

An introduction to shape and topology optimization

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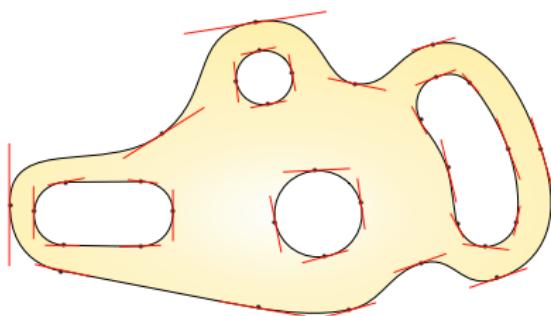
Foreword: geometric shape optimization

We have seen how to optimize shapes when they are **parametrized**:

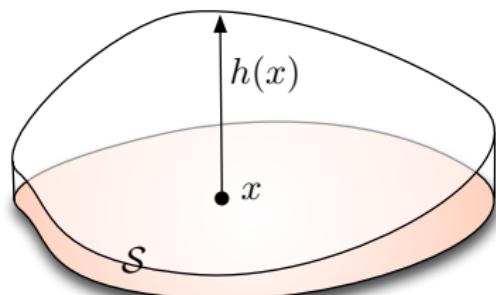
$$\min_h J(h) \text{ s.t. } C(h) \leq 0,$$

where the **design variable** h may be:

- A set of parameters in a finite-dimensional space (thickness, etc.);
- A function h in a suitable, infinite dimensional vector (Banach) space.



Description of a mechanical part via the control points of a CAD model.



Parametrization of a plate with cross-section S via the thickness function $h : S \rightarrow \mathbb{R}$.

Assets:

- In the considered examples, the state u_h lives in a fixed computational domain, which greatly simplifies the calculation of **derivatives with respect to the design**.
- Efficient methods from mathematical programming (optimization routines, etc.) are readily available in this context.

Drawbacks:

- This induces a strong **bias** in the sought shapes.
- It may be very difficult, and in practice cumbersome, to find which are the relevant parameters h of shapes.

⇒ It is often desirable to formulate shape optimization problems in terms of the **geometry** of shapes Ω :

$$\min J(\Omega) \text{ s.t. } C(\Omega) \leq 0.$$

Part III

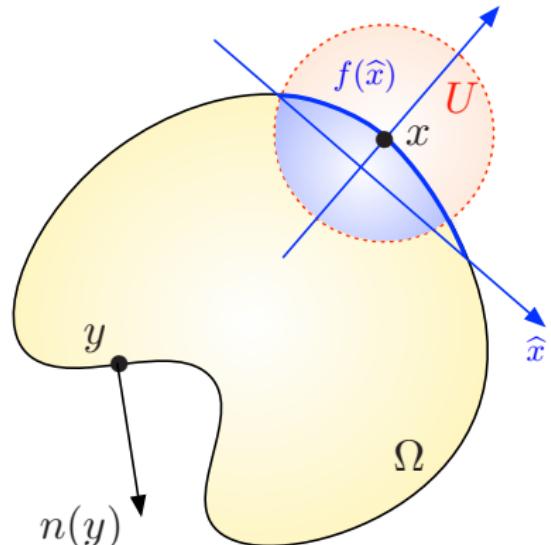
Geometric optimization problems

- 1 The method of Hadamard and shape derivatives
- 2 Shape derivatives of PDE-constrained functionals: the rigorous way, using Eulerian and material derivatives
- 3 Céa's method for calculating shape derivatives
- 4 Numerical aspects of geometric methods
- 5 The level set method for shape optimization

Let Ω be a bounded domain in \mathbb{R}^d ;

- $\partial\Omega$ is the **boundary** of Ω ;
 - $n : \partial\Omega \rightarrow \mathbb{R}^d$ denotes the **unit normal vector** to $\partial\Omega$, pointing outward Ω ;
 - The domain Ω is called **Lipschitz** (resp. of **class C^k**) if

“Near every point $x \in \partial\Omega$, Ω resembles the lower part of the graph of a Lipschitz function (resp. of a C^k function).”



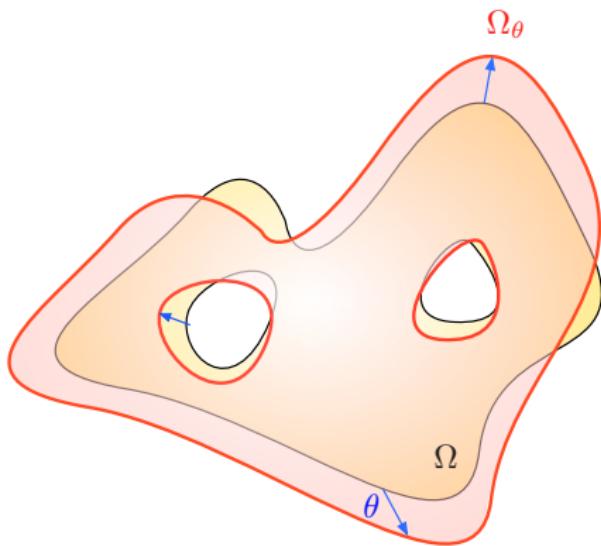
In a neighborhood U of each point $x \in \partial\Omega$, Ω "looks like" the lower part of the graph of some (Lipschitz or C^k) function $\hat{x} \mapsto f(\hat{x})$ defined for suitable $(d-1)$ -dimensional coordinates.

Differentiation with respect to the domain: Hadamard's method (I)

Hadamard's boundary variation method describes variations of a reference, bounded Lipschitz domain Ω of the form:

$$\Omega \mapsto \Omega_\theta := (\text{Id} + \theta)(\Omega),$$

for "small" vector fields $\theta \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$.



Lemma 1.

For $\theta \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ with norm $\|\theta\|_{W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)} < 1$, the mapping $(\text{Id} + \theta)$ is a Lipschitz diffeomorphism.

Definition 1.

Given a bounded Lipschitz domain Ω , a function $\Omega \mapsto J(\Omega) \in \mathbb{R}$ is **shape differentiable** at Ω if the mapping

$$W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d) \ni \theta \mapsto J(\Omega_\theta)$$

is Fréchet-differentiable at 0, i.e. the following expansion holds in the vicinity of 0:

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

The linear mapping $\theta \mapsto J'(\Omega)(\theta)$ is the **shape derivative** of J at Ω .

Remark Other spaces are often used in place of $W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$, made of **more regular** deformation fields θ , e.g.:

$$\mathcal{C}^{k,\infty}(\mathbb{R}^d, \mathbb{R}^d) := \left\{ \theta : \mathbb{R}^d \rightarrow \mathbb{R}^d \text{ of class } \mathcal{C}^k, \sup_{|\alpha| \leq k} \sup_{x \in \mathbb{R}^d} |\partial^\alpha \theta(x)| < \infty \right\}.$$

Theorem 2.

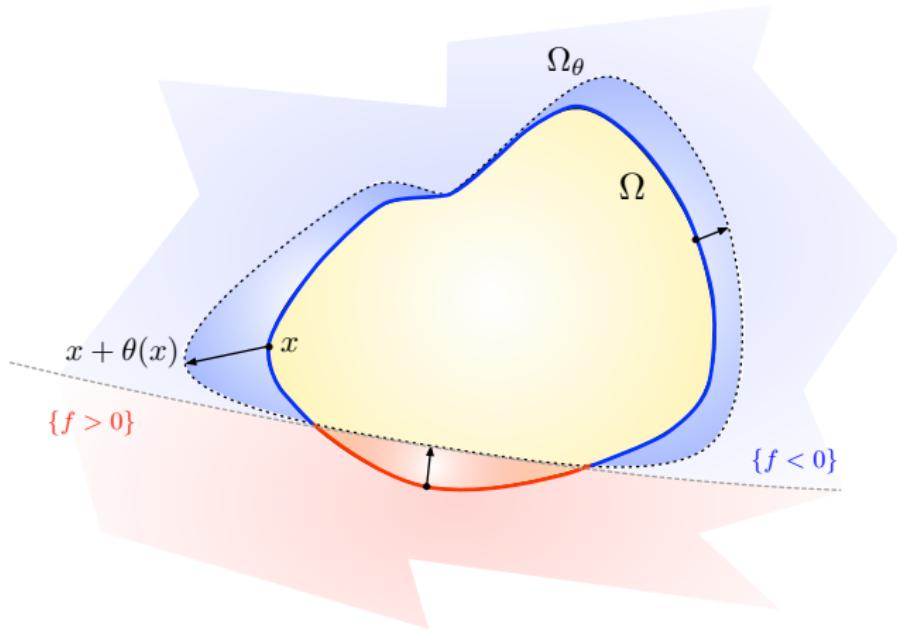
Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain, and let $f \in W^{1,1}(\mathbb{R}^d)$ be a fixed function. Consider the functional:

$$J(\Omega) = \int_{\Omega} f(x) \, dx;$$

then $J(\Omega)$ is shape differentiable at Ω and its shape derivative is:

$$\forall \theta \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d), \quad J'(\Omega)(\theta) = \int_{\partial\Omega} f(\theta \cdot n) \, ds.$$

First examples of shape derivatives (II)



Intuition: f takes negative (resp. positive) values on the blue (resp. red) part of the boundary $\partial\Omega$. The value $J(\Omega_\theta)$ is minimized from $J(\Omega)$ by adding the blue area, (i.e. $\theta \cdot n > 0$ where $f < 0$), and by removing the red area ($\theta \cdot n < 0$ where $f > 0$), weighted by f .

Remarks:

- This result is a particular case of the [Transport](#) (or [Reynolds](#)) theorem, used to derive the equations of motion from conservation principles in fluid mechanics (see the Appendix in [Lecture 1](#)).
- It allows to calculate the shape derivative of the [volume](#) functional

$$\text{Vol}(\Omega) = \int_{\Omega} 1 \, dx;$$

Indeed, it holds:

$$\forall \theta \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d), \quad \text{Vol}'(\Omega)(\theta) = \int_{\partial\Omega} \theta \cdot n \, ds = \int_{\Omega} \text{div}\theta \, dx.$$

In particular, if $\text{div}\theta = 0$, the volume is unchanged (at first order) when Ω is perturbed by θ .

First examples of shape derivatives (IV)

Proof: The formula proceeds from a **change of variables** in volume integrals:

$$J(\Omega_\theta) = \int_{(\text{Id} + \theta)(\Omega)} f(x) dx = \int_{\Omega} |\det(\text{Id} + \nabla \theta)| f \circ (\text{Id} + \theta) dx.$$

- The mapping $\theta \mapsto \det(\text{Id} + \nabla \theta)$ is Fréchet differentiable, and:

$$\det(\text{Id} + \nabla \theta) = 1 + \text{div} \theta + o(\theta), \text{ where } \frac{o(\theta)}{\|\theta\|_{W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)}} \xrightarrow{\theta \rightarrow 0} 0.$$

- If $f \in W^{1,1}(\mathbb{R}^d)$, $\theta \mapsto f \circ (\text{Id} + \theta)$ is also Fréchet differentiable and:

$$f \circ (\text{Id} + \theta) = f + \nabla f \cdot \theta + o(\theta).$$

- Combining those three identities and **Green's formula** leads to the result. □

Remark: This idea of

- ① Using the change of variables $\Omega \rightarrow (\text{Id} + \theta)(\Omega)$ to transport all integrals on the reference domain Ω ,
- ② Differentiating with respect to the deformation θ ,

is the “standard” way to calculate shape derivatives.

Theorem 3.

Let $\Omega \subset \mathbb{R}^d$ be a bounded domain of class C^2 , and let $g \in W^{2,1}(\mathbb{R}^d)$ be a **fixed** function. Consider the functional:

$$J(\Omega) = \int_{\partial\Omega} g(x) \, ds;$$

then $J(\Omega)$ is shape differentiable at Ω when deformations θ are chosen in

$$\mathcal{C}^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d) := \mathcal{C}^1(\mathbb{R}^d, \mathbb{R}^d) \cap W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d),$$

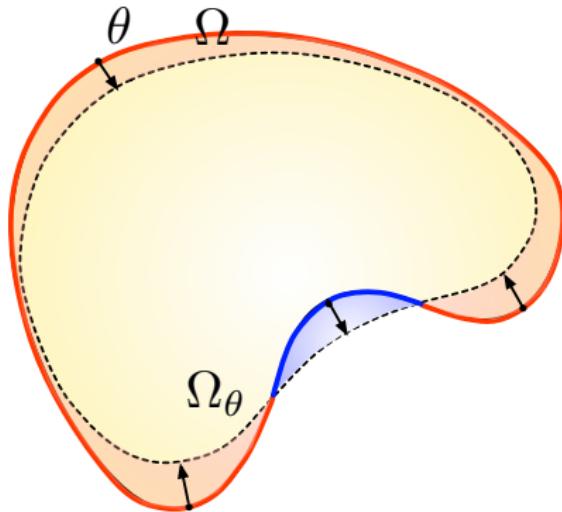
and the shape derivative is:

$$J'(\Omega)(\theta) = \int_{\partial\Omega} \left(\frac{\partial g}{\partial n} + \kappa g \right) (\theta \cdot n) \, ds,$$

where κ is the **mean curvature** of $\partial\Omega$.

Example: The shape derivative of the **perimeter** $\text{Per}(\Omega) = \int_{\partial\Omega} 1 \, ds$ is:

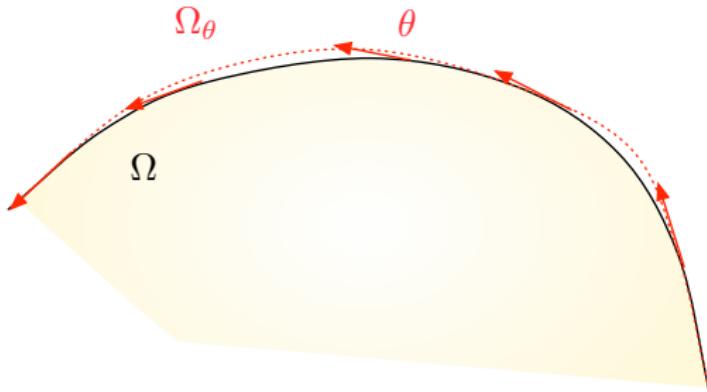
$$\text{Per}'(\Omega)(\theta) = \int_{\partial\Omega} \kappa (\theta \cdot n) \, ds.$$



Intuition: $\theta = -\kappa n$ is a *descent direction* for $\text{Per}(\Omega)$: it is reduced by smearing the *bumps* of $\partial\Omega$ (i.e. $\theta \cdot n < 0$ when $\kappa > 0$), and sealing its *holes* (i.e. $\theta \cdot n > 0$ when $\kappa < 0$).

Structure of shape derivatives (I)

Idea: The shape derivative $J'(\Omega)(\theta)$ of a “regular” functional $\Omega \mapsto J(\Omega)$ only depends on the normal component $\theta \cdot n$ of the vector field θ .



At first order, a **tangential** vector field θ , (i.e. $\theta \cdot n = 0$) only results in a **convection** of the shape Ω , and it is expected that $J'(\Omega)(\theta) = 0$.

Lemma 4.

Let Ω be a domain of class C^1 . Assume that the mapping

$$C^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d) \ni \theta \mapsto J(\Omega_\theta) \in \mathbb{R}$$

is of class C^1 . Then, for any vector field $\theta \in C^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ such that $\theta \cdot n = 0$ on $\partial\Omega$, one has: $J'(\Omega)(\theta) = 0$.

Corollary 5.

Under the same hypotheses, if $\theta_1, \theta_2 \in C^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ have the same normal component, i.e. $\theta_1 \cdot n = \theta_2 \cdot n$ on $\partial\Omega$, then:

$$J'(\Omega)(\theta_1) = J'(\Omega)(\theta_2).$$

Structure of shape derivatives (III)

- Actually, the shape derivatives of “many” integral objective functionals $J(\Omega)$ can be put under the **surface form**:

$$J'(\Omega)(\theta) = \int_{\partial\Omega} v_\Omega (\theta \cdot n) \, ds,$$

where the scalar field $v_\Omega : \partial\Omega \rightarrow \mathbb{R}$ depends on J and on the current shape Ω .

- This structure lends itself to the calculation of a **descent direction**: letting $\theta = -tv_\Omega n$, for a small enough **descent step** $t > 0$ in the definition of shape derivatives yields:

$$J(\Omega_{t\theta}) = J(\Omega) - t \int_{\partial\Omega} v_\Omega^2 \, ds + o(t) < J(\Omega).$$

- We shall return to this issue during our study of numerical algorithms.

Part III

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Shape derivatives of PDE constrained functionals

- Hitherto, we have studied the shape derivatives of functionals of the form

$$F_1(\Omega) = \int_{\Omega} f(x) dx, \text{ and } F_2(\Omega) = \int_{\partial\Omega} g(x) ds,$$

where $f, g : \mathbb{R}^d \rightarrow \mathbb{R}$ are given, smooth enough functions.

- We now intend to consider functions of the form

$$J_1(\Omega) = \int_{\Omega} j(u_{\Omega}(x)) dx, \text{ or } J_2(\Omega) = \int_{\partial\Omega} k(u_{\Omega}(x)) ds,$$

where $j, k : \mathbb{R} \rightarrow \mathbb{R}$ are given, smooth enough functions, and $u_{\Omega} : \Omega \rightarrow \mathbb{R}$ is the solution to a PDE posed on Ω .

- Doing so elaborates on the techniques from optimal control theory that we have seen in the parametric optimization context.

The considered framework

- For simplicity, we rely on the simplified model of the Laplace equation with Dirichlet boundary conditions: the state u_Ω is solution to:

$$\begin{cases} -\Delta u_\Omega = f & \text{in } \Omega \\ u_\Omega = 0 & \text{on } \partial\Omega, \end{cases}$$

for a smooth enough source $f : \mathbb{R}^d \rightarrow \mathbb{R}$.

- The associated variational formulation reads:

$$\forall v \in H_0^1(\Omega), \quad \int_{\Omega} \nabla u_\Omega \cdot \nabla v \, dx = \int_{\Omega} fv \, dx.$$

- In this setting:

- We calculate the “derivative” of the state $\Omega \mapsto u_\Omega$ in a sense to be defined.
- We infer the shape derivative of a shape functional of the form:

$$J(\Omega) = \int_{\Omega} j(u_\Omega) \, dx,$$

where $j : \mathbb{R} \rightarrow \mathbb{R}$ is a “smooth enough” function.

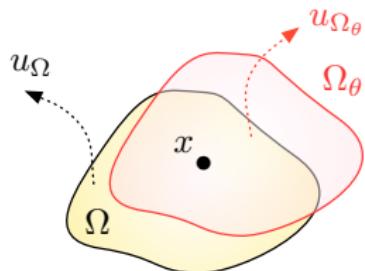
Eulerian and Lagrangian derivatives (I)

- The rigorous way to address this problem requires a notion of differentiation of functions $\Omega \mapsto u_\Omega$, which to a domain Ω associate a function defined on Ω .
- One could think of two ways of doing so:

The Eulerian point of view:

For a fixed $x \in \Omega$, $u'_\Omega(\theta)(x)$ is the derivative of the mapping

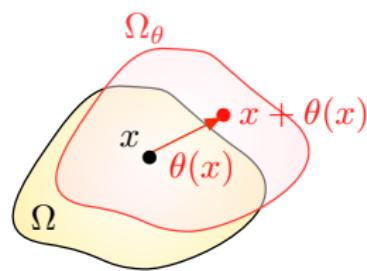
$$\theta \mapsto u_{\Omega_\theta}(x).$$



The Lagrangian point of view:

For a fixed $x \in \Omega$, $u_\Omega(\theta)(x)$ is the derivative of the mapping

$$\theta \mapsto u_{\Omega_\theta}((\text{Id} + \theta)(x)).$$



- The Eulerian notion of shape derivative, however more intuitive, is more difficult to define rigorously. In particular, differentiating the **boundary conditions** satisfied by u_Ω is awkward:

Even for “small” θ , $u_{\Omega_\theta}(x)$ may not make any sense if $x \in \partial\Omega$!

- The Lagrangian derivative $\mathring{u}_\Omega(\theta)$ can be rigorously defined, and lends itself to easier mathematical analysis.
- The rigorous mathematical trail consists in:
 - Defining properly the Lagrangian derivative $\mathring{u}_\Omega(\theta)$;
 - Defining the Eulerian derivative $u'_\Omega(\theta)$ is **defined** from $\mathring{u}_\Omega(\theta)$, via the formula:

$$u'_\Omega(\theta) = \mathring{u}_\Omega(\theta) - \nabla u_\Omega(x) \cdot \theta,$$

so that the expected **chain rule** holds for the expression $u_{(\text{Id}+\theta)(\Omega)} \circ (\text{Id} + \theta)$:

$$\forall x \in \Omega, \quad \mathring{u}_\Omega(\theta)(x) = u'_\Omega(\theta)(x) + \nabla u_\Omega(x) \cdot \theta(x).$$

Let $\Omega \mapsto u_\Omega \in H^1(\Omega)$ be a function which to a domain Ω , associates a function u_Ω defined on Ω .

Definition 2.

The mapping $u : \Omega \mapsto u_\Omega$ admits a **material**, or **Lagrangian** derivative $\dot{u}_\Omega(\theta) \in H^1(\Omega)$ at a particular domain Ω provided the **transported function**

$$W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d) \ni \theta \longmapsto \bar{u}(\theta) := u_{\Omega_\theta} \circ (\text{Id} + \theta) \in H^1(\Omega),$$

defined in the neighborhood of $0 \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$, is differentiable at $\theta = 0$.

This allows to *define* the notion of Eulerian derivative.

Definition 3.

The mapping $u : \Omega \mapsto u_\Omega$ has a **Eulerian derivative** $u'_\Omega(\theta)$ at a given domain Ω in the direction $\theta \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ if:

- ① It admits a material derivative $\dot{u}_\Omega(\theta)$ at Ω ;
- ② the quantity $\nabla u_\Omega \cdot \theta$ belongs to $H^1(\Omega)$.

One defines then:

$$u'_\Omega(\theta) = \dot{u}_\Omega(\theta) - \nabla u_\Omega \cdot \theta \in H^1(\Omega).$$

Once Lagrangian and Eulerian derivatives are known, the shape derivative of a quantity of interest involving u_Ω is readily obtained.

Proposition 6.

Let $\Omega \subset \mathbb{R}^d$ be a smooth bounded domain, and suppose that $\Omega \mapsto u_\Omega$ has a Lagrangian derivative \mathring{u}_Ω at Ω . If $j : \mathbb{R} \rightarrow \mathbb{R}$ is regular enough, the function

$$J(\Omega) = \int_{\Omega} j(u_\Omega) \, dx$$

is then **shape differentiable** at Ω , and:

$$\forall \theta \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d), \quad J'(\Omega)(\theta) = \int_{\Omega} (j'(u_\Omega) \mathring{u}_\Omega(\theta) + (\operatorname{div} \theta) j(u_\Omega)) \, dx.$$

If, in addition, $\Omega \mapsto u_\Omega$ has a Eulerian derivative u'_Ω at Ω , the “chain rule” holds:

$$J'(\Omega)(\theta) = \underbrace{\int_{\partial\Omega} j(u_\Omega) \theta \cdot n \, ds}_{\substack{\text{Derivative of the partial mapping} \\ \Omega \mapsto \int_{\partial\Omega} j(u_\Omega)}} + \underbrace{\int_{\Omega} j'(u_\Omega) u'_\Omega(\theta) \, dx}_{\substack{\text{Derivative of the partial mapping} \\ \Omega \mapsto \int_{\Omega} j(u_\Omega)}}$$

Eulerian and Lagrangian derivatives (VI)

Idea of the proof: As usual, a **change of variables** yields:

$$J(\Omega_\theta) = \int_{(\text{Id}+\theta)(\Omega)} j(u_{\Omega_\theta}) \, dx = \int_{\Omega} |\det(I + \nabla\theta)| j(\bar{u}(\theta)) \, dx.$$

- The mapping $\theta \mapsto |\det(I + \nabla\theta)|$ is Fréchet differentiable at $\theta = 0$ and

$$|\det(I + \nabla\theta)| = 1 + \text{div}\theta + o(\theta);$$

- The mapping $\theta \mapsto \bar{u}(\theta)$ is Fréchet differentiable at $\theta = 0$ and

$$\bar{u}(\theta) = u_\Omega + \mathring{u}_\Omega(\theta) + o(\theta);$$

Then, using the **chain rule**, $\theta \mapsto J(\Omega_\theta)$ is Fréchet differentiable at $\theta = 0$, and:

$$J'(\Omega)(\theta) = \int_{\Omega} ((\text{div}\theta)j(u_\Omega) + j'(u_\Omega)\mathring{u}_\Omega(\theta)) \, dx.$$

Now, if $\Omega \mapsto u_\Omega$ as a **Eulerian derivative**, the **definition** $u'_\Omega(\theta) = \mathring{u}_\Omega(\theta) - \nabla u_\Omega \cdot \theta$ combined with the Green's formula yields:

$$J'(\Omega)(\theta) = \int_{\partial\Omega} j(u_\Omega) \theta \cdot n \, ds + \int_{\Omega} j'(u_\Omega)u'_\Omega(\theta) \, dx.$$



Eulerian and Lagrangian derivatives (VII)

The calculation of the shape derivative $J'(\Omega)(\theta)$ thus rests on those of the Lagrangian and Eulerian derivatives of $\Omega \mapsto u_\Omega$, where

$$\begin{cases} -\Delta u_\Omega = f & \text{in } \Omega, \\ u_\Omega = 0 & \text{on } \partial\Omega. \end{cases}$$

The following result characterizes the **Lagrangian derivative** of $\Omega \mapsto u_\Omega$.

Theorem 7.

The mapping $\Omega \mapsto u_\Omega \in H_0^1(\Omega)$ has a **Lagrangian derivative** $\mathring{u}_\Omega(\theta)$, and for any $\theta \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$, $\mathring{u}_\Omega(\theta) \in H_0^1(\Omega)$ is the unique solution to the variational problem:

$$\begin{aligned} \forall v \in H_0^1(\Omega), \quad & \int_{\Omega} \nabla(u_\Omega(\theta)) \cdot \nabla v \, dx = \int_{\Omega} \operatorname{div}(f\theta)v \, dx \\ & - \int_{\Omega} (\operatorname{div}(\theta)\mathbf{I} - \nabla\theta - \nabla\theta^T) \nabla u_\Omega \cdot \nabla v \, dx, \end{aligned}$$

or, under classical form:

$$\begin{cases} -\Delta(\mathring{u}_\Omega(\theta)) = \operatorname{div}(f\theta) - \operatorname{div}((\operatorname{div}(\theta)\mathbf{I} - \nabla\theta - \nabla\theta^T)\nabla u_\Omega) & \text{in } \Omega, \\ \mathring{u}_\Omega(\theta) = 0 & \text{on } \partial\Omega. \end{cases}$$

Idea of the proof:

- The variational problem satisfied by u_{Ω_θ} is:

$$\forall v \in H_0^1(\Omega_\theta), \quad \int_{\Omega_\theta} \nabla u_{\Omega_\theta} \cdot \nabla v \, dx = \int_{\Omega_\theta} fv \, dx.$$

- By a change of variables, the **transported function** $\bar{u}(\theta) = u_{\Omega_\theta} \circ (\text{Id} + \theta)$ satisfies:

$$\forall v \in H_0^1(\Omega), \quad \int_{\Omega} A(\theta) \nabla \bar{u}(\theta) \cdot \nabla v \, dx = \int_{\Omega} |\det(I + \nabla \theta)| (f \circ (\text{Id} + \theta)) v \, dx,$$

where

$$A(\theta) := |\det(I + \nabla \theta)| (I + \nabla \theta)^{-1} (I + \nabla \theta)^{-T}.$$

- This variational problem features a **fixed domain** and a **fixed function space** $H_0^1(\Omega)$, and only the **coefficients of the formulation** depend on θ .

⇒ This structure lends itself to the use of the strategy based on the **Implicit Function theorem** to calculate the derivative of $\theta \mapsto \bar{u}(\theta)$.

- The problem can now be written as an equation for $\bar{u}(\theta)$:

$$\mathcal{F}(\theta, \bar{u}(\theta)) = \mathcal{G}(\theta),$$

for appropriate definitions of the operators:

- $\mathcal{F} : W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d) \times H_0^1(\Omega) \rightarrow H^{-1}(\Omega)$,
- $\mathcal{G} : W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d) \rightarrow H^{-1}(\Omega)$.
- The **implicit function theorem** shows that $\theta \mapsto \bar{u}(\theta)$ is differentiable at $\theta = 0$.
- The **Lagrangian derivative** $\dot{u}_\Omega(\theta)$ of the **transported mapping** $\bar{u}(\theta)$ can now be computed by taking derivatives inside the variational formula:

$$\begin{aligned} \forall v \in H_0^1(\Omega), \quad & \int_{\Omega} \nabla \dot{u}_\Omega(\theta) \cdot \nabla v \, dx = \int_{\Omega} \operatorname{div}(f\theta)v \, dx \\ & - \int_{\Omega} (\operatorname{div}(\theta)\mathbf{I} - \nabla\theta - \nabla\theta^T) \nabla u_\Omega \cdot \nabla v \, dx. \end{aligned}$$



Eulerian and Lagrangian derivatives (X)

- The Eulerian derivative of u_Ω can now be computed from its Lagrangian derivative. It satisfies (after elementary, but tedious calculations):

$$\begin{cases} -\Delta(u'_\Omega(\theta)) = 0 & \text{in } \Omega, \\ u'_\Omega(\theta) = -(\theta \cdot n) \frac{\partial u_\Omega}{\partial n} & \text{on } \partial\Omega. \end{cases}$$

- At this point, we have thus calculated the shape derivative of $J(\Omega)$ as:

$$J'(\Omega)(\theta) = \int_{\Omega} (j'(u_\Omega) \dot{u}_\Omega(\theta) + (\operatorname{div}\theta) j(u_\Omega)) \, dx,$$

or, involving the Eulerian derivative of $\Omega \mapsto u_\Omega$,

$$J'(\Omega)(\theta) = \int_{\partial\Omega} j(u_\Omega) \theta \cdot n \, ds + \int_{\Omega} j'(u_\Omega) u'_\Omega(\theta) \, dx.$$

- The identification of a descent direction θ for $J(\Omega)$ (i.e. such that $J'(\Omega)(\theta) < 0$) is awkward, since $\dot{u}_\Omega(\theta)$ and $u'_\Omega(\theta)$ depend implicitly on θ (via a PDE).

Idea: “**Lift**” the term of $J'(\Omega)(\theta)$ which features the Lagrangian (or the Eulerian) derivative of u_Ω by introducing an **adequate adjoint problem**.

Theorem 8.

The shape derivative $J'(\Omega)(\theta)$ rewrites (**volume form**):

$$J'(\Omega)(\theta) = \int_{\Omega} (\operatorname{div}\theta) j(u_\Omega) \, dx + \int_{\Omega} (\operatorname{div}(\theta)\mathbf{I} - \nabla\theta - \nabla\theta^T) \nabla u_\Omega \cdot \nabla p_\Omega \, dx$$

forme volumique

$$- \int_{\Omega} \operatorname{div}(f\theta)p_\Omega \, dx,$$

where the **adjoint state** $p_\Omega \in H_0^1(\Omega)$ is the solution to the equation:

$$\begin{cases} -\Delta p_\Omega = -j'(u_\Omega) & \text{in } \Omega, \\ p_\Omega = 0 & \text{on } \partial\Omega. \end{cases}$$

If u_Ω and p_Ω are **more regular** ($u_\Omega, p_\Omega \in H^2(\Omega)$), this rewrites under the equivalent **surface form**:

forme surfacique => plus simple pour direction descendante

$$J'(\Omega)(\theta) = \int_{\partial\Omega} j(u_\Omega)\theta \cdot n \, ds - \int_{\partial\Omega} \frac{\partial u_\Omega}{\partial n} \frac{\partial p_\Omega}{\partial n} \theta \cdot n \, ds - \int_{\partial\Omega} f p_\Omega \theta \cdot n \, ds.$$

Proof of the volume form.

- The shape derivative $J'(\Omega)(\theta)$ reads: u point inconnu !

$$J'(\Omega)(\theta) = \int_{\Omega} (j'(u_{\Omega}) \dot{u}_{\Omega}(\theta) + (\operatorname{div} \theta) j(u_{\Omega})) \, dx.$$

- Here, the Lagrangian derivative $\dot{u}_{\Omega}(\theta) \in H_0^1(\Omega)$ solves:

$$\forall v \in H_0^1(\Omega), \quad \int_{\Omega} \nabla \dot{u}_{\Omega}(\theta) \cdot \nabla v \, dx = \int_{\Omega} \operatorname{div}(f\theta) v \, dx \quad \text{u point solution equation}$$
$$- \int_{\Omega} (\operatorname{div}(\theta) I - \nabla \theta - \nabla \theta^T) \nabla u_{\Omega} \cdot \nabla v \, dx.$$

- This is to be compared with the variational formulation for p_{Ω} :

definition p pour le remplace dans J' $\forall v \in H_0^1(\Omega), \quad \int_{\Omega} \nabla p_{\Omega} \cdot \nabla v \, dx = - \int_{\Omega} j'(u_{\Omega}) v \, dx.$

Eulerian and Lagrangian derivatives (XIII): the adjoint method

- Thus,

$$\begin{aligned} J'(\Omega)(\theta) &= \int_{\Omega} (\operatorname{div} \theta) j(u_{\Omega}) \, dx + \int_{\Omega} j'(u_{\Omega}) \mathring{u}_{\Omega}(\theta) \, dx, \\ &= \int_{\Omega} (\operatorname{div} \theta) j(u_{\Omega}) \, dx - \int_{\Omega} \nabla p_{\Omega} \cdot \nabla \mathring{u}_{\Omega}(\theta) \, dx, \end{aligned}$$

where we have used the variational formulation for p_Ω with $\dot{u}_\Omega(\theta)$ as test function.

- Now taking p_Ω as test function in the variational formulation for $\dot{u}_\Omega(\theta)$ yields the desired result:

$$J'(\Omega)(\theta) = \int_{\Omega} (\operatorname{div}\theta) j(u_{\Omega}) \, dx + \int_{\Omega} (\operatorname{div}(\theta)\mathbf{I} - \nabla\theta - \nabla\theta^T) \nabla u_{\Omega} \cdot \nabla p_{\Omega} \, dx$$

theta explicite

$$- \int_{\Omega} \operatorname{div}(f\theta) p_{\Omega} \, dx.$$

theta explicite



Proof of the surface form. The main idea reads as follows:

- Since u_Ω and $p_\Omega \in H^2(\Omega)$, we perform integration by parts in the volume form to end up with an expression of the form:

$$J'(\Omega)(\theta) = \int_{\partial\Omega} v_\Omega \theta \cdot n \, ds + \int_{\partial\Omega} t_\Omega \cdot \theta_{\partial\Omega} \, ds + \int_{\Omega} S_\Omega \cdot \theta \, dx,$$

where:

- $v_\Omega : \partial\Omega \rightarrow \mathbb{R}$ is a scalar field;
- $t_\Omega : \partial\Omega \rightarrow \mathbb{R}^d$ is a vector field, acting on the tangential component of θ :

$$\theta_{\partial\Omega} := \theta - (\theta \cdot n)n;$$

- $S_\Omega : \Omega \rightarrow \mathbb{R}^d$ is a vector field,

whose expressions are explicit in terms of u_Ω and p_Ω .

- If we believe the **Structure theorem**, t_Ω and S_Ω must equal 0, ... which we verify.
- A tedious calculation eventually yields the result:

$$J'(\Omega)(\theta) = \int_{\partial\Omega} j(u_\Omega)\theta \cdot n \, ds - \int_{\partial\Omega} \frac{\partial u_\Omega}{\partial n} \frac{\partial p_\Omega}{\partial n} \theta \cdot n \, ds - \int_{\partial\Omega} f p_\Omega \theta \cdot n \, ds.$$

Eulerian and Lagrangian derivatives: volume form vs. surface form

- The volume form is easier to derive, and demands **minimal regularity** from u_Ω, p_Ω .
- For this reason, it is often more convenient for studying mathematical properties of shape derivatives (e.g. their finite element approximation).
- The volume form is explicit in terms of θ ... but it does not allow for a straightforward identification of a descent direction.
⇒ Need to rely on the "Hilbertian trick" to achieve this.

- The surface form requires **higher regularity** from u_Ω, p_Ω , which is often guaranteed by **elliptic regularity**, provided Ω and f are "smooth enough".
- The surface form has a more compact expression, which explicitly fulfills the **Structure theorem**.
⇒ A descent direction θ for $J(\Omega)$ is immediately revealed.

- Mathematically speaking, the above trail is the rigorous way to assess the differentiability of shape functionals.
- As we have seen, the techniques presented above (in particular the adjoint technique) exist in much more general frameworks than shape optimization, and pertain to the framework of optimal control theory.
- Calculating shape derivatives by these means requires tedious calculations.
- In practice, a version of Céa's method allows for a formal, simpler way to calculate shape derivatives. méthode informelle + simple pour dérivée de forme

Part III

Geometric optimization problems

- 1 The method of Hadamard and shape derivatives
- 2 Shape derivatives of PDE-constrained functionals: the rigorous way, using Eulerian and material derivatives
- 3 Céa's method for calculating shape derivatives
- 4 Numerical aspects of geometric methods
- 5 The level set method for shape optimization

Céa's method (I)

As we have seen, the philosophy of Céa's method comes from optimization theory:

- We express $J(\Omega)$ as the value of an Ω -dependent Lagrangian functional:

$$\mathcal{L}(\Omega, u, p) = \underbrace{\int_{\Omega} j(u) \, dx}_{\text{Objective function at stake}} + \underbrace{\int_{\Omega} (-\Delta u - f)p \, dx}_{u=u_{\Omega} \text{ is enforced as a constraint by penalization with the Lagrange multiplier } p},$$

at a saddle point $(u, p) = (u_{\Omega}, p_{\Omega})$.

- The “parameter” Ω , and the variables (u, p) must be independent.
- The nice features of the derivative of a saddle point value with respect to a parameter allow for significant simplifications in the calculation.

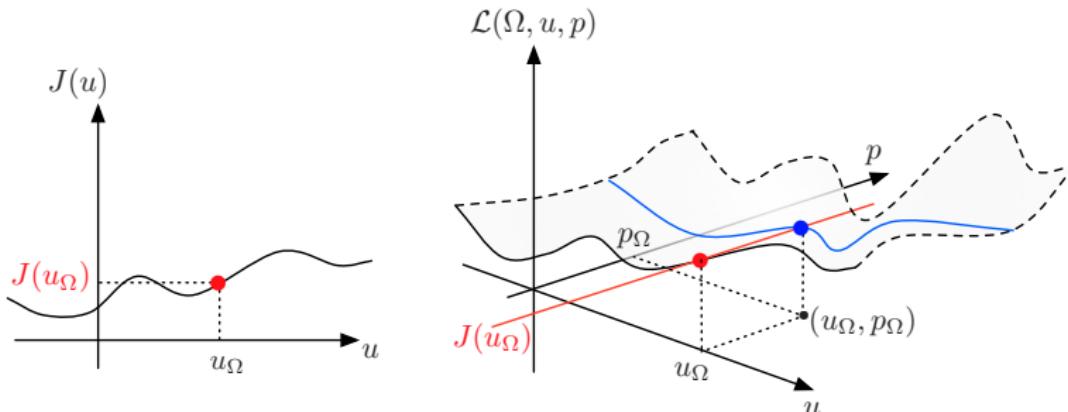
This method is formal: in particular, it assumes that we already know that $\Omega \mapsto u_{\Omega}$ is differentiable.

Céa's method (II)

- The objective function $J(\Omega)$ is expressed as the value

$$J(\Omega) = \mathcal{L}(\Omega, u_\Omega, p_\Omega),$$

of a suitably defined Lagrangian $\mathcal{L}(\Omega, u, p)$ at a saddle point (u_Ω, p_Ω) .



- The shape derivative $J'(\Omega)(\theta)$ reads, formally:

$$J'(\Omega)(\theta) = \underbrace{\frac{\partial \mathcal{L}}{\partial \Omega}(\Omega, u_\Omega, p_\Omega)(\theta)}_{\text{Shape derivative of } \Omega \mapsto \mathcal{L}(\Omega, u, p) \text{ taken at } (u, p) = (u_\Omega, p_\Omega)} + \underbrace{\frac{\partial \mathcal{L}}{\partial u}(\Omega, u_\Omega, p_\Omega)(u'_\Omega(\theta))}_{=0} + \underbrace{\frac{\partial \mathcal{L}}{\partial p}(\Omega, u_\Omega, p_\Omega)(p'_\Omega(\theta))}_{=0}.$$

car u et p sont des points selle

Céa's method: the Neumann case (I)

We first consider the case of Neumann boundary conditions:

$$\begin{cases} -\Delta u + \mathbf{u} = f & \text{in } \Omega, \\ \frac{\partial \mathbf{u}}{\partial n} = 0 & \text{on } \partial\Omega, \end{cases}$$

where the $+\mathbf{u}$ term is added for commodity, so that the system is well-posed in $H^1(\Omega)$ without any further assumption on f .

Consider the following **Lagrangian functional**:

$$\mathcal{L}(\Omega, \mathbf{u}, p) = \underbrace{\int_{\Omega} j(\mathbf{u}) dx}_{\text{Objective function where } u_{\Omega} \text{ is replaced by } \mathbf{u}} + \underbrace{\int_{\Omega} \nabla \mathbf{u} \cdot \nabla p dx + \int_{\Omega} \mathbf{u} p dx - \int_{\Omega} f p dx}_{\text{Penalization of the "constraint" } \mathbf{u}=u_{\Omega}: \int_{\Omega} (-\Delta \mathbf{u} + \mathbf{u} - f)p dx = 0}$$

which is defined for any shape $\Omega \in \mathcal{U}_{ad}$, and for any $\mathbf{u}, p \in H^1(\mathbb{R}^d)$, so that the variables Ω , \mathbf{u} and p are independent.

Céa's method: the Neumann case (II)

By construction, evaluating $\mathcal{L}(\Omega, u, p)$ with $u = u_\Omega$ yields:

$$\forall p \in H^1(\mathbb{R}^d), \quad \mathcal{L}(\Omega, u_\Omega, p) = \int_{\Omega} j(u_\Omega) dx = J(\Omega).$$

For a fixed shape Ω , we search for the **saddle points** $(u, p) \in \mathbb{R}^d \times \mathbb{R}^d$ of $\mathcal{L}(\Omega, \cdot, \cdot)$.
The first-order necessary conditions read:

- $\forall \hat{p} \in H^1(\mathbb{R}^d), \quad \frac{\partial \mathcal{L}}{\partial p}(\Omega, u, p)(\hat{p}) =$
$$\int_{\Omega} \nabla u \cdot \nabla \hat{p} dx + \int_{\Omega} u \hat{p} dx - \int_{\Omega} f \hat{p} dx = 0.$$
- $\forall \hat{u} \in H^1(\mathbb{R}^d), \quad \frac{\partial \mathcal{L}}{\partial u}(\Omega, u, p)(\hat{u}) =$
$$\int_{\Omega} j'(u) \hat{u} dx + \int_{\Omega} \nabla \hat{u} \cdot \nabla p dx + \int_{\Omega} \hat{u} p dx = 0.$$

Céa's method: the Neumann case (III)

Step 1: Identification of u :

$$\forall q \in H^1(\mathbb{R}^d), \int_{\Omega} \nabla u \cdot \nabla q \, dx + \int_{\Omega} uq \, dx - \int_{\Omega} fq \, dx = 0.$$

- Taking q as any \mathcal{C}^∞ function ψ with compact support in Ω yields:

$$\int_{\Omega} \nabla u \cdot \nabla \psi \, dx + \int_{\Omega} u\psi \, dx - \int_{\Omega} f\psi \, dx = 0 \Rightarrow \boxed{-\Delta u + u = f \text{ in } \Omega}.$$

- Now taking q as any \mathcal{C}^∞ function ψ and using Green's formula:

$$\int_{\partial\Omega} \frac{\partial u}{\partial n} \psi \, ds = 0 \Rightarrow \boxed{\frac{\partial u}{\partial n} = 0 \text{ on } \partial\Omega}.$$

Conclusion: $u = u_\Omega$.

Céa's method: the Neumann case (IV)

Step 2: Identification of p :

$$\forall v \in H^1(\mathbb{R}^d), \int_{\Omega} j'(u)v + \int_{\Omega} \nabla v \cdot \nabla p \, dx + \int_{\Omega} vp \, dx = 0.$$

- Taking v as any \mathcal{C}^∞ function ψ with compact support in Ω yields:

$$\int_{\Omega} \nabla p \cdot \nabla \psi \, dx + \int_{\Omega} vp \, dx + \int_{\Omega} j'(u)\psi \, dx = 0 \Rightarrow -\Delta p + p = -j'(u_\Omega) \text{ in } \Omega.$$

- Now taking v as any \mathcal{C}^∞ function ψ and using Green's formula:

$$\int_{\partial\Omega} \frac{\partial p}{\partial n} \psi \, ds = 0 \Rightarrow \frac{\partial p}{\partial n} = 0 \text{ on } \partial\Omega.$$

Conclusion: $p = p_\Omega$, solution to $\begin{cases} -\Delta p + p = -j'(u_\Omega) & \text{in } \Omega, \\ \frac{\partial p}{\partial n} = 0 & \text{on } \partial\Omega. \end{cases}$

Step 3: Calculation of the shape derivative $J'(\Omega)(\theta)$:

- We go back to the fact that:

$$\forall q \in H^1(\mathbb{R}^d), \quad \mathcal{L}(\Omega, u_\Omega, q) = \int_{\Omega} j(u_\Omega) \, dx = J(\Omega).$$

car si $u = u_{\Omega}$ est une penalisation s'améliore

- Differentiating with respect to Ω yields, thanks to the chain rule:

$$\forall \theta \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d), \quad J'(\Omega)(\theta) = \frac{\partial \mathcal{L}}{\partial \Omega}(\Omega, u_\Omega, q)(\theta) + \frac{\partial \mathcal{L}}{\partial u}(\Omega, u_\Omega, q)(u'_\Omega(\theta)),$$

where $u'_\Omega(\theta)$ is the Eulerian derivative of $\Omega \mapsto u_\Omega$ (assumed to exist).

- Now, choosing $q = p_\Omega$ produces, since $\frac{\partial \mathcal{L}}{\partial u}(\Omega, u_\Omega, p_\Omega) = 0$:

$$J'(\Omega)(\theta) = \frac{\partial \mathcal{L}}{\partial \Omega}(\Omega, u_\Omega, p_\Omega)(\theta).$$

Céa's method: the Neumann case (VI)

The last (partial) derivative boils down to that of a functional of the form:

$$\Omega \mapsto \int_{\Omega} f(x) \, dx,$$

where f is a fixed function.

théorème sur la dérivée de fonction
explicites de omega

Using Theorem 2, we end up with:

$$\forall \theta \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d),$$

$$J'(\Omega)(\theta) = \int_{\partial\Omega} \left(j(u_{\Omega}) + \nabla u_{\Omega} \cdot \nabla p_{\Omega} + u_{\Omega} p_{\Omega} - f p_{\Omega} \right) \theta \cdot n \, ds.$$

Céa's method: the Dirichlet case (I)

- We now consider the problem of calculating the derivative of:

$$J(\Omega) = \int_{\Omega} j(u_{\Omega}) \, dx, \text{ where } \begin{cases} -\Delta u = f & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega. \end{cases} .$$

- Warning:** When the state u_{Ω} satisfies **essential boundary conditions**, i.e. boundary conditions that are tied to the **definition space of functions** (here, $H_0^1(\Omega)$), an additional difficulty generally arises.
- It is no longer possible to rely on the Lagrangian

$$\mathcal{L}(\Omega, u, p) = \int_{\Omega} j(u) \, dx + \int_{\Omega} \nabla u \cdot \nabla p \, dx - \int_{\Omega} fp \, dx,$$

since it would have to be defined for $u, p \in H_0^1(\Omega)$.

espace dépend de omeg à cause the la CL !!

- In this case, the arguments Ω, u, p would not be **independent**.

Céa's method: the Dirichlet case (II)

Solution: Add an extra variable $p \in H^1(\mathbb{R}^d)$ to the Lagrangian to **penalize** the boundary condition: for all $u, p, \lambda \in H^1(\mathbb{R}^d)$; on se ramène à un espace H1 indépendant

$$\mathcal{L}(\Omega, u, p, \lambda) = \underbrace{\int_{\Omega} j(u) \, dx}_{\text{Objective function where } u_{\Omega} \text{ is replaced by } u} + \underbrace{\int_{\Omega} (-\Delta u - f)p \, dx}_{\text{penalization of the "constraint" } -\Delta u = f} + \underbrace{\int_{\partial\Omega} \lambda u \, ds}_{\text{penalization of the "constraint" } u=0 \text{ on } \partial\Omega} .$$

nouveau multiplicateur lambda pour enforcer la contrainte sur les bords

By Green's formula, $\mathcal{L}(u, p, \lambda)$ rewrites:

$$\mathcal{L}(\Omega, u, p, \lambda) = \int_{\Omega} j(u) \, dx + \int_{\Omega} \nabla u \cdot \nabla p \, dx - \int_{\Omega} fp \, dx + \int_{\partial\Omega} \left(\lambda u - \frac{\partial u}{\partial n} p \right) \, ds.$$

Of course, evaluating $\mathcal{L}(u, p, \lambda)$ with $u = u_{\Omega}$, it comes:

$$\forall p, \lambda \in H^1(\mathbb{R}^d), \quad \mathcal{L}(\Omega, u_{\Omega}, p, \lambda) = \int_{\Omega} j(u_{\Omega}) \, dx.$$

Céa's method: the Dirichlet case (III)

For a fixed shape Ω , we look for the **saddle points** $(u, p, \lambda) \in (H^1(\mathbb{R}^d))^3$ of the functional $\mathcal{L}(\Omega, \cdot, \cdot, \cdot)$. The first-order necessary conditions are:

- $\forall \hat{p} \in H^1(\mathbb{R}^d), \frac{\partial \mathcal{L}}{\partial p}(\Omega, u, p, \lambda)(\hat{p}) = \int_{\Omega} \nabla u \cdot \nabla \hat{p} \, dx - \int_{\Omega} f \hat{p} \, dx + \int_{\partial\Omega} \frac{\partial u}{\partial n} \hat{p} \, ds = 0.$
- $\forall \hat{u} \in H^1(\mathbb{R}^d), \frac{\partial \mathcal{L}}{\partial u}(\Omega, u, p, \lambda)(\hat{u}) = \int_{\Omega} j'(u) \hat{u} \, dx + \int_{\Omega} \nabla \hat{u} \cdot \nabla p \, dx + \int_{\partial\Omega} \left(\lambda \hat{u} - \frac{\partial \hat{u}}{\partial n} p \right) \, ds = 0.$
- $\forall \hat{\lambda} \in H^1(\mathbb{R}^d), \frac{\partial \mathcal{L}}{\partial \lambda}(\Omega, u, p, \lambda)(\hat{\lambda}) = \int_{\partial\Omega} \hat{\lambda} u \, ds = 0.$

Céa's method: the Dirichlet case (IV)

Step 1: Identification of u :

$$\forall q \in H^1(\mathbb{R}^d), \int_{\Omega} \nabla u \cdot \nabla q \, dx - \int_{\Omega} f q \, dx + \int_{\partial\Omega} \frac{\partial u}{\partial n} q \, ds = 0.$$

- Taking q as any \mathcal{C}^∞ function ψ with compact support in Ω yields:

$$\forall \psi \in \mathcal{C}_c^\infty(\Omega), \int_{\Omega} \nabla u \cdot \nabla \psi \, dx = \int_{\Omega} f \psi \, dx \Rightarrow \boxed{-\Delta u = f \text{ in } \Omega.}$$

- Using $\frac{\partial \mathcal{L}}{\partial \lambda}(\Omega, u, p, \lambda)(\mu) = 0$ for any $\mu = \psi \in \mathcal{C}_c^\infty(\mathbb{R}^d)$ yields:

$$\forall \psi \in \mathcal{C}_c^\infty(\mathbb{R}^d), \int_{\partial\Omega} \psi u \, ds = 0 \Rightarrow \boxed{u = 0 \text{ on } \partial\Omega.}$$

Conclusion: $u = u_\Omega$.

Céa's method: the Dirichlet case (V)

Step 2: Identification of p :

$$\forall v \in H^1(\mathbb{R}^d), \int_{\Omega} j'(u)v \, dx + \int_{\Omega} \nabla v \cdot \nabla p \, dx + \int_{\partial\Omega} \left(\lambda v - \frac{\partial v}{\partial n} p \right) \, ds = 0.$$

- Taking q as any \mathcal{C}^∞ function ψ with compact support in Ω yields:

$$\forall \psi \in \mathcal{C}_c^\infty(\Omega), \int_{\Omega} \nabla p \cdot \nabla \psi \, dx + \int_{\Omega} j'(u)\psi \, dx = 0$$

$$\Rightarrow \boxed{-\Delta p = -j'(u_\Omega) \text{ in } \Omega.}$$

- Now taking v as a \mathcal{C}^∞ function ψ and using Green's formula:

$$\forall \psi \in \mathcal{C}_c^\infty(\mathbb{R}^d), \int_{\partial\Omega} \frac{\partial p}{\partial n} \psi \, ds + \int_{\partial\Omega} \left(\lambda \psi - \frac{\partial \psi}{\partial n} p \right) \, ds = 0.$$

Step 2 (continued):

- Varying the normal trace $\frac{\partial \psi}{\partial n}$ while imposing $\psi = 0$ on $\partial\Omega$, one gets:

$$p = 0 \text{ on } \partial\Omega.$$

Conclusion: $p = p_\Omega$, solution to $\begin{cases} -\Delta p = -j'(u_\Omega) & \text{in } \Omega, \\ p = 0 & \text{on } \partial\Omega. \end{cases}$

- In addition, varying the trace of ψ on $\partial\Omega$ while imposing $\frac{\partial \psi}{\partial n} = 0$:

$$\lambda_\Omega = -\frac{\partial p_\Omega}{\partial n} \text{ on } \partial\Omega.$$

Step 3: Calculation of the shape derivative $J'(\Omega)(\theta)$:

- We return to the fact that:

$$\forall q, \mu \in H^1(\mathbb{R}^d), \quad \mathcal{L}(\Omega, u_\Omega, q, \mu) = \int_{\Omega} j(u_\Omega) \, dx.$$

- Differentiating with respect to Ω yields, for all $\theta \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$:

$$J'(\Omega)(\theta) = \frac{\partial \mathcal{L}}{\partial \Omega}(\Omega, u_\Omega, q, \mu)(\theta) + \frac{\partial \mathcal{L}}{\partial u}(\Omega, u_\Omega, q, \mu)(u'_\Omega(\theta)),$$

where $u'_\Omega(\theta)$ is the **Eulerian derivative** of $\Omega \mapsto u_\Omega$.

- Taking $q = p_\Omega$, $\mu = \lambda_\Omega$ produces, since $\frac{\partial \mathcal{L}}{\partial u}(\Omega, u_\Omega, p_\Omega, \lambda_\Omega) = 0$:

$$J'(\Omega)(\theta) = \frac{\partial \mathcal{L}}{\partial \Omega}(\Omega, u_\Omega, p_\Omega, \lambda_\Omega)(\theta).$$

Céa's method: the Dirichlet case (VIII)

Again, this (partial) shape derivative combines derivatives of functions of the form:

$$\Omega \mapsto \int_{\Omega} f(x) dx, \text{ or } \Omega \mapsto \int_{\partial\Omega} g(x) ds,$$

where f and g are fixed functions.

Using Theorems 2 and 3 (and after some calculation), we end up with:

$$\forall \theta \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d), \quad J'(\Omega)(\theta) = \int_{\partial\Omega} \left(j(u_{\Omega}) - \frac{\partial u_{\Omega}}{\partial n} \frac{\partial p_{\Omega}}{\partial n} \right) \theta \cdot n ds.$$

Part III

Geometric optimization problems

- 1 The method of Hadamard and shape derivatives
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Initialization: Start from an initial shape Ω^0 .

For $n = 0, \dots$ **convergence**,

- ① Calculate the **state** u_{Ω^n} (and the **adjoint** p_{Ω^n} if need be) on Ω^n .
- ② Compute the shape derivative $J'(\Omega^n)$ by evaluating the mathematical formula, and infer a **descent direction** θ^n for $J(\Omega)$.
- ③ **Advect** the shape Ω^n along the displacement field θ^n , for a small **pseudo-time step** τ^n , so as to obtain

$$\Omega^{n+1} = (\text{Id} + \tau^n \theta^n)(\Omega^n).$$

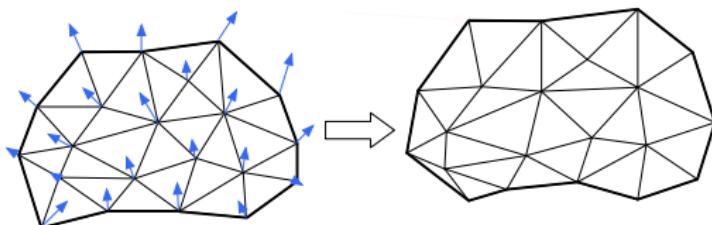
One possible implementation

- Each shape Ω^n is represented by a **simplicial mesh** \mathcal{T}^n (i.e. composed of triangles in $2d$ and of tetrahedra in $3d$).
- The **Finite Element method** is used on \mathcal{T}^n for computing u_{Ω^n} (and p_{Ω^n}).
- The descent direction θ^n is obtained from the **surface form** of the shape derivative:

$$J'(\Omega)(\theta) = \int_{\partial\Omega} v_{\Omega} \theta \cdot n \, ds \quad \Rightarrow \quad \theta^n = -v_{\Omega^n} n \text{ on } \partial\Omega.$$

- The **shape advection** step $\Omega^n \xrightarrow{(\text{Id} + \tau^n \theta^n)} \Omega^{n+1}$ is performed by **pushing the nodes** of \mathcal{T}^n along $\tau^n \theta^n$, to obtain the new mesh \mathcal{T}^{n+1} :

$$\forall \text{ vertex } x \in \mathcal{T}^n, \quad x \mapsto x + \tau^n \theta^n(x).$$



Deformation of a mesh by relocating its nodes to a prescribed final position.

Numerical examples (I)

- In the context of linear elasticity, one aims at minimizing the compliance $C(\Omega)$ of a cantilever beam:

$$C(\Omega) = \int_{\Omega} A e(u_{\Omega}) : e(u_{\Omega}) \, dx.$$

- An equality constraint on the volume $\text{Vol}(\Omega)$ of shapes is imposed by means of a fixed penalization procedure.

Numerical examples (II)

- In the context of **fluid mechanics** (Stokes equations), one aims at minimizing the **viscous dissipation** $D(\Omega)$ in a pipe:

$$D(\Omega) = 2\nu \int_{\Omega} D(u_{\Omega}) : D(u_{\Omega}) \, dx.$$

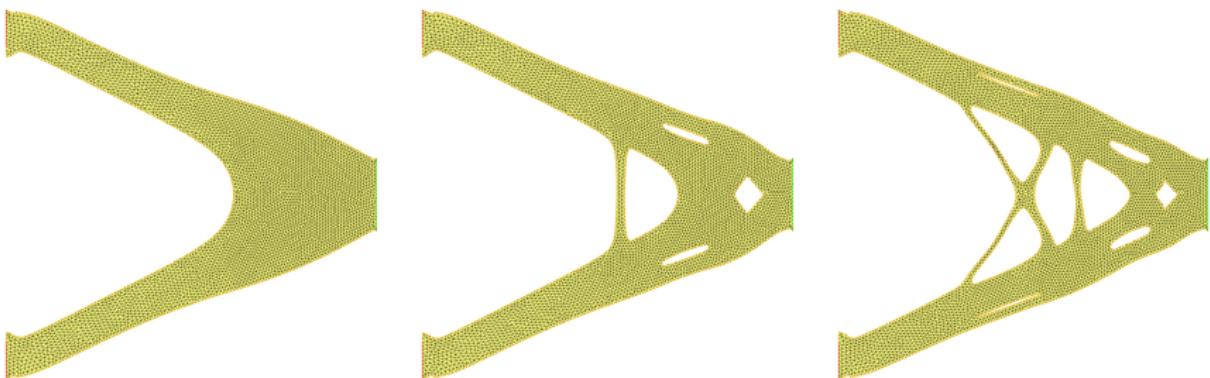
- A **volume constraint** is imposed by a *fixed* penalization of the function $D(\Omega)$.

Numerical examples (III)

- Still in **fluid mechanics**, the **viscous dissipation** $D(\Omega)$ of a double pipe system is minimized.
- A **volume constraint** is imposed.

I - Existence of many local minimizers:

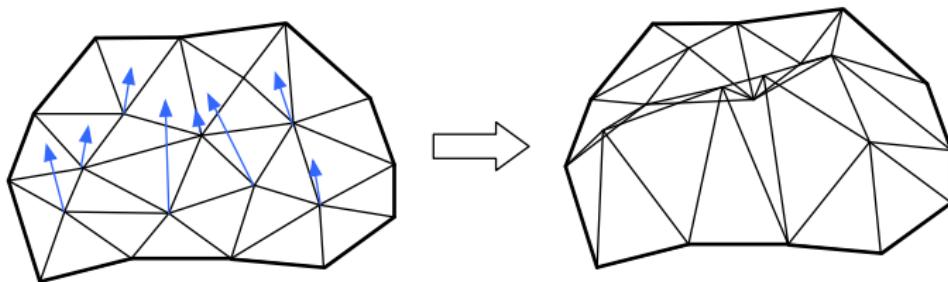
- In “most” shape optimization problems, no “true” global minimizer exists: the latter would have to be searched as a **homogenized design**;
- However, there exist many **local minimizers**;
- In practice, shape optimization algorithms are **very sensitive** to the initial design, to the size of the computational mesh, etc.



Several optimized cantilever beams associated to different initial designs.

II - The difficulty of mesh deformation:

- The update of the shape at each step $\Omega^n \mapsto (\text{Id} + \theta^n)(\Omega^n) = \Omega^{n+1}$ is realized by relocating each node $x \in \mathcal{T}^n$ to $x + \tau^n \theta^n(x) \in \mathcal{T}^{n+1}$.
- This may prove difficult, partly because it may cause inversion of elements, resulting in an invalid mesh.



Pushing nodes according to θ^n may result in an invalid configuration.

- For this reason, mesh deformation methods are generally preferred for accounting for “small displacements”.

III - Velocity extension:

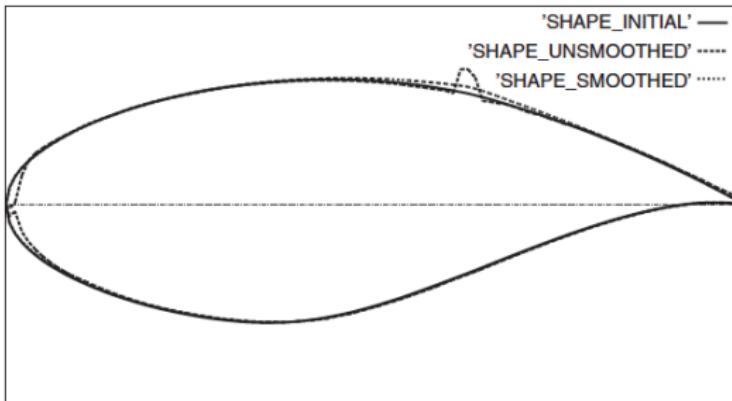
- A descent direction $\theta = -v_\Omega n$ from a shape Ω is inferred from the formula:

$$J'(\Omega)(\theta) = \int_{\partial\Omega} v_\Omega(\theta \cdot n) \, ds.$$

- The new shape $(Id + \theta)(\Omega)$ only depends on these values of θ on $\partial\Omega$.
- For many reasons, in numerical practice, it is crucial to extend θ to Ω (or even \mathbb{R}^d) in a “clever” way.
*on connaît v sur le bord du domaine mais pour level set method
on veut v pour tout omega*
(for instance, deforming a mesh of Ω using a “nice” vector field θ defined on the whole Ω may considerably ease the process)
- The “natural” extension of the formula $\theta = -v_\Omega n$, which is only legitimate on $\partial\Omega$ may not be a “good” choice.
=> direction irrégulière

IV - Velocity regularization:

- The descent direction $\theta = -v_\Omega n$ on $\partial\Omega$ may be very **irregular**, because of
 - **numerical artifacts** arising during the finite element analyses.
 - an inherent lack of regularity of $J'(\Omega)$ for the problem at stake.
- In numerical practice, it is often necessary to **smooth** this descent direction so that the considered shapes stay regular.



Irregularity of the shape derivative in the very sensitive problem of drag minimization of an airfoil (Taken from [MoPir]). In one iteration, using the unsmoothed shape derivative of $J(\Omega)$ produces large undesirable artifacts.

The Hilbertian method (I)

A popular idea: extend AND regularize the velocity field

- Suppose we aim at extending the *scalar* field $v_\Omega : \partial\Omega \rightarrow \mathbb{R}$ to Ω .
- **Idea:** (\approx Laplacian smoothing) Trade the “natural” inner product over $L^2(\partial\Omega)$ for a **more regular** inner product over functions on Ω .
- **Example:** Search the extended / regularized scalar field V as:

Find $V \in H^1(\Omega)$ s.t. $\forall w \in H^1(\Omega)$,

$$\alpha^2 \int_{\Omega} \nabla V \cdot \nabla w \, dx + \int_{\Omega} Vw \, dx = \int_{\partial\Omega} v_\Omega w \, ds.$$

J'(omeg) (définie sur le bord de omeg)

- The **regularizing parameter α** controls the balance between the fidelity of V to v_Ω and the intensity of smoothing.

- The resulting scalar field V is inherently defined on Ω and more regular than v_Ω .
- Multiple other **regularizing problems** are possible, associated to different inner products or different function spaces.
- A similar process also allows to:
 - extend v_Ω to a large computational box D (an inner product over functions defined on D is used),
 - extend the **vector velocity** $\theta = -v_\Omega n$ to Ω or D (an inner product over vector functions is used, e.g. that of linear elasticity).
- In particular, such a procedure allows to obtain a descent direction from the **volume form** of the shape derivative:

$$J'(\Omega)(\theta) = \int_{\Omega} (r_\Omega \cdot \theta + S_\Omega : \nabla \theta) \, dx,$$

where the fields $r_\Omega : \Omega \rightarrow \mathbb{R}^d$, $S_\Omega : \Omega \rightarrow \mathbb{R}^{d \times d}$ are known.

Part III

Geometric optimization problems

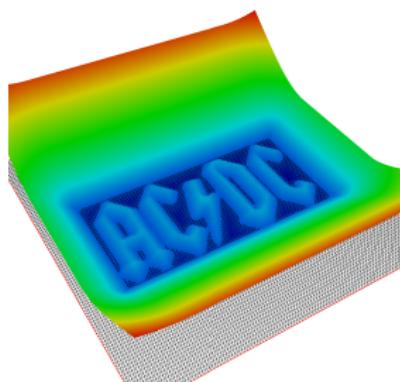
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The level set method

A paradigm: *the motion of an evolving domain is conveniently described in an **implicit** way.*

A domain $\Omega \subset \mathbb{R}^d$ is equivalently defined by a function $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ such that:

$$\phi(x) < 0 \quad \text{if } x \in \Omega \quad ; \quad \phi(x) = 0 \quad \text{if } x \in \partial\Omega \quad ; \quad \phi(x) > 0 \quad \text{if } x \in {}^c\overline{\Omega}$$



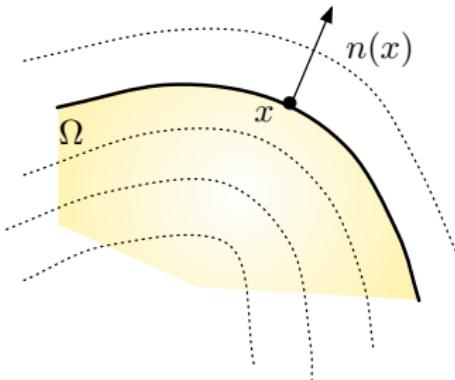
A domain $\Omega \subset \mathbb{R}^2$ (left), some level sets of an associated level set function (right).

Level set functions and geometry (I)

If $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ is a **level set function** of class C^2 for Ω , such that $\nabla\phi(x) \neq 0$ on a neighborhood of $\partial\Omega$,

- The **normal vector** n to $\partial\Omega$ pointing outward Ω reads:

$$\forall x \in \partial\Omega, \quad n(x) = \frac{\nabla\phi(x)}{|\nabla\phi(x)|}.$$



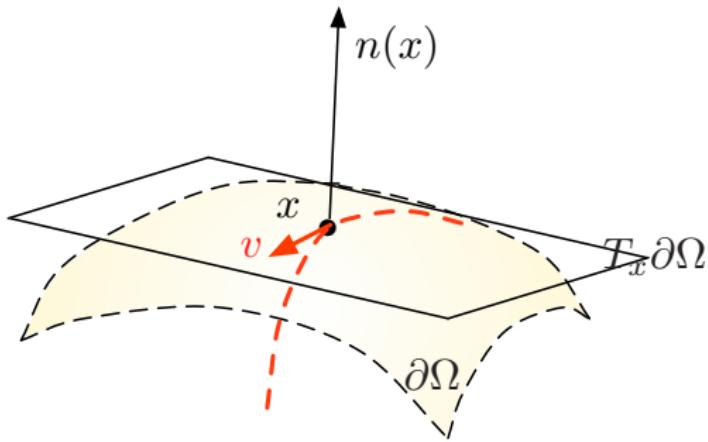
Normal vector to a domain Ω ; some isolines of the function ϕ are dotted.

- The second fundamental form II of $\partial\Omega$ is:

$$\forall x \in \partial\Omega, \quad \text{II}(x) = \nabla \left(\frac{\nabla \phi(x)}{|\nabla \phi(x)|} \right).$$

- The mean curvature κ of $\partial\Omega$ is:

$$\forall x \in \partial\Omega, \quad \kappa(x) = \operatorname{div} \left(\frac{\nabla \phi(x)}{|\nabla \phi(x)|} \right).$$



$\Pi_x(v, v)$ is the curvature of a curve drawn on $\partial\Omega$ with tangent vector v at x .

Evolution of domains with the level set method

- Let $\Omega(t) \subset \mathbb{R}^d$ be a domain moving along a velocity field $v(t, x) \in \mathbb{R}^d$.
- Let $\phi(t, x)$ be a level set function for $\Omega(t)$.
- The motion of $\Omega(t)$ translates in terms of ϕ as the **level set advection equation**:

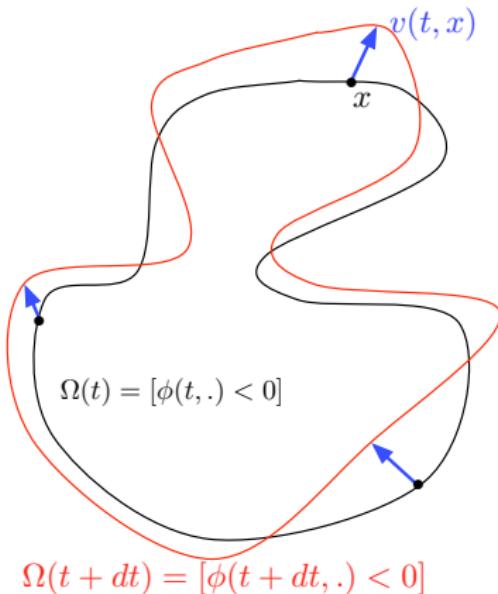
$$\frac{\partial \phi}{\partial t}(t, x) + v(t, x) \cdot \nabla \phi(t, x) = 0$$

- If $v(t, x)$ is normal to the boundary $\partial\Omega(t)$, i.e.:

$$v(t, x) := V(t, x) \frac{\nabla \phi(t, x)}{|\nabla \phi(t, x)|},$$

this rewrites as a **Hamilton-Jacobi equation**:

$$\frac{\partial \phi}{\partial t}(t, x) + V(t, x) |\nabla \phi(t, x)| = 0$$



The level set method in the context of shape optimization (I)

- A **fixed** computational domain D is meshed once and for all (e.g. with triangular or quadrilateral elements).
- Each shape Ω^n is represented by a **level set function** ϕ^n , defined at the nodes of the mesh.
- As soon as a descent direction θ^n from Ω^n is available, the **advection step**

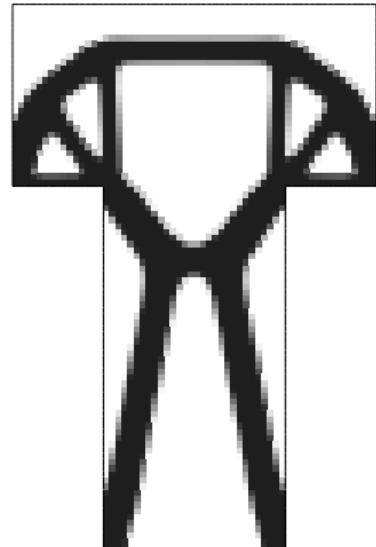
$$\Omega^n \mapsto \Omega^{n+1} = (\text{Id} + \tau^n \theta^n)(\Omega^n)$$

is achieved by solving the **advection-like equation**

$$\begin{cases} \frac{\partial \phi}{\partial t} + \theta^n \cdot \nabla \phi = 0 & t \in (0, \tau^n), x \in D \\ \phi(0, \cdot) = \phi^n \end{cases}$$

or if $\theta^n = v^n n$ is normal, the **Hamilton-Jacobi equation**:

$$\begin{cases} \frac{\partial \phi}{\partial t} + v^n |\nabla \phi| = 0 & t \in (0, \tau^n), x \in D \\ \phi(0, \cdot) = \phi^n \end{cases}$$



Shape accounted for by a level set description (from [AlJouToa])

Problem: At each iteration n , no mesh of Ω^n is available to solve the finite element problems needed in the calculation of the shape gradient.

Solution: The state and adjoint PDE problems posed on Ω^n are approximated by a problem posed on the whole box D

⇒ Use of a Fictitious domain method.

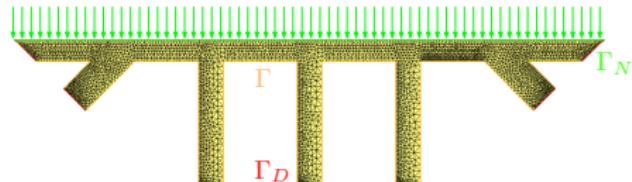
The ersatz material approximation in linearized elasticity (I)

- In the linear elasticity context, the optimized part of the boundary Γ (i.e. that represented with the level set method) is often **traction-free**.
 - The **ersatz material method** approximates the elastic displacement $u_\Omega : \Omega \rightarrow \mathbb{R}^d$ by that $u_{\Omega,\varepsilon} : D \rightarrow \mathbb{R}^d$ of the total domain D when the **void** $D \setminus \overline{\Omega}$ is filled with a very 'soft' material:

where the approximate Hooke's tensor A_ε reads:

$$A_\varepsilon = \chi_\Omega A + (1 - \chi_\Omega)\varepsilon A, \quad \varepsilon \ll 1.$$

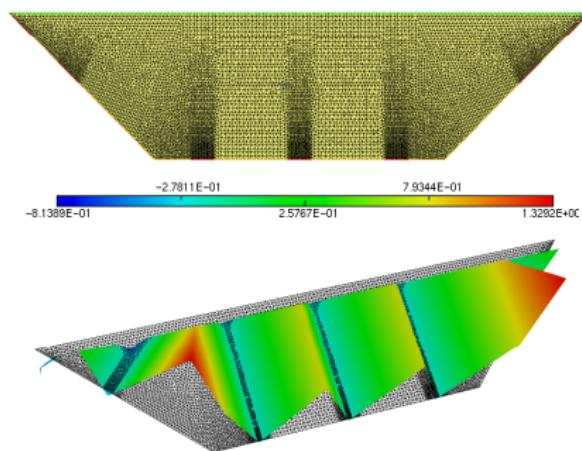
The ersatz material approximation in linearized elasticity (II)



Physical situation of a bridge



Deformed configuration of the bridge



Implicit definition of the bridge on a mesh of D



Deformed configuration of the domain D

Example: optimization of a 2d bridge using the level set method

- In the context of linear elasticity, the compliance of a bridge is minimized

$$C(\Omega) = \int_{\Omega} A e(u_{\Omega}) : e(u_{\Omega}) \, dx.$$

- A constraint on the volume $\text{Vol}(\Omega)$ of shapes is imposed.

Technical appendix

The Sobolev space $W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$

Definition 4.

The space $W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ is equivalently defined as:

- The space of **bounded** and **Lipschitz** vector fields $\theta : \mathbb{R}^d \rightarrow \mathbb{R}^d$, i.e. there exists $C > 0$ such that:

$$\forall x \in \mathbb{R}^d, |\theta(x)| \leq C, \text{ and } \forall x, y \in \mathbb{R}^d, |\theta(x) - \theta(y)| \leq C|x - y|.$$

- The **Sobolev space** of uniformly bounded functions, with uniformly bounded derivatives:

$$\left\{ \theta \in L^\infty(\mathbb{R}^d), \frac{\partial \theta_i}{\partial x_j} \in L^\infty(\mathbb{R}^d), i, j = 1, \dots, d \right\}.$$

The space $W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ is equipped with the norm:

$$\begin{aligned} \|\theta\|_{W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)} &= \sup_{\substack{x, y \in \mathbb{R}^d \\ x \neq y}} \left(|\theta(x)| + \frac{|\theta(x) - \theta(y)|}{|x - y|} \right) \\ &= \|\theta\|_{L^\infty(\mathbb{R}^d)} + \sup_{x \in \mathbb{R}^d} |\nabla \theta(x)|. \end{aligned}$$

Change of variable formulas (I)

The next theorem is an extension of the usual [change of variables](#) formula (involving a \mathcal{C}^1 diffeomorphism) to the case of a [Lipschitz](#) diffeomorphism; see [EGar], Chap. 3.

Theorem 9 (Lipschitz change of variables in volume integrals).

Let $\Omega \subset \mathbb{R}^d$ be a Lipschitz bounded domain, and $\varphi : \Omega \rightarrow \mathbb{R}^d$ be a Lipschitz diffeomorphism of \mathbb{R}^d . Then, for any function $f \in L^1(\varphi(\Omega))$, $f \circ \varphi$ is in $L^1(\Omega)$ and:

$$\int_{\varphi(\Omega)} f \, dx = \int_{\Omega} |\det(\nabla \varphi)| f \circ \varphi \, dx.$$

Remark: The Jacobian determinant $|\det(\nabla \varphi)|$ exists a.e. in Ω , as a consequence of the [Rademacher theorem](#):

A Lipschitz function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ is almost everywhere differentiable.

Change of variable formulas (II)

The following theorem is a version of the change of variables formula adapted to [surface integrals](#); see [HenPi], Prop. 5.4.3.

Theorem 10 (Change of variables in surface integrals).

Let $\Omega \subset \mathbb{R}^d$ be a bounded domain of class C^1 with boundary Γ and unit normal vector n pointing outward Ω . Let $\varphi : \Omega \rightarrow \mathbb{R}^d$ be a C^1 diffeomorphism of \mathbb{R}^d . Then, for any function $g \in L^1(\varphi(\Gamma))$, $g \circ \varphi$ belongs to $L^1(\Gamma)$ and:

$$\int_{\varphi(\Gamma)} g \, ds = \int_{\Gamma} |\text{Com}(\nabla \varphi)n| g \circ \varphi \, ds,$$

where $\text{Com}(M)$ is the cofactor matrix of a $d \times d$ matrix.

Remark: The integrand

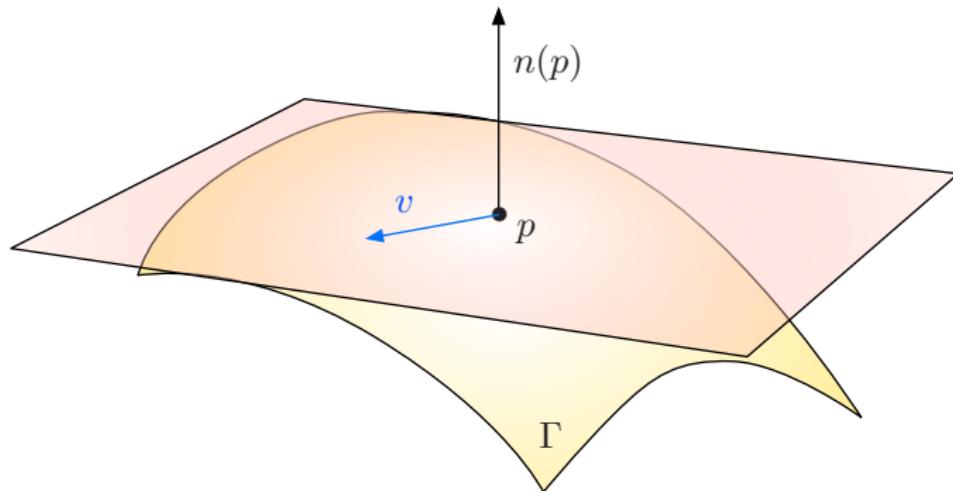
$$|\text{Com}(\nabla \varphi)n| = |\det(\nabla \varphi)| |\nabla \varphi^{-T} n|$$

is sometimes called the **tangential Jacobian** of the diffeomorphism φ .

Surfaces and curvature (I)

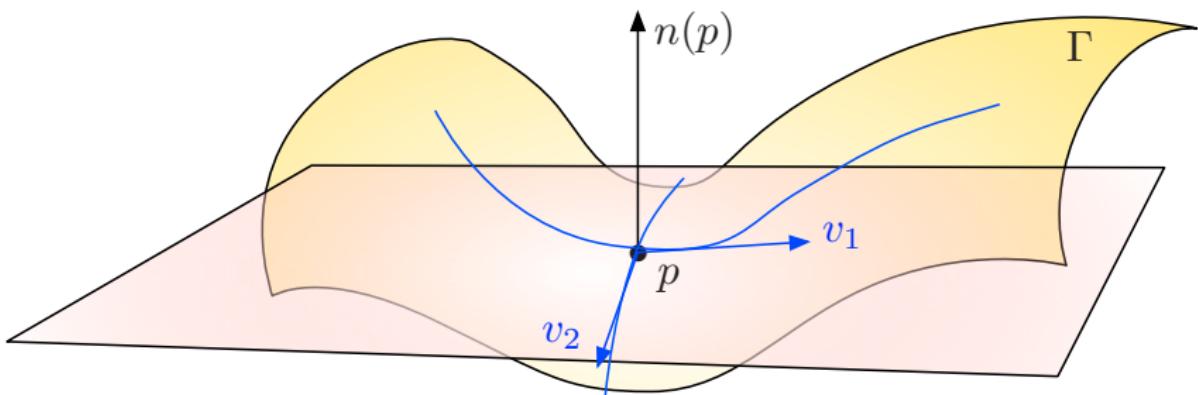
At first order, in the neighborhood of a point $p \in \Gamma$, a surface Γ behaves like a plane, the **tangent plane**,

- With **normal vector** $n(p)$,
- Which contains the **tangential directions** to Γ .



Surfaces and curvature (II)

- At second order in the neighborhood of $p \in \Gamma$, the surface Γ has one **curvature** in each tangential direction.
- The **principal directions** at p are those tangential directions $v_1(p)$ et $v_2(p)$ associated to the lower and larger curvatures $\kappa_1(p)$ et $\kappa_2(p)$.
- The **mean curvature** $\kappa(p)$ is the sum $\kappa(p) = \kappa_1(p) + \kappa_2(p)$.



The implicit function theorem

Let us recall the [implicit function theorem](#); see [La], Chap. I, Th. 5.9.

Theorem 11 (Implicit function theorem).

Let Θ, E, F be Banach spaces, $\mathcal{V} \subset \Theta$, $U \subset E$ be open sets, and $\mathcal{F} : \mathcal{V} \times U \rightarrow G$ be a function of class \mathcal{C}^p for $p \geq 1$. Let $(\theta_0, u_0) \in \mathcal{V} \times U$ be such that $\mathcal{F}(\theta_0, u_0) = 0$ and assume that:

$d_u \mathcal{F}(\theta_0, u_0) : F \rightarrow G$ is a linear isomorphism.

Then there exist an open subset $\mathcal{V}' \subset \mathcal{V}$ of θ_0 in Θ and a mapping $g : \mathcal{V}' \rightarrow U$ of class \mathcal{C}^p satisfying the properties:

- ① $g(\theta_0) = u_0$,
- ② For all $\theta \in \mathcal{V}'$, the equation $\mathcal{F}(\theta, u) = 0$ has a unique solution $u \in E$, given by $u = g(\theta)$.

A glimpse of elliptic regularity

- Existence and uniqueness of the solution u to an **elliptic equation** (e.g. the **conductivity equation**, the **linear elasticity system**) is often guaranteed by the **Lax-Milgram theory**.
- In general, this theory only supplies “weak” solutions, in a Sobolev space with “low” regularity (typically $H^1(\Omega)$).
- It turns out that this solution is in general “as regular as permitted by the data”.
- **Elliptic regularity** is a general phenomenon, which roughly states:

The solution u to a second-order **elliptic equation** posed in a **smooth** domain Ω , with **smooth** coefficients, is twice more regular than the data f :

$$f \in H^k(\Omega) \Rightarrow u \in H^{k+2}(\Omega), \text{ and } \|u\|_{H^{k+2}(\Omega)} \leq C \|f\|_{H^k(\Omega)}.$$

Theorem 12.

Let $\Omega \subset \mathbb{R}^d$ be a bounded domain of class C^{k+2} , and let $f \in H^k(\Omega)$. Then, the unique solution $u \in H_0^1(\Omega)$ to the equation

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

belongs to $H^{k+2}(\Omega)$, and the following estimate holds:

$$\|u\|_{H^{k+2}(\Omega)} \leq C \|f\|_{H^k(\Omega)},$$

for a constant $C > 0$ which only depends on k and Ω .

- This is an avatar of a very general phenomenon; similar statements hold for
 - Other types of **boundary conditions** (Neumann, Robin, ...),
 - Other **equations**: the **linearized elasticity system**, the **Stokes equations**, etc.
- We only provide a short sketch of proof; see [?], §9.6 for a comprehensive treatment.

Sketch of proof

Hint of proof: We proceed in three steps:

- (i) Interior regularity: We prove that for every cut-off function $\chi \in \mathcal{C}_c^\infty(\Omega)$,

$$\chi u \in H^2(\Omega), \text{ and } \|\chi u\|_{H^2(\Omega)} \leq C \|f\|_{L^2(\Omega)},$$

for a constant $C > 0$ depending only on χ and Ω .

- (ii) Regularity near the boundary: We prove that for any point $x_0 \in \partial\Omega$, there exists a bounded open set $\bar{\mathcal{O}}$ containing x_0 such that for any cutoff function $\chi \in \mathcal{C}_c^\infty(\mathbb{R}^d)$ with compact support inside $\bar{\mathcal{O}}$,

$$\chi u \in H^2(\Omega), \text{ and } \|\chi u\|_{H^2(\Omega)} \leq C \|f\|_{L^2(\Omega)}.$$

- (iii) Global regularity: Using a **partition of unity** argument, we “glue” the local results from Steps (i) and (ii).

Proof of the interior regularity statement (I)

Proof of Step (i): Interior regularity

- By a simple calculation, the function χu satisfies the equation:

$$-\Delta(\chi u) = g, \text{ where } g := -(\Delta\chi)u - 2\nabla\chi \cdot \nabla u - \chi f \in L^2(\mathbb{R}^d). \quad (\text{SF})$$

Under variational form, χu is the unique solution in $H_0^1(\Omega)$ to the problem:

$$\forall v \in H_0^1(\Omega), \int_{\Omega} \nabla(\chi u) \cdot \nabla v \, dx = \int_{\Omega} gv \, dx. \quad (\text{VF})$$

- Intuitively, because $g \in L^2(\Omega)$ and $\text{supp}(g)$ is a compact of Ω , for $i = 1, \dots, d$, $\frac{\partial g}{\partial x_i} \in H^{-1}(\Omega)$. By the standard Lax-Milgram theory, the variational problem

$$\forall v \in H_0^1(\Omega), \int_{\Omega} \nabla w_i \cdot \nabla v \, dx = \left\langle \frac{\partial g}{\partial x_i}, v \right\rangle_{H^{-1}(\Omega), H_0^1(\Omega)},$$

obtained by formally taking derivatives in (SF) or (VF), has a unique solution $w_i \in H_0^1(\Omega)$, which it is tempting to identify with $\frac{\partial}{\partial x_i}(\chi u)$.

- Making this argument rigorous relies on the method of translations of L. Nirenberg.

Proof of the interior regularity statement (II)

For a function $u : \Omega \rightarrow \mathbb{R}$, a point $x \in \Omega$, and a direction $h \in \mathbb{R}^d$ such that $|h| < d(x, \partial\Omega)$, we define the **difference quotient**:

$$D_h u(x) = \frac{u(x + h) - u(x)}{|h|}.$$

Theorem 13 (The method of translations).

The following statements are equivalent:

① $u \in H^1(\Omega)$;

② There exists $C > 0$ such that:

$$\forall i = 1, \dots, d, \quad \forall \varphi \in C_c^\infty(\Omega), \quad \left| \int_{\Omega} u \frac{\partial \varphi}{\partial x_i} \, dx \right| \leq C \|\varphi\|_{L^2(\Omega)}.$$

③ There exists $C > 0$ such that for any open subset $\omega \Subset \Omega$, and any vector $h \in \mathbb{R}^d$ with $|h| < \text{dist}(\omega, \partial\Omega)$,

$$\|D_h u\|_{L^2(\omega)} \leq C.$$

In addition, one may take $C = \|\nabla u\|_{L^2(\Omega)^d}$ in the last two statements.

Proof of the interior regularity statement (III)

- Taking $v = D_{-h}D_h(\chi u)$ as test function in the variational formulation for χu is possible because $\text{supp}(\chi u)$ is a compact of Ω ; this yields:

$$\int_{\Omega} \nabla(\chi u) \cdot \nabla(D_{-h}D_h(\chi u)) \, dx = \int_{\Omega} g D_{-h}D_h(\chi u) \, dx.$$

- Performing a discrete integration by parts (i.e. a change of variables), we get:

$$\int_{\Omega} \nabla(D_h(\chi u)) \cdot \nabla(D_h(\chi u)) \, dx = \int_{\Omega} g D_{-h}D_h(\chi u) \, dx.$$

The Cauchy-Schwarz inequality and the translation theorem ((i) \Rightarrow (iii)) lead to:

$$\|\nabla(D_h(\chi u))\|_{L^2(\Omega)^d}^2 \leq \|g\|_{L^2(\Omega)} \|\nabla(D_h(\chi u))\|_{L^2(\Omega)^d},$$

and so:

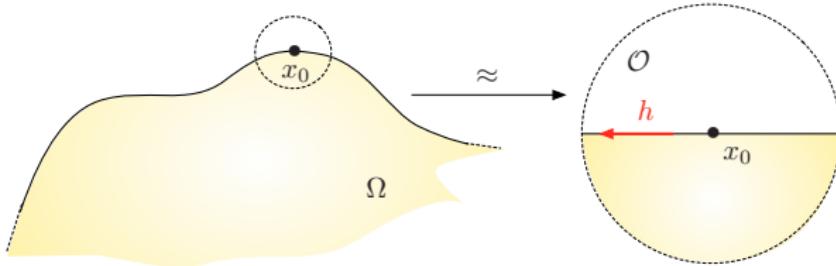
$$\|D_h(\nabla(\chi u))\|_{L^2(\Omega)^d} \leq \|g\|_{L^2(\Omega)}.$$

- Eventually, the translation theorem ((iii) \Rightarrow (i)) implies from this inequality that $\nabla(\chi u) \in H^1(\Omega)^d$ with the desired estimate.

Proof of the boundary regularity statement

Proof of Step (ii):

- Let $x_0 \in \partial\Omega$. Because $\partial\Omega$ is “smooth”, we may take \mathcal{O} so small that $\partial\Omega$ is “nearly flat” around x_0 (say, Ω coincide with the lower half-space near x_0).



- The same argument as before (with “horizontal” translations h), shows that:

$$\forall i = 1, \dots, d-1, \frac{\partial(\chi u)}{\partial x_i} \in H^1(\Omega), \text{ and } \left\| \frac{\partial}{\partial x_i} (\chi u) \right\|_{H^1(\Omega)} \leq C \|f\|_{L^2(\Omega)}.$$

- It remains to prove that $\frac{\partial^2}{\partial x_d^2} (\chi u) \in L^2(\Omega)$: we re-use the original equation:

$$\frac{\partial^2}{\partial x_d^2} (\chi u) = g - \sum_{i=1}^{d-1} \frac{\partial^2}{\partial x_i^2} (\chi u).$$

End of the proof

Proof of Step (iii).

- By compactness of $\bar{\Omega}$, there exist open subsets $\mathcal{O}_0 \Subset \Omega$, and $\mathcal{O}_1, \dots, \mathcal{O}_N \subset \mathbb{R}^d$ as in the statement of Step (ii) such that:

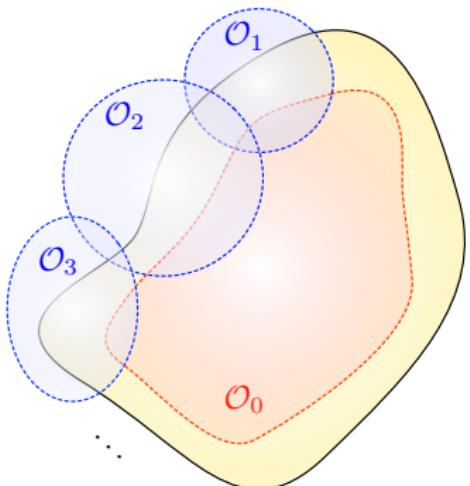
$$\overline{\Omega} \subset \bigcup_{i=0}^N \mathcal{O}_i.$$

- Let $\{\theta_i\}_{i=0,\dots,N}$ be a **partition of unity** associated to the covering $\{\mathcal{O}_i\}_{i=0,\dots,N}$, i.e.

$$\forall i, \theta_i \in \mathcal{C}_c^\infty(\mathcal{O}_i), \theta_i \geq 0, \text{ and } \sum_{i=0}^N \theta_i = 1 \text{ on } \overline{\Omega}.$$

- Then:

$$u = \underbrace{\theta_0 u}_{\in H^2(\Omega), \text{ by Step (i) and} \\ ||\theta_0 u||_{H^2(\Omega)} \leq C ||f||_{L^2(\Omega)}} + \sum_{i=1}^N \underbrace{\theta_i u}_{\in H^2(\Omega), \text{ by Step (ii) and} \\ ||\theta_i u||_{H^2(\Omega)} \leq C ||f||_{L^2(\Omega)}}$$



The Sobolev imbedding theorem

The **Sobolev imbedding theorem** states conditions for Sobolev class functions to be **regular** in the “classical” sense, i.e. for their belonging to a **Hölder space** $\mathcal{C}^{k,\sigma}(\Omega)$:

$$u \in \mathcal{C}^{k,\sigma}(\Omega) \Leftrightarrow \|u\|_{\mathcal{C}^{k,\sigma}(\Omega)} := \|u\|_{\mathcal{C}^k(\Omega)} + \sup_{|\alpha|=k} \sup_{\substack{x,y \in \Omega \\ x \neq y}} \frac{|\partial^\alpha u(x) - \partial^\alpha u(y)|}{|x-y|^\sigma} < \infty.$$

Theorem 14 (Sobolev imbedding theorem).

Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain. Let $0 \leq k, 1 \leq m$ be two integers, $1 \leq p < \infty$ be an exponent, such that there exists $\sigma \in (0, 1)$ satisfying:

$$k + \sigma \leq m - \frac{d}{p}.$$

Then, the space $W^{m,p}(\Omega)$ is continuously embedded in $\mathcal{C}^{k,\sigma}(\Omega)$, and there exists a constant $C > 0$ such that:

$$\forall u \in W^{m,p}(\Omega), \|u\|_{\mathcal{C}^{k,\sigma}(\Omega)} \leq C \|u\|_{W^{m,p}(\Omega)}.$$

Roughly speaking, functions in $W^{m,p}(\Omega)$ have “a little less” than m classical derivatives, and “tend to have m classical derivatives” as $p \rightarrow \infty$.

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