Seminar for Applied Mathematics SAM

ETH Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

# Reasonable Shape Gradient Approximations

Alberto Paganini and Sahar Sargheini
alberto.paganini@sam.math.ethz.ch

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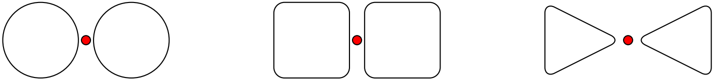
# Motivation

Nano antennae: cavities for LSP.



● : Strongly localized field in sub-wavelength region.

Possible applications: Sensing, enhancing solar cells, ...

Issue: Production inaccuracies can drastically affect optical behavior.

$\longrightarrow$ Sensitivity analysis is crucial!

It tells us the robustness of a design.

# Perturbation of domains



Transformation $T_{\mathcal{V}} \; : \; \Omega \longrightarrow T_{\mathcal{V}}(\Omega)$

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

Family of admissible domains:

$$\mathcal{U}_{\mathrm{ad}}(\Omega) := \{ T_{\mathcal{V}}(\Omega); \|\mathcal{V}\|_{C^1} < 1 \}.$$

[1] Conception optimale de structures, 2007.

# Shape Differentiable Functionals

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A shape functional

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

is shape differentiable if the map

$$\mathcal{V} \mapsto \mathcal{J}\left(T_{\mathcal{V}}(\Omega)\right)$$

is Fréchet differentiable in 0 in the Banach space $C^1(\mathbb{R}^N; \mathbb{R}^N)$, i.e., there is a linear continuous map (shape gradient)

$$d\mathcal{J}(\Omega; \cdot) : C^1(\mathbb{R}^N; \mathbb{R}^N) \to \mathbb{R}$$

so that

$$\lim_{\mathcal{V}\to 0} \frac{\mathcal{J}\left(T_{\mathcal{V}}(\Omega)\right) - \mathcal{J}(\Omega)}{\|\mathcal{V}\|_{C^1}} = d\mathcal{J}(\Omega; \mathcal{V}).$$

# Differentiation of domain integrals

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EXAMPLE: Consider $\mathcal{J}(\Omega) = \int_\Omega f\, d\mathbf{x}$, with $f \in W^{1,1}(\mathbb{R}^N)$.

$$d\mathcal{J}(\Omega; \mathcal{V}) = \lim_{\mathcal{V}\to 0} \frac{1}{\|\mathcal{V}\|_{C^1}} \left( \int_{T_\mathcal{V}(\Omega)} f\, d\mathbf{x} - \int_\Omega f\, d\mathbf{x} \right),$$

$$= \lim_{\mathcal{V}\to 0} \frac{1}{\|\mathcal{V}\|_{C^1}} \left( \int_\Omega (f \circ T_\mathcal{V})\, |\det DT_\mathcal{V}| - f\, d\mathbf{x} \right),$$

$$= \int_\Omega \dot{f} + f\ \mathrm{div}(\mathcal{V})\, d\mathbf{x}\,.$$

Material derivative: $\dot{f} := \lim_{\mathcal{V}\to 0} \frac{f\circ T_\mathcal{V} - f}{\|\mathcal{V}\|_{C^1}} = \nabla f \cdot \mathcal{V}\,.$

Gauss's Theorem $\Rightarrow d\mathcal{J}(\Omega; \mathcal{V}) = \int_{\partial\Omega} f\, \mathcal{V} \cdot \mathbf{n}\, dS$.

# Differentiation of boundary integrals

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EXAMPLE: Consider $\mathcal{J}(\Omega) = \int_{\partial\Omega} f \, d\mathbf{x}$, with $f \in W^{2,1}(\mathbb{R}^N)$.

**Lemma**:

$$\int_{T_{\mathcal{V}}(\partial\Omega)} f \, dS = \int_{\partial\Omega} (f \circ T_{\mathcal{V}}) |\det DT_{\mathcal{V}}| \, \|(DT_{\mathcal{V}})^{-t}\mathbf{n}\|_{\mathbb{R}^N} \, dS$$

$$\Rightarrow d\mathcal{J}(\Omega; \mathcal{V}) = \int_{\partial\Omega} \nabla f \cdot \mathcal{V} + f \underbrace{(\operatorname{div}(\mathcal{V}) - D\mathcal{V}\mathbf{n} \cdot \mathbf{n})}_{:= \operatorname{div}_\Gamma \mathcal{V}} \, dS \, .$$

Assuming $\Omega$ piecewise smooth, and defining $\mathcal{V}_\tau := \mathcal{V} - (\mathcal{V} \cdot \mathbf{n})\mathbf{n}$,

# Differentiation of boundary integrals(2)

it holds,

$$\int_{\partial\Omega} \nabla f \cdot \mathcal{V} + f \ \mathrm{div}_\Gamma \mathcal{V} \, dS = \sum_{i=1}^{M} \int_{\partial\Omega_i} \nabla f \cdot \mathcal{V} + f \ \mathrm{div}_\Gamma \mathcal{V} \, dS$$

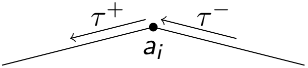
$$\overset{*}{=} \sum_{i=1}^{M} \int_{\partial\Omega_i} \mathcal{V} \cdot \mathbf{n} \Big( \frac{\partial f}{\partial \mathbf{n}} + f \mathrm{K} \Big) + \frac{\partial f}{\partial \tau} \tau \cdot \mathcal{V}_\tau + f \, \mathrm{div}_\Gamma \mathcal{V}_\tau \, dS$$

$$= \sum_{i=1}^{M} \int_{\partial\Omega_i} \mathcal{V} \cdot \mathbf{n} \Big( \frac{\partial f}{\partial \mathbf{n}} + f \mathrm{K} \Big) + \mathrm{div}_\Gamma (f \mathcal{V}_\tau) \, dS$$

$$\overset{**}{=} \int_{\partial\Omega} \mathcal{V} \cdot \mathbf{n} \Big( \frac{\partial f}{\partial \mathbf{n}} + f \mathrm{K} \Big) \, dS + \sum_{i=1}^{M} f(a_i) \mathcal{V}(a_i) \cdot (\tau^-(a_i) - \tau^+(a_i))$$

*: $\mathrm{div}_\Gamma \mathcal{V} = \mathrm{div}_\Gamma \mathcal{V}_\tau + \mathrm{K} \mathcal{V} \cdot \mathbf{n}$,

**: Stokes' Theorem,



# The Hadamard's Structure Theorem

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

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

Proof: following closely Allaire's intuitive proof

- if $\mathcal{V} \cdot \mathbf{n} = 0$, then $T_\mathcal{V}(\partial\Omega) = \partial\Omega$,
- $T_\mathcal{V}$ is a homeomorphism, thus $T_\mathcal{V}(\Omega) = \Omega$
- which implies $\mathcal{J}(T_\mathcal{V}(\Omega)) = \mathcal{J}(\Omega)$.

□

# PDE constrained Shape Functionals



Consider

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

with $j \in C^{1,1}(\mathbb{R};\mathbb{R})$ and $u \in H^2(\Omega)$ solution of

$$\left\{\begin{array}{rcll} -\Delta u + u & = & f & \text{in } \Omega\,, \\ u & = & g & \text{on } \partial\Omega\,, \end{array}\right. \quad \Big\}\ \text{State problem}$$

where $f \in H^1(\mathbb{R}^N)$, $g \in H^2(\mathbb{R}^N)$, Then

$$d\mathcal{J}(\Omega;\mathcal{V}) = \int_\Omega j'(u)\dot{u} + j(u)\ \operatorname{div}(\mathcal{V})\, d\mathbf{x}\,,$$

but

$$\dot{u} \neq \nabla u \cdot \mathcal{V}\ !$$

# Differentiation with Lagrangian Approach

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We introduce the Lagrangian

$$\mathscr{L}(\Omega, v, q, \lambda) := \int_\Omega j(v) + (\Delta v - v + f)q \, d\mathbf{x} + \int_{\partial\Omega} \lambda(g - v) \, dS \,,$$

where the functions $v$, $q$ and $\lambda$ are in $H^2(\mathbb{R}^N)$. The saddle point of $\mathscr{L}(\Omega, \cdot, \cdot, \cdot)$ is characterized by

$$\langle \frac{\partial \mathscr{L}(\Omega, v, q, \lambda)}{\partial v}, \phi \rangle = \langle \frac{\partial \mathscr{L}(\Omega, v, q, \lambda)}{\partial q}, \phi \rangle = \langle \frac{\partial \mathscr{L}(\Omega, v, q, \lambda)}{\partial \lambda}, \phi \rangle = 0$$

for all $\phi \in H^2(\mathbb{R}^N)$.

# Characterisation of saddle points

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By density we retrieve

$$\left\{\begin{array}{rcll} -\Delta v + v & = & f & \text{in } \Omega\,, \\ v & = & g & \text{on } \partial\Omega\,, \end{array}\right\} \text{State problem}$$

$$\left\{\begin{array}{rcll} -\Delta q + q & = & j'(v) & \text{in } \Omega\,, \\ q & = & 0 & \text{on } \partial\Omega\,, \end{array}\right\} \begin{array}{l}\text{Adjoint problem,} \\ \text{solution } p\end{array}$$

$$\lambda = -\frac{\partial q}{\partial \mathbf{n}} \quad \text{on } \partial\Omega\,,$$

weakly in $H^1(\mathbb{R}^N)$. Thus, for $\Omega$ fixed,

$$\mathcal{J}(\Omega) = \min_{v \in H^2(\mathbb{R}^N)} \max_{q,\lambda \in H^2(\mathbb{R}^N)} \mathscr{L}(\Omega, v, q, \lambda)\,,$$

because

$$\mathcal{J}(\Omega) = \mathscr{L}(\Omega, u, q, \lambda) \quad \text{for all } q, \lambda \text{ in } H^2(\mathbb{R}^N)\,.$$

# Volume and boundary representations

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Correa-Seeger[2]: we can swap $d$ and min max.

$$d\mathcal{J}(\Omega;\mathcal{V}) = \lim_{\mathcal{V}\to 0} \frac{\mathscr{L}(T_{\mathcal{V}}(\Omega), v, q, \lambda) - \mathscr{L}(\Omega, v, q, \lambda)}{\|\mathcal{V}\|_{C^1}}\bigg|_{(v,q,\lambda)=(u,p,-\frac{\partial p}{\partial \mathbf{n}})},$$

$$= \int_\Omega \big(\nabla u \cdot (D\mathcal{V} + D\mathcal{V}^T)\nabla p - \nabla p \cdot \nabla \dot{g} + \big(j'(u) - p\big)\dot{g} + \dot{f}p + \operatorname{div}(\mathcal{V})\,(j(u) - \nabla u \cdot \nabla p - u\,p + fp)\big)\, d\mathbf{x},$$

$$\stackrel{*}{=} \int_{\partial\Omega} \mathcal{V}\cdot\mathbf{n}\left(j(u) + \frac{\partial p}{\partial \mathbf{n}}\frac{\partial(u-g)}{\partial \mathbf{n}}\right) dS\,.$$

*: Gauss's theorem and integration by parts on boundaries.

[2] Directional derivatives of a minimax function, 1985.

# Reasonable Approximations

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Let's define

$$d\mathcal{J}(\Omega, u, p; \mathcal{V})^{\mathrm{Vol}} := \int_{\Omega} \Big( \nabla u \cdot (D\mathcal{V} + D\mathcal{V}^T) \nabla p + \ldots \Big) \, d\mathbf{x} \,,$$

$$d\mathcal{J}(\Omega, u, p; \mathcal{V})^{\mathrm{Bdry}} := \int_{\partial\Omega} \mathcal{V} \cdot \mathbf{n} \left( j(u) + \frac{\partial p}{\partial \mathbf{n}} \frac{\partial (u - g)}{\partial \mathbf{n}} \right) \, dS \,.$$

Note that

$$d\mathcal{J}(\Omega, \mathcal{V}) = d\mathcal{J}(\Omega, u, p; \mathcal{V})^{\mathrm{Vol}} = d\mathcal{J}(\Omega, u, p; \mathcal{V})^{\mathrm{Bdry}} \,.$$

Question : $u_h \approx u$ and $p_h \approx p \Rightarrow d\mathcal{J}(\ldots)^{\mathrm{Vol}}$ vs $d\mathcal{J}(\ldots)^{\mathrm{Bdry}}$?

# Convergence theorem

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Let $u_h$ and $p_h$ be Ritz–Galerkin linear Lagrangian finite elements approximations of the solutions $u$ and $p$ . Furthermore, assume that the source function $f$ and that the boundary data $g$ are restrictions of $H^1(\mathbb{R}^2)$-, $H^2(\mathbb{R}^2)$-functions, respectively, and that the state problem is 2-regular. Then

$$|d\mathcal{J}(\Omega,\mathcal{V}) - d\mathcal{J}(\Omega,u_h,p_h;\mathcal{V})^{\mathrm{Vol}}| \leq C(\Omega,f,g,j)\|\mathcal{V}\|_{C^1}\mathcal{O}(h^2),$$

where $h$ is the meshwidth of the mesh.
In addition to the previous hypothesis, let assume that

$$\|u\|_{W^2_p(\Omega)} \leq C\|f\|_{L^p(\Omega)}$$

for $1 < p < \mu$, $\mu > d$, where $d = 2$ is the dimension of $\Omega$. Then

$$|d\mathcal{J}(\Omega,\mathcal{V}) - d\mathcal{J}(\Omega,u_h,p_h;\mathcal{V})^{\mathrm{Bdry}}| \leq C'(\Omega,f,g,j)\|\mathcal{V}\cdot\mathbf{n}\|_{C^0}\mathcal{O}(h).$$

# Key steps for a proof

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- $$|d\mathcal{J}(\Omega,\mathcal{V}) - d\mathcal{J}(\Omega,u_h,p_h;\mathcal{V})^{\mathrm{Vol}}|$$

$$\leq \|\mathcal{V}\|_{C^1}\Big(|\int_\Omega (\nabla f\cdot\mathbf{1} + f - \nabla g\cdot\mathbf{1})(p-p_h)\,d\mathbf{x}| \quad \text{CS}$$

$$\text{Taylor, CS} \quad + |\int_\Omega j(u) - j(u_h) + \big(j'(u) - j'(u_h)\big)\,\nabla g\cdot\mathbf{1}\,d\mathbf{x}|$$

$$\text{Gal. Orth.} \quad + |\int_\Omega \nabla u\cdot\nabla p + up - \nabla u_h\cdot\nabla p_h - u_h p_h\,d\mathbf{x}|$$

$$\text{Duality} \quad + |\int_\Omega \nabla(p-p_h)\cdot(\nabla(\nabla g\cdot\mathbf{1}) + (\nabla g\cdot\mathbf{1})\mathbf{1})\;d\mathbf{x}|$$

$$\text{Duality} \quad + 2|\int_\Omega \nabla u\cdot\mathbb{1}\nabla p - \nabla u_h\cdot\mathbb{1}\nabla p_h\,d\mathbf{x}|\Big),$$

- $W^{1,\infty}(\Omega)$ approximation properties of FEM, cf. [Brenner Scott]

□

# NumExp: setup

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Discretization: Piecewise linear nodal FE on triangular meshes.

$$\begin{cases} -\Delta u + u = f & \text{in } \Omega\,, \\ u = g & \text{on } \partial\Omega\,. \end{cases} \qquad \mathcal{J}(\Omega) = \int_\Omega u^2 \, d\mathbf{x}\,,$$

Tracked

$$\mathrm{err}^{\mathrm{Vol}} := \frac{|d\mathcal{J}(\Omega,\mathcal{V}) - d\mathcal{J}(\Omega,u_h,p_h;\mathcal{V})^{\mathrm{Vol}}|}{|d\mathcal{J}(\Omega,\mathcal{V})|}$$

and

$$\mathrm{err}^{\mathrm{Bdry}} := \frac{|d\mathcal{J}(\Omega,\mathcal{V}) - d\mathcal{J}(\Omega,u_h,p_h;\mathcal{V})^{\mathrm{Bdry}}|}{|d\mathcal{J}(\Omega,\mathcal{V})|}$$

on different nested meshes generated through uniform refinement, for

$$\mathcal{V}_1 = \begin{pmatrix} x \\ y \end{pmatrix}, \qquad \mathcal{V}_2 = \begin{pmatrix} 2x - y \\ y^2 - x \end{pmatrix}.$$

# NumExp: smooth domain

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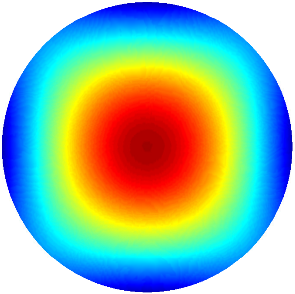
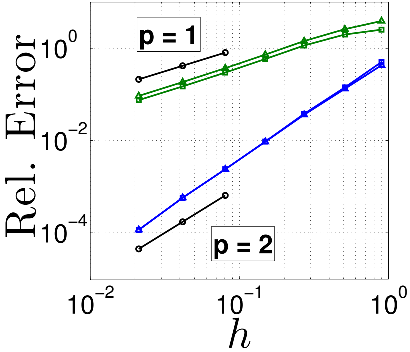
Sorce function and boundary data from solution $u = \cos(x)\cos(y)$.





# NumExp: Lipschitz domain

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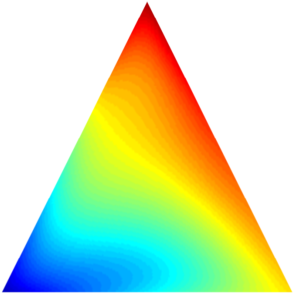
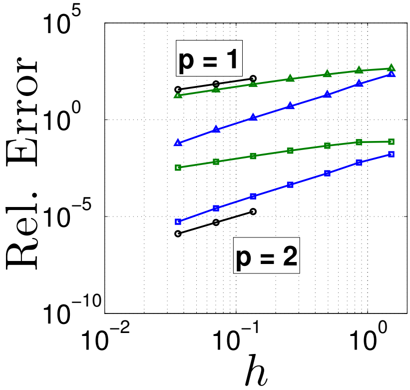
Source function: $f = x^2 - y^2$ , boundary data: $g = x + y$ .



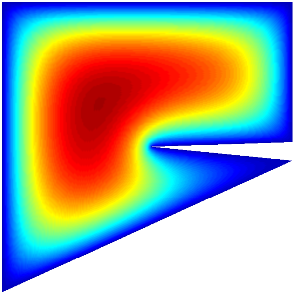


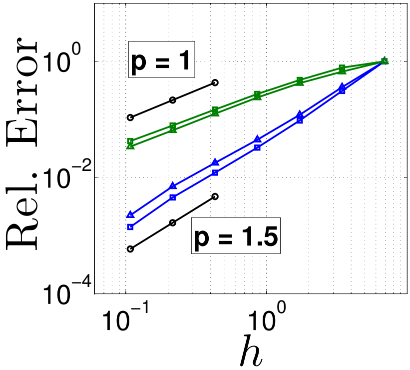
# NumExp: Reentrant corner



State problem:

$$\begin{cases} -\Delta u + u = 1 & \text{in } \Omega\,, \\ u = 0 & \text{on } \partial\Omega\,. \end{cases}$$





# NumExp: Neumann Boundary Conditions

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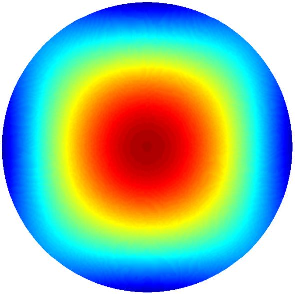
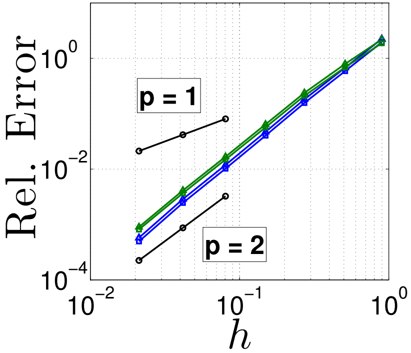
Sorce function and boundary data from solution $u = \cos(x)\cos(y)$.

$$d\mathcal{J}(\Omega, \mathcal{V}) = \int_{\partial\Omega} \mathcal{V} \cdot \mathbf{n} \left( j(u) - \nabla_\Gamma u \nabla_\Gamma p - up + fp + \mathrm{K}gp \right) dS \,,$$





# Summary

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- Sensitivity of a design can be investigated with Shape Gradients,
- Shape Gradients belong to the dual of $C^1(\mathbb{R}^N; \mathbb{R}^N)$,
- Formulas in volume are better suited for FEM-based approximations,
- Smoothness of boundary is not strictly necessary, what is relevant is the 2-regularity of the state problem,
- Approximations of formulation on boundary work surprisingly well when the constraint is a Neumann BVP.

Thanks for your attention!