Shape Optimization by Constrained First-Order System Least Mean Approximation

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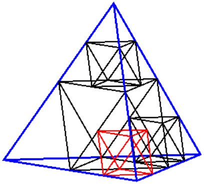

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Overview

Shape Optimality As L^p Best Approximation

Structure of the Least Mean Approximation Problem

Discretization by Finite Elements

Shape Gradient Iteration

GS:
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To Appear in *SIAM Journal on Scientific Computing*
(in about 4 - 6 weeks)

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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:

$$u_\Omega \in H^1_0(\Omega): \quad (\nabla u_\Omega, \nabla v)_{L^2(\Omega)} = (f, v)_{L^2(\Omega)} \text{ for all } v \in H^1_0(\Omega)$$

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

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

$y_\Omega \in H^1_0(\Omega)$: solution of the adjoint problem

$$(\nabla y_\Omega, \nabla z) = -(j'(u_\Omega), z) \text{ for all } z \in H^1_0(\Omega)$$

[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] [8]

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)

[8] M. Berggren: Comput. Methods Appl. Sci., Springer **15** (2010)

Shape Optimality As L^p Best Approximation

Shape derivative in volume expression:

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

In general, u_Ω and y_Ω only slightly more regular than $H^1(\Omega)$

$$\Longrightarrow \nabla u_\Omega \,,\ \nabla y_\Omega \text{ only slightly better than } L^2(\Omega; \mathbb{R}^d)$$

$J'(\Omega)[\chi]$ may only be defined on $W^{1,p}(\Omega; \mathbb{R}^d)$ for large p

Shape Optimality As L^p Best Approximation

Shape derivative in volume expression:

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

Shape 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][3]

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

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

[3] A. Laurain, P. T. P. Lopes, J. C. Nakasato: ESAIM Control Optim. Calc. Var. **29** (2023)

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.

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

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

Suitable norm of the shape derivative:

$$\sup_{\chi \in W^{1,p^*}(\Omega;\mathbb{R}^d)} \frac{J'(\Omega)[\chi]}{\|\nabla \chi\|_{L^{p^*}(\Omega)}} := \eta_p(\Omega) \qquad \left(\frac{1}{p} + \frac{1}{p^*} = 1\right)$$

Exists if $K(u_\Omega, y_\Omega) \in L^p(\Omega; \mathbb{R}^{d \times d})$, $p \in (1, 2]$ (may be close to 1)

Restrict χ to
$\Theta^{p^*} = \{\chi \in W^{1,p^*}(\Omega; \mathbb{R}^d) : (\chi, e) = 0 \; \forall \text{ constant } e \in \mathbb{R}^d\}$

Assume that $\qquad J'(\Omega)[e] = (f \nabla y_\Omega, e) = 0 \qquad$ (barycenter known)

Shape Optimality As L^p Best Approximation

Necessary condition for $\theta \in \Theta^{p^*}$ with

$$\frac{J'(\Omega)[\theta]}{\|\nabla\theta\|_{L^{p^*}(\Omega)}} = \sup_{\chi \in \Theta^{p^*}} \frac{J'(\Omega)[\chi]}{\|\nabla\chi\|_{L^{p^*}(\Omega)}} \quad \text{by differentiating:}$$

$$(|\nabla\theta|^{p^*-2}\nabla\theta, \nabla\chi) = J'(\Omega)[\chi] \quad \text{for all} \quad \chi \in \Theta^{p^*}$$

Define $S := K(u_\Omega, y_\Omega) - |\nabla\theta|^{p^*-2}\nabla\theta \ (\in L^p(\Omega; \mathbb{R}^{d\times d}))$, then

$$\|S - K(u_\Omega, y_\Omega)\|^p_{L^p(\Omega)} = \int_\Omega |\nabla\theta|^{(p^*-1)p} dx = \int_\Omega |\nabla\theta|^{p^*} dx = \|\nabla\theta\|^{p^*}_{L^{p^*}(\Omega)}$$

and

$$(S, \nabla\chi) = (K(u_\Omega, y_\Omega), \nabla\chi) - J'(\Omega)[\chi] = -(f\nabla y_\Omega, \chi) - (j(u_\Omega), \mathrm{div}\chi)$$

$$S \in \Sigma^{p,0}_{f,j} := \{T \in L^p(\Omega; \mathbb{R}^{d\times d}) :$$
$$(\mathrm{div}\, T, \chi) = (f\, \nabla y_\Omega, \chi) + (j(u_\Omega), \mathrm{div}\, \chi)\ ,\ \langle T \cdot n, \chi|_{\partial\Omega}\rangle = 0\ \forall \chi\}$$

Shape Optimality As L^p Best Approximation

$$\Sigma_{f,j}^{p,0} := \{ T \in L^p(\Omega;\mathbb{R}^{d\times d}) :$$
$$(\mathrm{div}\, T, \chi) = (f\,\nabla y_\Omega, \chi) + (j(u_\Omega), \mathrm{div}\,\chi)\,,\ \langle T\cdot n,\, \chi|_{\partial\Omega}\rangle = 0\ \forall \chi\}$$

For all $T \in \Sigma_{f,j}^{p,0}$ and for all $\chi \in \Theta^{p^*}$:

$$\frac{J'(\Omega)[\chi]}{\|\nabla\chi\|_{L^{p^*}(\Omega)}} = \frac{(K(u_\Omega, y_\Omega) - T, \nabla\chi)}{\|\nabla\chi\|_{L^{p^*}(\Omega)}} \le \|K(u_\Omega, y_\Omega) - T\|_{L^p(\Omega)}$$

On the other hand:

$$\frac{J'(\Omega)[\theta]}{\|\nabla\theta\|_{L^{p^*}(\Omega)}} = \frac{(K(u_\Omega, y_\Omega) - S, \nabla\theta)}{\|\nabla\theta\|_{L^{p^*}(\Omega)}}$$
$$= \|\nabla\theta\|_{L^{p^*}(\Omega)}^{p^*-1} = \|\nabla\theta\|_{L^{p^*}(\Omega)}^{p^*/p} = \|K(u_\Omega, y_\Omega) - S\|_{L^p(\Omega)}$$

We have shown: $\eta_p(\Omega) = \inf\{\|T - K(u_\Omega, y_\Omega)\|_{L^p(\Omega)} : T \in \Sigma_{f,j}^{p,0}\}$

Overview

Structure of the Least Mean Approximation Problem

$$S \in \Sigma^{p,0} := \{ T \in L^p(\Omega; \mathbb{R}^{d\times d}) : \operatorname{div} T \in L^p(\Omega; \mathbb{R}^d),\ T \cdot n|_{\partial\Omega} = 0 \}$$

Optimality system (for $\|S - K(u_\Omega, y_\Omega)\|_{L^p(\Omega)} \to \min!$):

$$(|S - K(u_\Omega, y_\Omega)|^{p-2}(S - K(u_\Omega, y_\Omega)), T) + (\operatorname{div} T, \theta) = 0 \ \forall T \in \Sigma^{p,0}$$
$$(\operatorname{div} S, \chi) = (f \nabla y_\Omega, \chi) + (j(u_\Omega), \operatorname{div} \chi) \qquad \forall \chi \in \Theta^{p^*}$$

This is hopefully enough justification for me to give this talk here!

Lagrange multipl. by Helmholtz decomposition in $L^{p^*}(\Omega; \mathbb{R}^{d\times d})$:[1][2]

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

The above optimality system has a unique solution

$$(S, \theta) \in \Sigma^{p,0} \times \Theta^{p^*}$$

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

[2] E. Fabes, O. Mendez, M. Mitrea: J. Funct. Anal. **159** (1998)

Structure of the Least Mean Approximation Problem

Main Theorem:
Let $p \in (1, 2]$ and assume $K(u_\Omega, y_\Omega) \in L^p(\Omega; \mathbb{R}^{d \times d})$ and that the compatibility condition $(f \nabla y_\Omega, e) = 0$ for all const. $e \in \mathbb{R}^d$ holds. Then, the Lagrange multiplier $\theta \in \Theta^{p^*}$ satisfies

$$\frac{J'(\Omega)[\theta]}{\|\nabla\theta\|_{L^{p^*}(\Omega)}} = \inf_{\chi \in \Theta^{p^*}} \frac{J'(\Omega)[\chi]}{\|\nabla\chi\|_{L^{p^*}(\Omega)}}$$
$$= -\eta_p(\Omega) = -\|S - K(u_\Omega, y_\Omega)\|_{L^p(\Omega)}$$

This provides an alternative route to W^{1,p^*} shape gradients[3] [4] [5] [6]

Proof consists basically in going backwards in the derivation of the previous section.

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[3] P. M. Müller, N. Kühl, M. Siebenborn, K. Deckelnick, M. Hinze, T. Rung: Struct. Multid. Optim. **64** (2021)
[4] K. Deckelnick, P. J. Herbert, M. Hinze: ESAIM Control Optim. Calc. Var. **28** (2022)
[5] K. Deckelnick, P. J. Herbert, M. Hinze: arXiv:2301.08690 (2023)
[6] K. Deckelnick, P. J. Herbert, M. Hinze: arXiv:2310.15078 (2023)

Structure of the Least Mean Approximation Problem

Example 1

$D_R = \{x \in \mathbb{R}^2 : |x| < R\}$

$$f \equiv 1/2 - \mathbf{1}_{D_1}$$
$$j(u_\Omega) = u_\Omega/2$$

$$u_R(x) = \begin{cases} \frac{R^2+|x|^2}{8} - \frac{1}{4} - \frac{1}{2}\ \ln R & ,\ 0 \le |x| < 1\,, \\ \frac{R^2-|x|^2}{8} + \frac{1}{2}(\ln|x| - \ln R) & ,\ 1 < |x| < R \end{cases}$$

$$y_R(x) = (|x|^2 - R^2)/8$$

$$\nabla u_R(x) = \begin{cases} \frac{1}{4}\,x & ,\ 0 \le |x| < 1\,, \\ -\frac{1}{4}\,x + \frac{1}{2}\ \frac{x}{|x|^2} & ,\ 1 < |x| < R\,, \end{cases} \quad ,\ \nabla y_R(x) = \frac{1}{4}x$$

$$K(u_R, y_R) = (\nabla u_R \cdot \nabla y_R)\,I - \nabla y_R \otimes \nabla u_R - \nabla u_R \otimes \nabla y_R$$
$$= \begin{cases} \frac{1}{16}|\mathrm{id}|^2 I - \frac{1}{8}\mathrm{id} \otimes \mathrm{id} & ,0 \le |x| < 1\,, \\ \left(\frac{1}{8} - \frac{1}{16}|\mathrm{id}|^2\right) I - \left(\frac{1}{4\,|\mathrm{id}|^2} - \frac{1}{8}\right) \mathrm{id} \otimes \mathrm{id} & ,1 < |x| < R \end{cases}$$

Structure of the Least Mean Approximation Problem

$$K(u_R, y_R) = (\nabla u_R \cdot \nabla y_R)\, I - \nabla y_R \otimes \nabla u_R - \nabla u_R \otimes \nabla y_R$$
$$= \begin{cases} \frac{1}{16}|\mathrm{id}|^2 I - \frac{1}{8}\mathrm{id} \otimes \mathrm{id} & , 0 \le |x| < 1\,, \\ \left(\frac{1}{8} - \frac{1}{16}|\mathrm{id}|^2\right) I - \left(\frac{1}{4\,|\mathrm{id}|^2} - \frac{1}{8}\right) \mathrm{id} \otimes \mathrm{id} & , 1 < |x| < R \end{cases}$$

$$\mathrm{div}\, K(u_R, y_R) = \left\{ \begin{matrix} -\frac{1}{4}\mathrm{id} & , 0 \le |x| < 1\,, \\ \frac{1}{4}\mathrm{id} - \frac{1}{4\,|\mathrm{id}|^2}\,\mathrm{id} & , 1 < |x| < R \end{matrix} \right\} = f\, \nabla y_R - \nabla j(u_R)$$

$$K(u_R, y_R) \cdot n = \left(\frac{1}{8} - \frac{R^2}{16}\right) n - \left(\frac{1}{4} - \frac{R^2}{8}\right) n \text{ on } \partial D_R$$

Optimality conditions satisfied for $R = \sqrt{2}$

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Discretization by Finite Elements

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

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

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

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

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

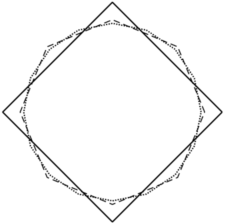
Approximation space $\Theta_{b,h}$: Piecewise constant on $\partial\Omega$

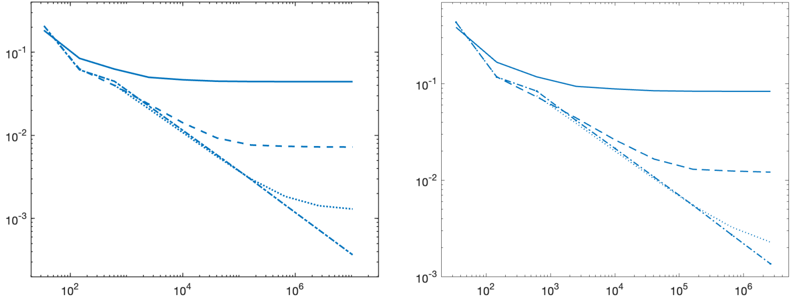
Discretization by Finite Elements

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:

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

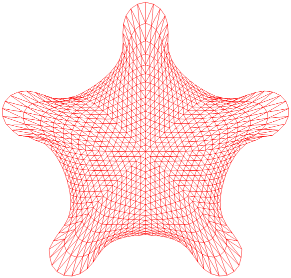
[1] R. Stenberg: RAIRO Modél. Math. Anal. Numér. **25** (1991)

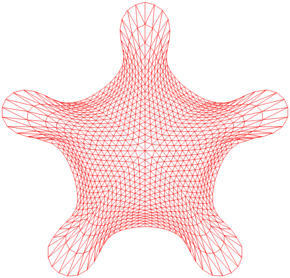
Shape Gradient Iteration

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

$\lvert\mathcal{T}_h\rvert$	2048	8192	32768	131072
$J(\Omega_h^\diamond)$	$-1.4147 \cdot 10^{-2}$	$-1.4594 \cdot 10^{-2}$	$-1.4887 \cdot 10^{-2}$	$-1.4951 \cdot 10^{-2}$
$\eta_{2,h}(\Omega_h^\diamond)$	$2.6914 \cdot 10^{-3}$	$1.9698 \cdot 10^{-3}$	$9.0139 \cdot 10^{-4}$	$2.9399 \cdot 10^{-4}$

$p = 1.1$: shape iteration converges

$\lvert\mathcal{T}_h\rvert$	2048	8192	32768	131072
$J(\Omega_h^\diamond)$	$-1.4295 \cdot 10^{-2}$	$-1.4748 \cdot 10^{-2}$	$-1.4911 \cdot 10^{-2}$	$-1.4953 \cdot 10^{-2}$
$\eta_{1.1,h}(\Omega_h^\diamond)$	$2.8951 \cdot 10^{-3}$	$1.4649 \cdot 10^{-3}$	$7.1925 \cdot 10^{-4}$	$3.7628 \cdot 10^{-4}$

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

Conclusions and Outlook

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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. $W^{1,p^*}(p^* > 2)$

Extension: Replace $\|\nabla\theta\|$ by elasticity norm $\|\varepsilon(\theta)\|$
(see talk by Laura Hetzel on Wednesday morning)

Laura Hetzel, GS: *Constrained L^p Approximation of Shape Tensors and its Role for the Determination of Shape Gradients*
arXiv: 2406.14405