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Error-Controlled Shape Optimization by Constrained First-Order System Least ~~Squares~~ Mean

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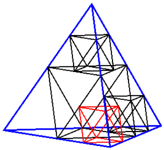

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Overview

Shape Optimality As L^p Best Approximation

Structure of the Least Mean Approximation Problem

Discretization by Finite Elements

Shape Gradient Iteration

Error Analysis

GS: *Shape Optimization by Constrained First-Order System Least Mean Approximation* arXiv: 2309.13595

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Shape Optimality As L^p Best Approximation

$$J(\Omega) = \int_\Omega j(u_\Omega)\, dx \longrightarrow \min!$$

subject to PDE constraint:

$$u_\Omega \in H_0^1(\Omega) : \quad (\nabla u_\Omega, \nabla v)_{L^2(\Omega)} = (f, v)_{L^2(\Omega)} \text{ for all } v \in H_0^1(\Omega)$$

Shape derivative (under certain assumptions on Ω, f and $j(\,\cdot\,)$): [1]

$$J'(\Omega)[\chi] = \left(\left((\operatorname{div} \chi)\, I - \left(\nabla \chi + (\nabla \chi)^T \right) \right) \nabla u_\Omega, \nabla y_\Omega \right) \\ + (f\, \nabla y_\Omega, \chi) + (j(u_\Omega), \operatorname{div} \chi)\ ,$$

$y_\Omega \in H_0^1(\Omega)$: solution of the adjoint problem

$$(\nabla y_\Omega, \nabla z) = -(j'(u_\Omega), z) \text{ for all } z \in H_0^1(\Omega)$$

[1] G. Allaire, C. Dapogny, F. Jouve: Handbook Numer. Anal. **22** (2021)

Shape Optimality As L^p Best Approximation

Shape derivative in volume expression:

$$J'(\Omega)[\chi] = \Big(\Big((\operatorname{div} \chi)\, I - \Big(\nabla\chi + (\nabla\chi)^T \Big) \Big) \nabla u_\Omega, \nabla y_\Omega \Big) + (f\, \nabla y_\Omega, \chi) + (j(u_\Omega), \operatorname{div} \chi) \ ,$$

studied and used a lot recently, e.g. [1] [2] [3] [4] [5] [6] [7]

Advantages (compared to surface expression):
Less demands on regularity, less danger of mesh deterioration

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[1] K. Deckelnick, P. J. Herbert, M. Hinze: ESAIM Control Optim. Calc. Var. **28** (2022)
[2] S. Bartels, G. Wachsmuth: SIAM J. Sci. Comput. **42** (2020)
[3] T. Etling, R. Herzog, E. Loayza, G. Wachsmuth: SIAM J. Sci. Comput. **42** (2020)
[4] M. Eigel, K. Sturm: Optim. Methods Softw. **33** (2018)
[5] V. Schulz, M. Siebenborn, K. Welker: SIAM J. Optim. **26** (2016)
[6] A. Laurain, K. Sturm: ESAIM Math. Model. Numer. Anal. **50** (2016)
[7] R. Hiptmair, A. Paganini, S. Sargheini: BIT **55** (2015)

Shape Optimality As L^p Best Approximation

Shape derivative in volume expression:

$$J'(\Omega)[\chi] = \Big(\Big((\mathrm{div}\,\chi)\, I - \Big(\nabla\chi + (\nabla\chi)^T\Big)\Big)\, \nabla u_\Omega, \nabla y_\Omega\Big) + (f\,\nabla y_\Omega, \chi) + (j(u_\Omega), \mathrm{div}\,\chi)\ ,$$

Tensor representation:[1]

$$J'(\Omega)[\chi] = (K(u_\Omega, y_\Omega), \nabla\chi) + (f \nabla y_\Omega, \chi) + (j(u_\Omega), \mathrm{div}\,\chi)$$
$$\text{with } K(u_\Omega, y_\Omega) = (\nabla u_\Omega \cdot \nabla y_\Omega)\, I - \nabla y_\Omega \otimes \nabla u_\Omega - \nabla u_\Omega \otimes \nabla y_\Omega$$

Follows basically from (for $x, y \in \mathbb{R}^d, A \in \mathbb{R}^{d\times d}$):

$$y \cdot (Ax) = \mathrm{tr}(y^T A x) = \mathrm{tr}(x y^T A) = A : (y \otimes x)$$

Tensor representation available for many shape optimiz. problems[2]

[1] A. Laurain, K. Sturm: ESAIM Math. Model. Numer. Anal. **50** (2016)

[2] A. Laurain: J. Math. Pures Appl. **134** (2020)

Shape Optimality As L^p Best Approximation

Stationarity: Find

$\Omega \in \mathcal{S} = \{\Omega = (\mathrm{id} + \theta)\Omega_0 : \theta, (\mathrm{id} + \theta)^{-1} - \mathrm{id} \in W^{1,\infty}(\Omega; \mathbb{R}^d)\}$ s.t.

$$J'(\Omega)[\chi] = (K(u_\Omega, y_\Omega), \nabla\chi) + (f \nabla y_\Omega, \chi) + (j(u_\Omega), \operatorname{div} \chi) = 0$$

for all $\chi \in W^{1,\infty}(\Omega; \mathbb{R}^d)$

$$\Longleftrightarrow$$

$$\begin{aligned} (\operatorname{div} K(u_\Omega, y_\Omega), \chi) &= (f \, \nabla y_\Omega, \chi) - (j(u_\Omega), \operatorname{div} \chi) \quad && \forall \chi \\ \langle K(u_\Omega, y_\Omega) \cdot n, \, \chi|_{\partial\Omega} \rangle_{\partial\Omega} &= 0 && \forall \, \chi|_{\partial\Omega} \end{aligned}$$

$$\Longleftrightarrow$$

$\exists S \in \Sigma^1 := \{ T \in L^1(\Omega; \mathbb{R}^{d \times d}) : \operatorname{div} T \in L^1(\Omega; \mathbb{R}^d)\}$ s.t.

$$\begin{aligned} (\operatorname{div} S, \chi) &= (f \, \nabla y_\Omega, \chi) + (j(u_\Omega), \operatorname{div} \chi) \quad && \forall \chi \\ \langle S \cdot n, \, \chi|_{\partial\Omega} \rangle &= 0 && \forall \, \chi|_{\partial\Omega} \\ S - K(u_\Omega, y_\Omega) &= 0 \end{aligned}$$

Shape Optimality As L^p Best Approximation

$p > 1$: $S \in \Sigma^p := \{ T \in L^p(\Omega; \mathbb{R}^{d\times d}) : \mathrm{div}\, T \in L^p(\Omega; \mathbb{R}^d)\}$ s.t.

$$\begin{aligned} (\mathrm{div}\, S, \chi) &= (f\, \nabla y_\Omega, \chi) + (j(u_\Omega), \mathrm{div}\, \chi) \; \forall \chi \\ \langle S \cdot n, \chi|_{\partial\Omega} \rangle &= 0 \qquad \forall\, \chi|_{\partial\Omega} \\ S - K(u_\Omega, y_\Omega) &= 0 \end{aligned}$$

$$\eta_p(\Omega) = \inf\{\| T - K(u_\Omega, y_\Omega)\|_{L^p(\Omega)} : T \in \Sigma^p \text{ satisfying}$$
$$(\mathrm{div}\, T, \chi) = (f\, \nabla y_\Omega, \chi) + (j(u_\Omega), \mathrm{div}\, \chi) \; \forall \chi \in W^{1,p^*}(\Omega; \mathbb{R}^d)$$
$$\langle T \cdot n, \chi|_{\partial\Omega} \rangle = 0 \; \forall\, \chi|_{\partial\Omega} \} \qquad \left(\tfrac{1}{p} + \tfrac{1}{p^*} = 1 \,,\; p \in (1,\infty) \right)$$

In words: $\eta_p(\Omega)$ is the $L^p(\Omega; \mathbb{R}^{d\times d})$-mean approximation to the Laurain-Sturm shape tensor $K(u_\Omega, y_\Omega)$ out of the affine space

$$\Sigma^p_{\mathrm{adm}} = \{ T \in \Sigma^p : (\mathrm{div}\, T, \chi) = (f\, \nabla y_\Omega, \chi) + (j(u_\Omega), \mathrm{div}\, \chi) \; \forall \chi \}$$

Shape Optimality As L^p Best Approximation

Wellposedness ($p \in (1,2]$): Assume the compatibility condition $(f\,\nabla y_\Omega, e) = 0\,\forall\, e \in \mathbb{R}^d$ to hold, then there is a unique $S \in \Sigma^p$ s.t.

$$\eta_p(\Omega) = \|S - K(u_\Omega, y_\Omega)\|_{L^p(\Omega)}$$

Existence:
$\Sigma^p_{\mathrm{adm}} \neq \emptyset$ since it contains $\bar{S} = \nabla\psi$ where $\psi \in H^1(\Omega;\mathbb{R}^d)$ solves

$$(\nabla\psi, \nabla\chi) = -(f\,\nabla y_\Omega, \chi) - (j(u_\Omega), \mathrm{div}\,\chi)\forall\chi \in H^1(\Omega;\mathbb{R}^d)$$

Uniqueness: $L^p(\Omega;\mathbb{R}^{d\times d})$ is strictly normed for $1 < p < \infty$

Geometric meaning of compatibility condition: 0 known barycenter

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$$S \in \Sigma^{p,0} := \{ T \in \Sigma^p : \langle T \cdot n, \chi|_{\partial\Omega} \rangle = 0 \text{ for all } \chi \in W^{1,p^*}(\Omega; \mathbb{R}^d) \}$$

Optimality system:

$$(|S - K(u_\Omega, y_\Omega)|^{p-2}(S - K(u_\Omega, y_\Omega)), T) + (\text{div } T, \theta) = 0 \, \forall T \in \Sigma^{p,0}$$

$$(\text{div } S, \chi) = (f \, \nabla y_\Omega, \chi) + (j(u_\Omega), \text{div } \chi) \qquad \forall \chi \in W^{1,p^*}$$

Lagrange multiplier by Helmholtz decomposition in $L^{p^*}(\Omega; \mathbb{R}^{d \times d})$:[1]

$$|S - K(u_\Omega, y_\Omega)|^{p-2}(S - K(u_\Omega, y_\Omega)) = \nabla \theta$$

The above optimality system has a solution

$$(S, \theta) \in \Sigma^{p,0} \times W^{1,p^*}(\Omega; \mathbb{R}^d)$$

which is unique up to additive constant vectors for θ

[1] D. Fujiwara, H. Morimoto: J. Fac. Sci. Univ. Tokyo Sect. IA Math. **24** (1977)

Structure of the Least Mean Approximation Problem

Main Theorem:

Let $p \in (1,\infty)$ and assume that $K(u_\Omega, y_\Omega) \in L^p(\Omega; \mathbb{R}^{d\times d})$, $f \in L^\infty(\Omega)$, $j(u_\Omega) \in L^2(\Omega)$ and that the compatibility condition $(f\,\nabla y_\Omega, e) = 0$ for all constant $e \in \mathbb{R}^d$ hold.
Then, the Lagrange multiplier $\theta \in W^{1,p^*}(\Omega; \mathbb{R}^d)$ satisfies

$$-\frac{J'(\Omega)[\theta]}{\|\nabla\theta\|_{L^{p^*}(\Omega;\mathbb{R}^{d\times d})}} = \sup_{\chi \in W^{1,p^*}(\Omega;\mathbb{R}^d)} \frac{J'(\Omega)[\chi]}{\|\nabla\chi\|_{L^{p^*}(\Omega;\mathbb{R}^{d\times d})}} = \eta_p(\Omega)$$

This provides an alternative route to W^{1,p^*} shape gradients[2] [3]

Sketch of Proof:

$$\begin{aligned} J'(\Omega)[\chi] &= (K(u_\Omega, y_\Omega), \nabla\chi) + (j(u_\Omega), \operatorname{div}\chi) + (f\,\nabla y_\Omega, \chi) \\ &= (K(u_\Omega, y_\Omega), \nabla\chi) + (\operatorname{div} S, \chi) \\ &= (K(u_\Omega, y_\Omega) - S, \nabla\chi) + \langle S\cdot n, \chi\rangle = -(S - K(u_\Omega, y_\Omega), \nabla\chi) \end{aligned}$$

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[2] K. Deckelnick, P. J. Herbert, M. Hinze: ESAIM Control Optim. Calc. Var. **28** (2022)

[3] K. Deckelnick, P. J. Herbert, M. Hinze: arXiv:2301.08690 (2023)

Structure of the Least Mean Approximation Problem

Sketch of Proof (continued):

Insert Lagrange multipl. θ into $J'(\Omega)[\chi] = -(S - K(u_\Omega, y_\Omega), \nabla\chi)$:

$$\begin{aligned} J'(\Omega)[\theta] &= -(S - K(u_\Omega, y_\Omega), |S - K(u_\Omega, y_\Omega)|^{p-2}(S - K(u_\Omega, y_\Omega))) \\ &= -\|S - K(u_\Omega, y_\Omega)\|^p_{L^p(\Omega;\mathbb{R}^{d\times d})} \end{aligned}$$

Observe that $\|\nabla\theta\|_{L^{p^*}(\Omega;\mathbb{R}^d)} = \|S - K(u_\Omega, y_\Omega)\|^{p-1}_{L^p(\Omega;\mathbb{R}^{d\times d})}$

Combine this to

$$\begin{aligned} &-\frac{J'(\Omega)[\theta]}{\|\nabla\theta\|_{L^{p^*}(\Omega;\mathbb{R}^{d\times d})}} = \|S - K(u_\Omega, y_\Omega)\|_{L^p(\Omega;\mathbb{R}^{d\times d})} \\ &\quad\geq \sup_{\chi\in W^{1,p^*}(\Omega;\mathbb{R}^d)} \frac{(S - K(u_\Omega, y_\Omega), \nabla\chi)}{\|\nabla\chi\|_{L^{p^*}(\Omega;\mathbb{R}^{d\times d})}} \\ &\quad= \sup_{\chi\in W^{1,p^*}(\Omega;\mathbb{R}^d)} \frac{J'(\Omega)[\chi]}{\|\nabla\chi\|_{L^{p^*}(\Omega;\mathbb{R}^{d\times d})}} \geq -\frac{J'(\Omega)[\theta]}{\|\nabla\theta\|_{L^{p^*}(\Omega;\mathbb{R}^{d\times d})}} \qquad \Box \end{aligned}$$

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Discretization by Finite Elements

Triangulation $\mathcal{T}_h$: Polygonal approximation Ω_h to Ω
Approximation space Σ_h^p for S: (Lowest-order) Raviart-Thomas
Approximation space Θ_h^p for θ: Piecewise constant functions

$$\eta_{p,h}(\Omega_h) = \|S_h - K(u_{\Omega,h}, y_{\Omega,h})\|_{L^p(\Omega_h)}$$

Find $S_h \in \Sigma_h^p$, $\theta_h \in \Theta_h$, $\theta_{b,h} \in \Theta_{b,h}$ such that

$$\begin{aligned}(|S_h - K(u_{\Omega,h}, y_{\Omega,h})|^{p-2}(S_h - K(u_{\Omega,h}, y_{\Omega,h})), T_h) + (\operatorname{div} T_h, \theta_h)& \\ + \langle T_h \cdot n, \theta_{b,h}\rangle &= 0 \\ (\operatorname{div} S_h, \chi_h) - (f\, \nabla y_{\Omega,h}, \chi_h) + (\nabla j(u_{\Omega,h}), \chi_h) &= 0 \\ \langle S_h \cdot n, \chi_{b,h}\rangle - \langle j(u_{\Omega,h}), \chi_{b,h} \cdot n\rangle &= 0\end{aligned}$$

holds for all $T_h \in \Sigma_h^p$, $\chi_h \in \Theta_h$, $\chi_{b,h} \in \Theta_{b,h}$

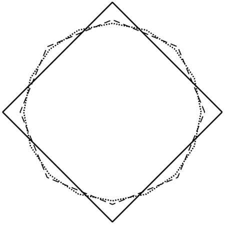
Approximation space $\Theta_{b,h}^p$: Piecewise constant on $\partial\Omega$

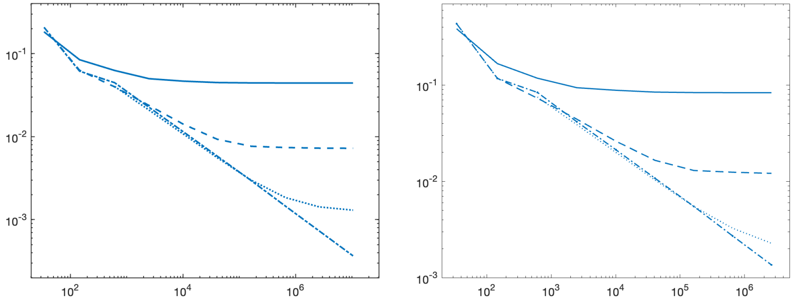
Discretization by Finite Elements

Example 1

$f \equiv 1/2 - \mathbf{1}_D$, D unit disk
$j(u_\Omega) = u_\Omega / 2$

Optimal shape: $\{x \in \mathbb{R}^2 : |x| < \sqrt{2}\}$





$\eta_p(\Omega_h)$ vs. number of degrees of freedom for $p = 2$ (left) and $p = 1.1$ (right)

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Shape Gradient Iteration

Aim:
Continuous deformation $\theta_h^\diamond \in W^{1,p^*}(\Omega;\mathbb{R}^d)$ from $\theta_h \in L^{p^*}(\Omega;\mathbb{R}^d)$

Local potential reconstruction procedure:[1]
1. Compute, for each element $\tau \in \mathcal{T}_h$, $\nabla\theta_h^\square\big|_\tau \in \mathbb{R}^{d\times d}$ such that

$$\|\nabla\theta_h^\square - |S_h - K(u_{\Omega,h}, y_{\Omega,h})|^{p-2}(S_h - K(u_{\Omega,h}, y_{\Omega,h}))\|_{L^{p^*}(\tau)} \longrightarrow \min!$$

2. Compute, for each $\tau \in \mathcal{T}_h$, $\theta_h^\square$ with $\nabla\theta_h^\square\big|_\tau$ given by 1. such that

$$\|\theta_h^\square - \theta_h\|_{L^{p^*}(\tau)} \longrightarrow \min!$$

3. Compute $\theta_h^\diamond$ pcw. linear, contin., by averaging at the vertices:

$$\theta_h^\diamond(\nu) = \frac{1}{|\{\tau \in \mathcal{T}_h : \nu \in \tau\}|} \sum_{\tau\in\mathcal{T}_h:\nu\in\tau} \theta_h^\square(\nu|_\tau)\,.$$

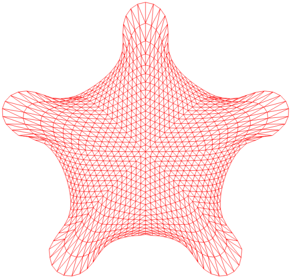
[1] R. Stenberg: RAIRO Modél. Math. Anal. Numér. **25** (1991)

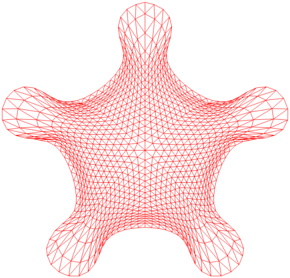
Shape Gradient Iteration

Example 2[1]

$$f(x) = -\frac{1}{2} + \frac{4}{5}|x|^2 + 2\sum_{i=1}^{5} \exp\left(-8\,|x - y^{(i)}|^2\right) - \sum_{i=1}^{5} \exp\left(-8\,|x - z^{(i)}|^2\right),$$

$$y^{(i)} = (\sin(\frac{(2i+1)\pi}{5}), \cos(\frac{(2i+1)\pi}{5})), z^{(i)} = \frac{6}{5}(\sin(\frac{2i\pi}{5}), \cos(\frac{2i\pi}{5})), i = 1, \ldots, 5$$





Final iterate for $p(= p^*) = 2$ on the left and $p = 1.1$ ($p^* = 11$) on the right

[1] S. Bartels, G. Wachsmuth: SIAM J. Sci. Comput. **42** (2020)

Shape Gradient Iteration

Example 2

$p = 2$: shape iteration terminates due to degenerate mesh

$\|\mathcal{T}_h\|$	2048	8192	32768	131072
$J(\Omega_h^\diamond)$	-0.01457574	-0.01490224	-0.01495978	-0.01496720
$\eta_{2,h}(\Omega_h^\diamond)$	2.6914e-3	1.7784e-3	6.0273e-4	3.0347e-4
iterations	69	46	59	66

$p = 1.1$: shape iteration converges

$\|\mathcal{T}_h\|$	2048	8192	32768	131072
$J(\Omega_h^\diamond)$	-0.01485067	-0.01493147	-0.01495993	-0.01496731
$\eta_{1.1,h}(\Omega_h^\diamond)$	2.6551e-3	1.4609e-3	7.4356e-4	3.7225e-4
iterations	42	86	62	59

Observation: $\eta_{p,h} = O(h)$

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We have shown that $\eta_p(\Omega)$ indicates how close to stationarity Ω is.

But we can only compute $\eta_{p,h}(\Omega)$ (based on $u_{\Omega,h}, y_{\Omega,h}$ and S_h)!

Are they close to each other?

Theorem:
For $p \in (1, 2]$, assume that Ω is such that
$\{u_\Omega, y_\Omega\} \subset H^2(\Omega) \cap W^{1,q}(\Omega)$ (with $q = 2p/(2-p)$).
Then, if $f \in H^1(\Omega) \cap L^q(\Omega)$ and $j'(u_\Omega) \in H^1(\Omega) \cap L^q(\Omega)$,

$$|\eta_p(\Omega) - \eta_{p,h}(\Omega)| \leq Ch$$

holds with a constant C (independently of h).

Error Analysis

Proof Ingredients:

$$\|K(u_\Omega, y_\Omega) - K(u_{\Omega,h}, y_{\Omega,h})\|_{L^p(\Omega)}$$
$$\leq (2d)^{1/2} \big(\|\nabla u_\Omega\|_{L^q(\Omega)} \|\nabla (y_\Omega - y_{\Omega,h})\|_{L^2(\Omega)}$$
$$+ \|\nabla y_\Omega\|_{L^q(\Omega)} \|\nabla (u_\Omega - u_{\Omega,h})\|_{L^2(\Omega)} \big)$$

S: L^p projection of $K(u_\Omega, y_\Omega)$ onto Σ^p_{adm}
S_h: L^p projection of $K(u_{\Omega,h}, y_{\Omega,h})$ onto

$$\Sigma^p_{\mathrm{adm},h} = \{ T_h \in \Sigma^p_h : \operatorname{div} T = P^0_h f \, \nabla y_{\Omega,h} - P^0_h j'(u_{\Omega,h}) \, \nabla j(u_{\Omega,h}) \, ,$$
$$T_h \cdot n|_{\partial\Omega} = P^{0,b}_h j(u_{\Omega,h}) \, n\Big|_{\partial\Omega} \}$$

gives $\|S - S_h\|_{L^p(\Omega)} \leq \|K(u_\Omega, y_\Omega) - K(u_{\Omega,h}, y_{\Omega,h})\|_{L^p(\Omega)} + C\, h$

$$|\eta_p(\Omega) - \eta_{p,h}(\Omega)| \leq \|S - S_h\|_{L^p(\Omega)} + \|K(u_\Omega, y_\Omega) - K(u_{\Omega,h}, y_{\Omega,h})\|_{L^p(\Omega)}$$

Conclusions and Outlook

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arXiv: 2309.13595

Two main messages of this contribution:

1. $\eta_{p,h}(\Omega) = \|S_h - K(u_{\Omega,h}, y_{\Omega,h})\|_{L^p(\Omega_h)}$ provides a computable way of estimating the "closeness to stationarity" of Ω
2. Lagrange multiplier θ_h can be reconstructed to steepest descent deformation $\theta^\diamond$ w.r.t. $W^{1,p^*}(p^* > 2)$

Two (of the many) things to do next:

1. Combine this with adaptive techniques (for computing $u_{\Omega_h}, y_{\Omega_h}$ and S_h)
2. Incorporate constraints (prescribed volume, prescribed perimeter etc.)