdot) : X \to X^*$ and $d^2\mathcal{J}(\cdot) : X \to L(X, X^*)$ continuous,
- optimal point $r^* \in X$ satisfing $d\mathcal{J}(r^*) = 0\,(\in X^*)$.

Uniqueness in $\overline{B^X_{\delta_1}(r^*)}$ guaranteed by

- bicontinuity of $d^2\mathcal{J}(r)[\cdot,\cdot] \quad \forall\, r \in \overline{B^X_{\delta_2}(r^*)}$, $\delta_2 > \delta_1$,
- coercivity of $d^2\mathcal{J}(r^*)[\cdot,\cdot]$,
- technical assumption on $d^2\mathcal{J}(\cdot)$,

with respect to a Hilbert Space $H^s \supset X$.

Approximations, theory

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Reference: Eppler, Harbrecht, and Schneider, *On convergence in elliptic shape optimization*, SIAM J. Control Optim. 46 (2007).

Ritz method: Let $\{V_N\}_{N=0}^{\infty}$ be a sequence of conforming nested finite dimensional trial spaces with certain continuous embedding, inverse and approximation properties, and let

$$r_N* := \underset{r_N \in V_N \cap \overline{B^X_{\delta_1}(r^*)}}{\operatorname{argmin}} \mathcal{J}(r_N)\,.$$

Then r_N* exists, is unique, and satisfies [Thm. 3.9]

$$\|r_N^* - r^*\|_{H^s} \leq C \inf_{r_N \in V_N} \|r_n - r^*\|_{H^s}$$

for $N > N_0$.

Approximations, practice

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Ansatz:

$$r_N = \sum_{i=1}^{N} c_i \mathbf{B}_i, \quad V_N := \mathrm{span}\{\mathbf{B}_i\}_{i=1}^N .$$

Iterative schemes: $\mathbf{c}_{(n)} := (c_1^{(n)}, \dots, c_N^{(n)})^T$

- First order

$$\mathbf{c}^{(n+1)} = \mathbf{c}^{(n)} - \delta^{(n)} \{d\mathcal{J}(\Omega; \mathbf{B}_i)\}_{i=1}^N$$

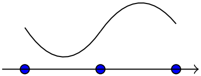
- Second order

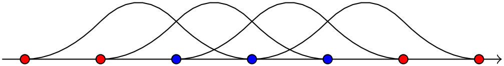
$$\{d^2\mathcal{J}(\Omega; \mathbf{B}_i; \mathbf{B}_j)\}_{i,j=1}^N \left(\mathbf{c}^{(n+1)} - \mathbf{c}^{(n)}\right) = -\{d\mathcal{J}(\Omega; \mathbf{B}_i)\}_{i=1}^N$$

- Quasi-Newton

$$\{\widetilde{d^2\mathcal{J}}(\Omega; \mathbf{B}_i; \mathbf{B}_j)\}_{i,j=1}^N \left(\mathbf{c}^{(n+1)} - \mathbf{c}^{(n)}\right) = -\{d\mathcal{J}(\Omega; \mathbf{B}_i)\}_{i=1}^N$$

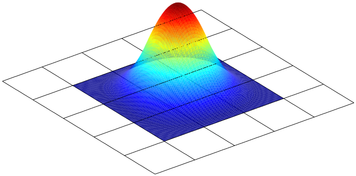
Trial Space

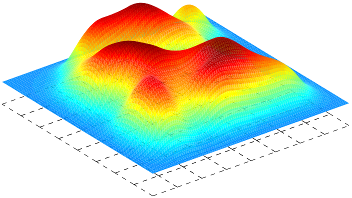




V_N = multivariate Spline space

Basis: tensorized uniform B-Splines of degree ≥ 2.





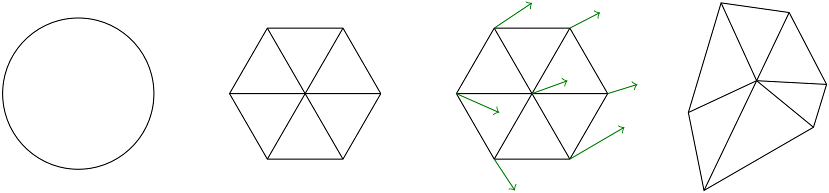
E.g.: $\mathcal{V}_N = \sum_{i=1}^{N} c_i^x \binom{\mathbf{B}_i}{0} + c_i^y \binom{0}{\mathbf{B}_i}$.

A Simple Numerical Approach

PDE CONSTRAINED PROBLEM:

$$\mathcal{J}(\Omega) = \int_\Omega j(u)\,\mathrm{d}\mathbf{x}\,, \mathcal{A}(u) = f \quad \text{in } \Omega \Rightarrow d\mathcal{J}(\Omega;\mathcal{V}) = d\mathcal{J}(\Omega, u;\mathcal{V})\,.$$

Mesh moving method:

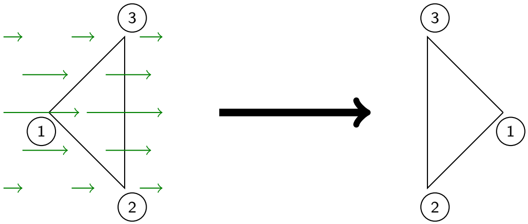


Ω $\quad$ Ω_h $\quad$ $\{d\mathcal{J}(\Omega_h, u_h; \mathbf{B}_i)\}_{i=1}^N$ $\quad$ $\Omega_h^{(1)}$

$$T_{\mathcal{V}_N} = \mathcal{I} - \sum_{i=1}^{N} d\mathcal{J}(\Omega_h, u_h; \mathbf{B}_i)\mathbf{B}_i$$

Issue

Mesh deteriorates, and there might be flipped triangles:

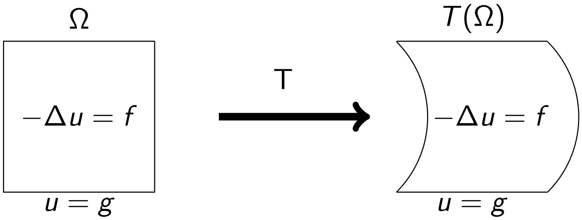


Know in: Shape Optimization, Computer Graphics, R-adaptivity, ...

Remedies in the literature are technical and based on heuristic.
Sometimes remeshing can not be avoided.

Pullbacks

Let T be a diffeomorphism.



Let $\hat{u} := T^*(u)$. Then $\hat{u}$ is the solution of

$$\begin{cases} -\operatorname{div}_\Omega \left(|\det DT| (DT)^{-1} (DT)^{-T} \, \mathbf{grad}_\Omega \, \hat{u} \right) = |\det DT| \, T^*(f) & \text{in } \Omega\,, \\ \hat{u} = T^*(g) & \text{on } \partial\Omega\,. \end{cases}$$

Then $u = \hat{u} \circ T^{-1}$.

Reformulation of Optimization Problem

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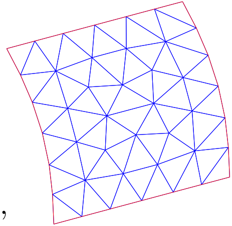
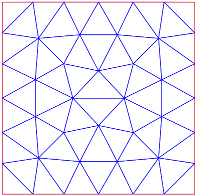
Instead of

$$\mathcal{J}(T) = \int_{T(\Omega)} j(u)\,\mathrm{d}T(\mathbf{x})$$



$$d\mathcal{J}(\Omega, u; \mathcal{V}), \quad \begin{cases} -\Delta u = f & \text{in } T(\Omega), \\ u = g & \text{on } T(\partial\Omega), \end{cases}$$



we consider

$$\mathcal{J}(T) = \int_{\Omega} j(\hat{u})|\det DT|\mathrm{d}\mathbf{x}, \quad d\mathcal{J}(\Omega, \hat{u}; \mathcal{V}),$$

$$\begin{cases} -\operatorname{div}_{\Omega}(\cdots \mathbf{grad}_{\Omega}\,\hat{u}) = |\det DT|\, T^*(f) & \text{in } \Omega, \\ \hat{u} = T^*(g) & \text{on } \partial\Omega. \end{cases}$$

Algorithm

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Initialization ($T = \mathcal{I}$)

Repeat until $\mathcal{J}(T(\Omega))$ small enough

- solve state problem (depends on T),
- evaluate $d\mathcal{J}(T(\Omega), \mathbf{B}_i)$ for all $i = 1, \ldots, N$,
- find optimal direction $\mathcal{V} = \sum_{i=1}^{N} c_i^{\mathrm{opt}} \mathbf{B}_i$,
- update T.

Algorithm

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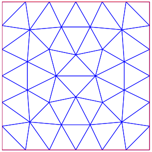
Initialization ($T = \mathcal{I}$)



Repeat until $\mathcal{J}(T(\Omega))$ small enough

- **solve state problem (depends on T),**
- evaluate $d\mathcal{J}(T(\Omega), \mathbf{B}_i)$ for all $i = 1, \ldots, N$,
- find optimal direction $\mathcal{V} = \sum_{i=1}^{N} c_i^{\mathrm{opt}} \mathbf{B}_i$,
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Algorithm

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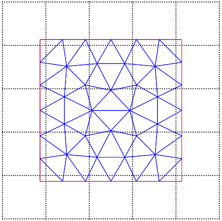

Initialization ($T = \mathcal{I}$)

Repeat until $\mathcal{J}(T(\Omega))$ small enough

- solve state problem (depends on T),
- **evaluate** $d\mathcal{J}(T(\Omega), \mathbf{B}_i)$ **for all** $i = 1, \ldots, N$**,**
- **find optimal direction** $\mathcal{V} = \sum_{i=1}^{N} c_i^{\mathrm{opt}} \mathbf{B}_i$**,**
- update T.

Algorithm

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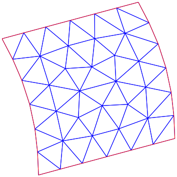
Initialization ($T = \mathcal{I}$)



Repeat until $\mathcal{J}(T(\Omega))$ small enough

- solve state problem (depends on T),
- evaluate $d\mathcal{J}(T(\Omega), \mathbf{B}_i)$ for all $i = 1, \dots, N$,
- find optimal direction $\mathcal{V} = \sum_{i=1}^{N} c_i^{\mathrm{opt}} \mathbf{B}_i$,
- **update T.**

Algorithm

Initialization ($T = \mathcal{I}$)

Repeat until $\mathcal{J}(T(\Omega))$ small enough

- solve state problem (depends on T),
- evaluate $d\mathcal{J}(T(\Omega), \mathbf{B}_i)$ for all $i = 1, \dots, N$,
- find optimal direction $\mathcal{V} = \sum_{i=1}^{N} c_i^{\mathrm{opt}} \mathbf{B}_i$,
- update T.

Enjoy the new design.

Hadamard-Zolésio Theorem

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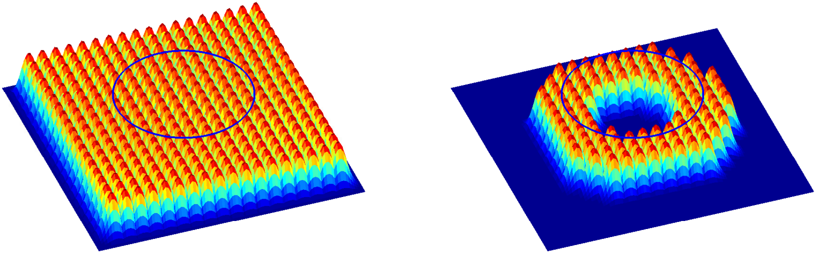
If Ω is smooth, there is a scalar distribution $g(\Omega)$ in $C^1(\partial\Omega)'$ so that

$$d\mathcal{J}(\Omega;\mathcal{V}) = \langle g(\Omega), \gamma_\Gamma \mathcal{V}\cdot\mathbf{n}\rangle_{C^1(\partial\Omega)'\times C^1(\partial\Omega)}.$$

Idea: drop B-splines whose support does not intersect $T(\partial\Omega)$.



Benchmark Problem

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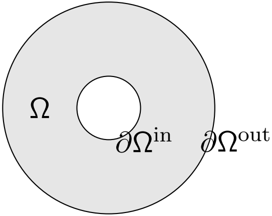
Exterior Bernoulli problem: find $\partial\Omega^{\mathrm{out}}$ so that



$$\begin{cases} -\Delta u &= 0 \quad \text{in } \Omega\,, \\ u &= 0 \quad \text{on } \partial\Omega^{\mathrm{out}}\,, \\ -\frac{\partial u}{\partial \mathbf{n}} &= g \quad \text{on } \partial\Omega^{\mathrm{out}} \\ u &= 1 \quad \text{on } \partial\Omega^{\mathrm{in}}\,. \end{cases}$$

Shape Optimization: find $\partial\Omega^{\mathrm{out}}$ that minimizes

$$\mathcal{J}(\Omega) = \int_\Omega \|\nabla u\|^2 + g^2 \mathrm{d}\mathbf{x}\,, \quad \text{st} \quad \begin{cases} -\Delta u &= 0 \quad \text{in } \Omega\,, \\ u &= 0 \quad \text{on } \partial\Omega^{\mathrm{out}}\,, \\ u &= 1 \quad \text{on } \partial\Omega^{\mathrm{in}}\,. \end{cases}$$

Well-posedness: stable unique minimum for constant $g > 0$ if optimal $\partial\Omega^{\mathrm{out}}$ is convex from inside.

- Discretization by piecewise linear Lagrangian finite elements on quasi-uniform triangular meshes (uniform refinement).

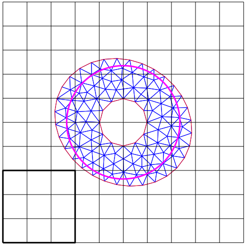
Accuracy of Shape Gradient[3]:

$$|d\mathcal{J}(\Omega, u; \mathcal{V}) - d\mathcal{J}(\Omega, u_h; \mathcal{V})^{\mathrm{Vol}}| \leq C(\Omega, g)\|\mathcal{V}\|_{W^{2,4}}\mathcal{O}(h^2)\,.$$

- Integrals in the domain computed by a 7-point quadrature rule in each triangle.
- The boundary of the computational domains is approximated by a polygon.

[3] Hiptmair, Paganini, and Sargheini, *Comparison of approximate shape gradients*, BIT (accepted).

1^{st} Run

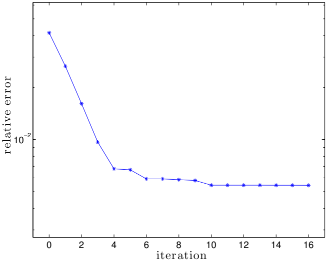


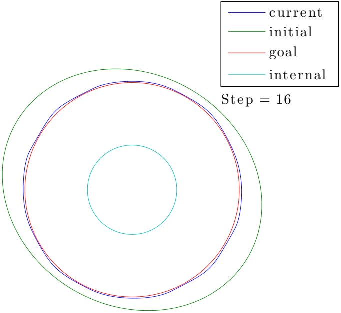
121 Vertices,

198 Elements,

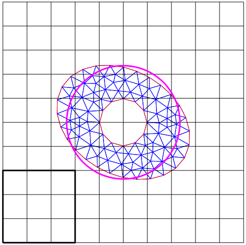
319 Edges,

$2 \cdot 46$ active B-splines.





2^{nd} Run

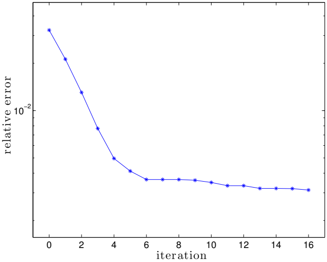


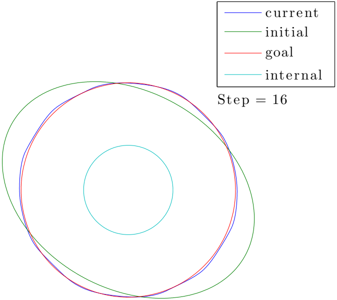
98 Vertices,

156 Elements,

254 Edges,

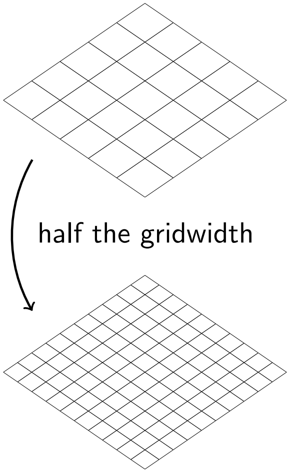
$2 \cdot 44$ active B-splines.

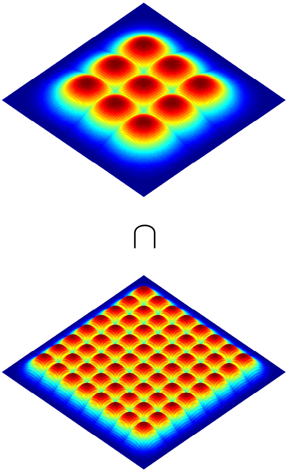




Refinement in Space of Shapes

Hierarchical Splines[4]:





[4] Höllig and Hörner, *Approximation and Modeling with B-Splines*, 2013.

1^{st} Run with SoS Refinement

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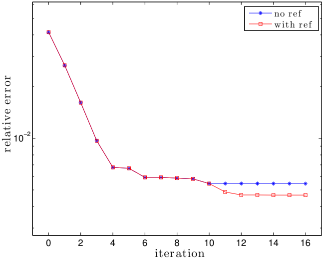
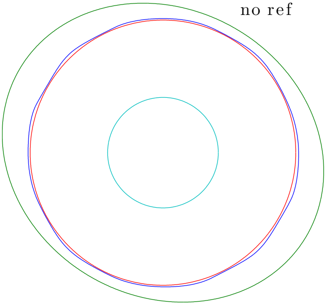
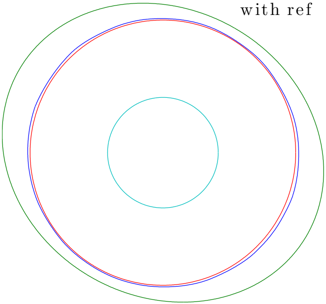
SoS refinement at 10^{th} step:

$2 \cdot 46 \to 2 \cdot 130$ B-splines.







Mesh Refinement: quadratic

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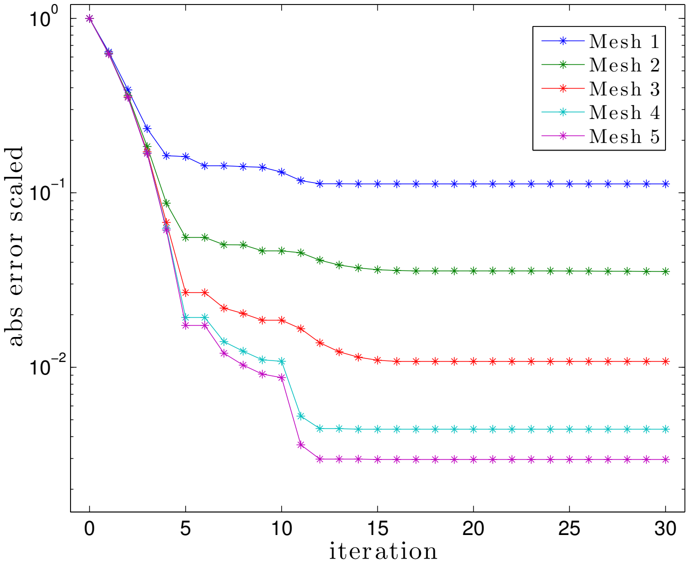

Mesh Refinement: cubic

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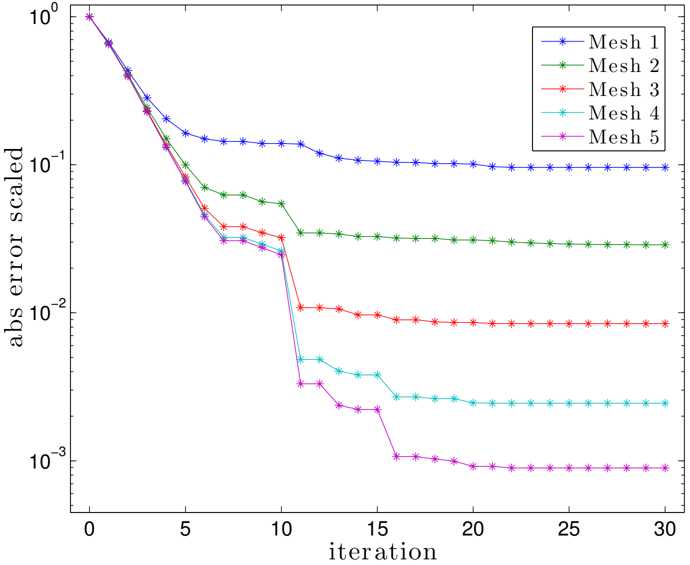

Mesh Refinement: cubic

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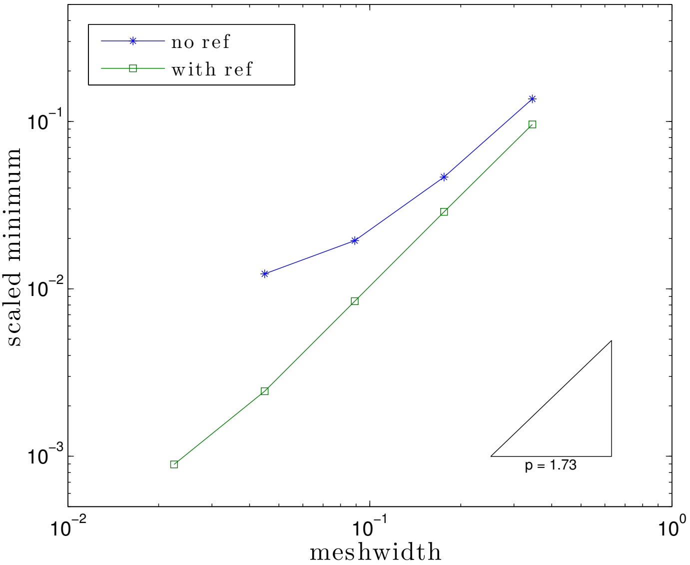
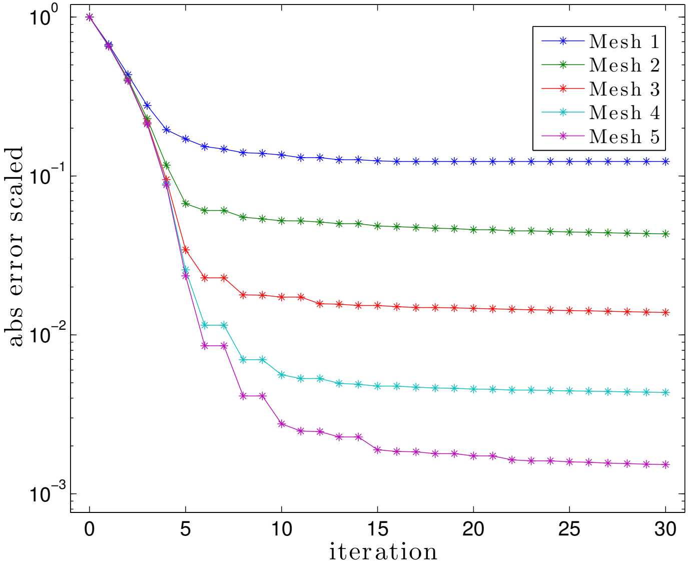
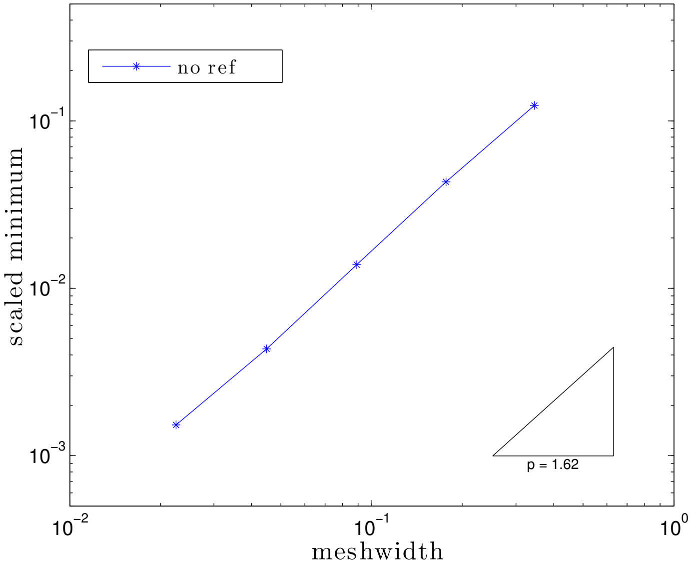


Mesh Refinement: degree4



Mesh Refinement: degree4



Shape optimisation by pursuing diffeomorphisms:

$$\Omega^*_{N,h} = \underset{\|\sum_{i=1}^N c_i \mathbf{B}_i\|_{C^1} \leq 1-\varepsilon}{\operatorname{argmin}} \mathcal{J}\left(\Omega_h + \sum_{i=1}^N c_i \mathbf{B}_i(\Omega_h)\right) .$$

Pros:

- accuracy,
- reliability (no flipping triangles),
- versatility,

Cons:

- complexity (numerical integration).

Summary

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Shape optimisation by pursuing diffeomorphisms:

$$\Omega^*_{N,h} = \operatorname*{argmin}_{\|\sum_{i=1}^N c_i \mathbf{B}_i\|_{C^1} \leq 1-\varepsilon} \mathcal{J}\left(\Omega_h + \sum_{i=1}^{N} c_i \mathbf{B}_i(\Omega_h)\right) .$$

Pros:

- accuracy,
- reliability (no flipping triangles),
- versatility,

Cons:

- complexity (numerical integration).

Next:

- optimization algorithm,
- inverse problems,
- FEM-BEM coupling,
- C++ library.

Thanks for your attention!

Trial Space Update

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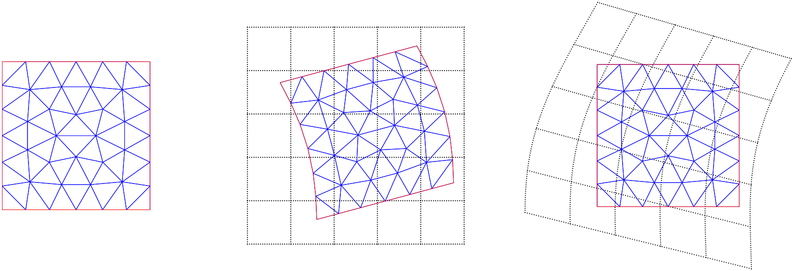
Heuristic idea: $V_N^{(1)}$ depends on transformation $T^{(1)}$.



Pros: $V_N^{(i)}$ adapted to $T^{(i)}(\Omega)$.

Cons: infinite dimensional problem $\Rightarrow$ complexity (see below).

Complexity Issue and Remedy

After k iterations

$$T^{(k)} = (\mathcal{I} + \sum_{i=1}^{N} c_i^{(k)} \mathbf{B}_i) \circ \cdots \circ (\mathcal{I} + \sum_{i=1}^{N} c_i^{(1)} \mathbf{B}_i) \,.$$

Issue: exponential complexity in k for solving the state problem!

Remedy: projection onto $V_N^{(0)}$

$$\widetilde{T}^{(k)} := (\mathcal{I} + \sum_{i=1}^{N} \tilde{c}_i^{(k)} \mathbf{B}_i) \approx (\mathcal{I} + \sum_{i=1}^{N} c_i^{(k)} \mathbf{B}_i) \circ \widetilde{T}^{(k-1)} \,.$$

Drawback: "worse" descent direction.

Algorithm

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Initialization ($T = \mathcal{I}$)

Repeat until $\mathcal{J}(T(\Omega))$ small enough

- solve state problem (depends on T),
- evaluate $d\mathcal{J}(T(\Omega), \mathbf{B}_i)$ $\forall i$ st $\mathrm{supp}(\mathbf{B}_i) \cap T(\partial\Omega) \neq \emptyset$,
- find optimal direction $\mathcal{V} = \sum_{i=1}^{N} c_i^{\mathrm{opt}} \mathbf{B}_i$,
- project $T \approx (\mathcal{I} + \mathcal{V}) \circ T$.

Enjoy the new design.