Lecture 8: Shape derivatives of arbitrary functionals. Complete shape optimization algorithms.

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Given a Lipschitz domain Ω, we parameterize deformations of Ω by a continuous vector field $\boldsymbol{\theta}$:

$$\Omega_{\boldsymbol{\theta}} := (I + \boldsymbol{\theta})\Omega = \{x + \boldsymbol{\theta}(x) \,|\, x \in \Omega\}$$

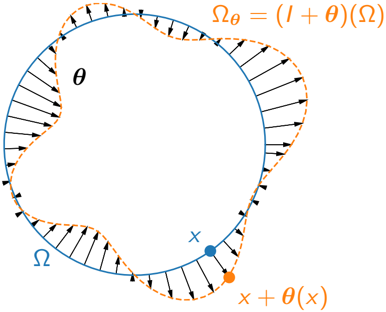


Figure: Deformation of a domain Ω with the method of Hadamard. A small vector field $\boldsymbol{\theta}$ is used to deform Ω into $\Omega_{\boldsymbol{\theta}} = (I + \boldsymbol{\theta})\Omega$.

Recap

Let $J(\Omega)$ denote a shape functional arising e.g. in a shape optimization problem

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

Definition 1

A shape functional $J(\Omega)$ is said shape differentiable if the mapping

$$\begin{array}{ccc} W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d) & \longrightarrow & \mathbb{R} \\ \boldsymbol{\theta} & \longmapsto & J(\Omega_{\boldsymbol{\theta}}) \end{array}$$

is Fréchet differentiable at $\boldsymbol{\theta} = 0$, *i.e.* if there exists a continuous linear form

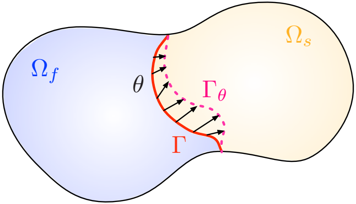
$$\mathrm{D}J(\Omega) \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)^*$$

such that the following asymptotics holds true:

$$J(\Omega_{\boldsymbol{\theta}}) = J(\Omega) + \mathrm{D}J(\Omega)(\boldsymbol{\theta}) + o(\boldsymbol{\theta}), \qquad \text{where } \frac{|o(\boldsymbol{\theta})|}{||\boldsymbol{\theta}||_{W^{1,\infty}(\mathbb{R}^d,\mathbb{R}^d)}} \xrightarrow{\boldsymbol{\theta}\to 0} 0.$$

The **linear form** $\mathrm{D}J(\Omega)$ is called the shape derivative of J on the domain Ω.

$$\min_{\Gamma} \; J(\Gamma)$$



$$\Gamma_{\boldsymbol{\theta}} = (I + \boldsymbol{\theta})\Gamma, \text{ with } \theta \in W_0^{1,\infty}(D, \mathbb{R}^d), \;\; ||\boldsymbol{\theta}||_{W^{1,\infty}(\mathbb{R}^d,\mathbb{R}^d)} < 1.$$

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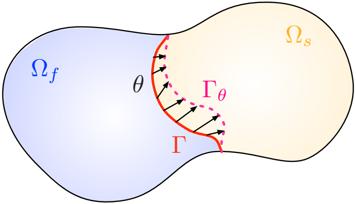
Under suitable regularity assumptions, Hadamard structure theorem holds:

$$\frac{\mathrm{d}J}{\mathrm{d}\boldsymbol{\theta}}(\Gamma)(\boldsymbol{\theta}) = \int_\Gamma v_J(\Gamma)\, \boldsymbol{\theta}\cdot\boldsymbol{n}\mathrm{d}\sigma$$

for some $v_J(\Gamma) \in L^1(\Gamma)$.

If $\boldsymbol{\theta}\cdot\boldsymbol{n} = -v_J(\Gamma)$ on Γ, then $J(\Gamma_{\boldsymbol{\theta}}) = J(\Gamma) - t\int_\Gamma |v_J(\Gamma)|^2 \mathrm{d}\sigma + o(t) < J(\Gamma)$; $\boldsymbol{\theta}$ is a descent direction.

$$\min_{\Gamma} \; J(\Gamma)$$



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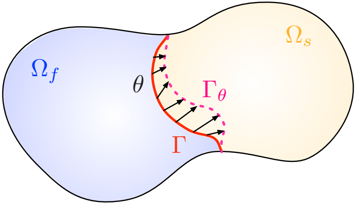

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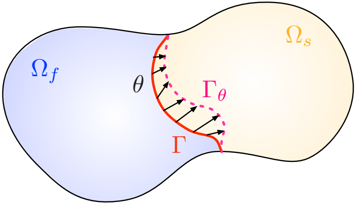

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Outline

1. Shape derivatives of arbitrary functionals
2. Optimization on manifolds

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Manifold structure of shape optimization

Generically, a design optimization problem arises under the form

$$\min_{\Omega \subset D} \quad J(\Omega)$$
$$s.t. \begin{cases} G_i(\Omega) = 0, & 1 \leq i \leq p \\ H_j(\Omega) \leq 0, & 1 \leq j \leq q \end{cases}$$

where

- Ω is an **open domain** sought to be optimized
- J is an **objective function** to minimize (corresponding to a measure of the performance)
- G_i and H_j are respectively p and q **equality and inequality constraints** (corresponding e.g. to industrial specifications to meet)

In industrial applications, $J(\Omega)$, $G_i(\Omega)$ or $H_j(\Omega)$ involve the solution u_Ω defined with respect to a PDE model posed on Ω.
In the previous lectures, we have learned how to compute shape derivatives of the functionals $J(\Omega)$, $G_i(\Omega)$, $H_i(\Omega)$ with respect to **arbitrary** shape deformations

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Today, we see how to adapt the null space optimization algorithm to this infinite dimensional setting.

Manifold structure of shape optimization

In the first lecture, we have considered

$$\begin{aligned} \min_{x \in \mathcal{X}} \quad & J(x) \\ \text{s.t.} \quad & \begin{cases} \boldsymbol{g}(x) = 0 \\ \boldsymbol{h}(x) \leq 0, \end{cases} \end{aligned} \tag{1}$$

with $J : \mathcal{X} \to \mathbb{R}$, $\boldsymbol{g} : \mathcal{X} \to \mathbb{R}^p$ and $\boldsymbol{h} : \mathcal{X} \to \mathbb{R}^q$ Fréchet differentiable.

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$\widetilde{I}(x)$ the set of violated constraints:

$$\widetilde{I}(x) = \{i \in \{1, \dots, q\} \mid h_i(x) \geqslant 0\}.$$

$$\boldsymbol{C}_{\widetilde{I}(x)} = \left[\boldsymbol{g}(x) \quad | \quad (h_i(x))_{i\in\widetilde{I}(x)}\right]^T$$

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The gradient ∇ and the transpose $\mathcal{T}$ are defined with respect to the inner product $a(\cdot,\cdot)$ of V:

$$\begin{aligned} \langle \nabla J, \boldsymbol{\xi} \rangle_V &= \mathrm{D}J(x)\cdot\boldsymbol{\xi} \text{ for any } \boldsymbol{\xi} \in V, \\ \langle \mathrm{D}\boldsymbol{C}(x)^{\mathcal{T}}\boldsymbol{\mu}, \boldsymbol{\xi} \rangle_V &= \boldsymbol{\mu}^T \mathrm{D}\boldsymbol{C}(x)\cdot\boldsymbol{\xi}, \qquad \text{for any } \boldsymbol{\xi} \in V. \end{aligned}$$

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$\mathcal{X}$ is not a Hilbert space !
However $\mathcal{X}$ has some manifold structure that allows for optimization.

Definition 2

- A "manifold" is a set $\mathcal{M}$ such that at any $x \in \mathcal{M}$, there exist a **tangent vector space** $\mathcal{T}_x$ and a mapping

$$\rho_x \,:\, \mathcal{T}_x \to \mathcal{M}$$

defined on a neighborhood of zero satisfying the consistency condition

$$\rho_x(0) = x.$$

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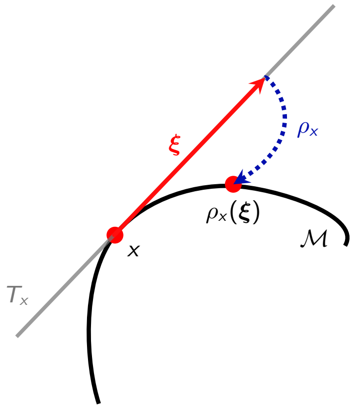

Figure: Optimization on a manifold $\mathcal{M}$: the retraction ρ_x projects tangential motions $\boldsymbol{\xi} \in T_x$ from $x \in \mathcal{M}$ back onto the optimization domain $\mathcal{M}$.

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Assuming $\mathcal{M} = \mathbb{R}^k$ and using the chain rule, eq. (2) is similar to the consistency condition
$$\forall \boldsymbol{\xi} \in \mathcal{T}_x, \qquad \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \rho_x(t\boldsymbol{\xi}) = \boldsymbol{\xi}.$$

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eq. (2) is the definition of shape derivative for
$$\mathcal{M} = \{\Omega \subset D \,|\, \Omega \text{ Lipschitz}\}$$
with $\mathcal{T}_\Omega = W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ and $\rho_\Omega(\boldsymbol{\theta}) = (I + \boldsymbol{\theta})\Omega$.

Manifold structure of shape optimization

If further, $\mathcal{T}_x$ is a **Hilbert space**, then it is possible to implement the null space gradient flow

$$\dot{x} = -\alpha_J \boldsymbol{\xi}_J(x) - \alpha_C \boldsymbol{\xi}_C(x)$$

by considering the following Euler step:

$$x_{n+1} = \rho_{x_n}(\Delta t \boldsymbol{\xi}_n) \text{ with } \boldsymbol{\xi}_n = -\alpha_J \boldsymbol{\xi}_J(x_n) - \alpha_C \boldsymbol{\xi}_C(x_n).$$

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with γ proportional to the mesh size `hmin`.

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- γ tunes the level of diffusion of the shape derivative from the boundary Γ.
- Gradient $\nabla J(\Omega)$ vs. differential $\mathrm{D}J(\Omega)$:

$$\langle \nabla J(\Omega), \boldsymbol{\theta}' \rangle_V = \mathrm{D}J(\Omega) \cdot \boldsymbol{\theta}' \text{ for all } \boldsymbol{\theta}' \in V.$$

Manifold structure of shape optimization

Remark 1

For enforcing non-optimizable regions $\omega \subset \Omega$, we need the descent direction $\boldsymbol{\theta}$ to satisfy

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The identification of $\nabla J(\Omega)$ amounts to solve a Laplace equation with zero boundary Dirichlet condition on ω.

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In practice, the design update is performed with the level-set method, and/or remeshing, which is still consistent at first order.