An introduction to shape and topology optimization

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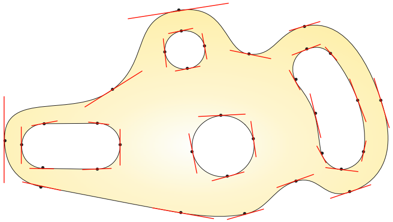
Foreword: geometric shape optimization

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

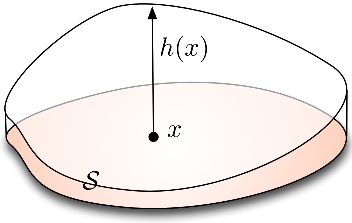
$$\min_h J(h) \text{ s.t. } C(h) \leq 0,$$

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 $\mathcal{S}$ via the thickness function $h : \mathcal{S} \to \mathbb{R}$.

Foreword: geometric shape optimization (II)

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.

$\Rightarrow$ It is often desirable to formulate shape optimization problems in terms of the geometry of shapes Ω:

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

Part III

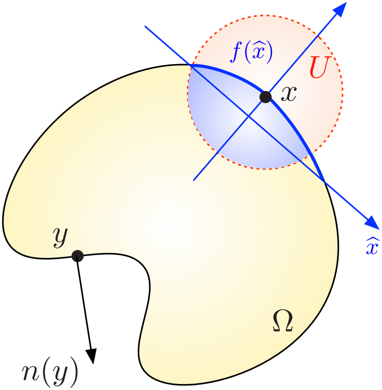
Geometric optimization problems

Preliminary notations

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

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

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



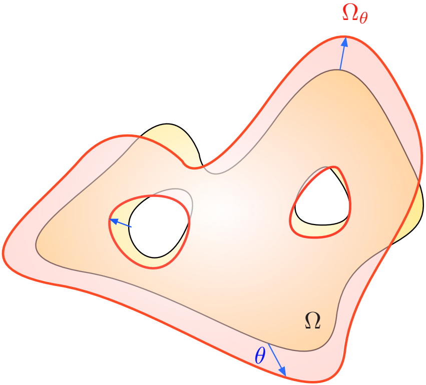
In a neighborhood U of each point $x \in \partial\Omega$, Ω "looks like" the lower part of the graph of some (Lipschitz or $\mathcal{C}^k$) function $\widehat{x} \mapsto f(\widehat{x})$ defined for suitable $(d-1)$-dimensional coordinates.

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

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

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 $(\mathrm{Id} + \theta)$ 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:

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

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.:

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

Theorem 2.

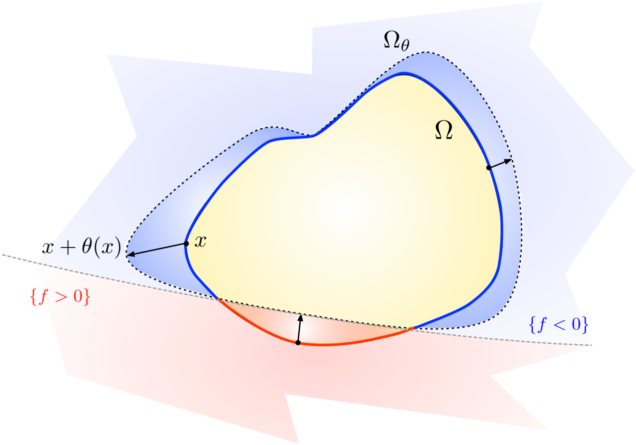
Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain, and let $f \in W^{1,1}(\mathbb{R}^d)$ be a fixed function. Consider the functional:

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

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

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

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 decreased 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
$$\mathrm{Vol}(\Omega) = \int_\Omega 1 \,\mathrm{d}x.$$
Indeed, one has:
$$\forall \theta \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d), \;\; \mathrm{Vol}'(\Omega)(\theta) = \int_{\partial\Omega} \theta \cdot n \,\mathrm{d}s = \int_\Omega \mathrm{div}\theta \,\mathrm{d}x.$$
In particular, if $\mathrm{div}\theta = 0$, 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:

$$J(\Omega_\theta) = \int_{(\mathrm{Id}+\theta)(\Omega)} f(x)\,\mathrm{d}x = \int_\Omega |\det(\mathrm{I}+\nabla\theta)|\, f\circ(\mathrm{Id}+\theta)\,\mathrm{d}x.$$

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

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

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

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

- Combining those three identites and Green's formula leads to the result.

□

Remark: This idea of

1. Using the change of variables $\Omega \to (\mathrm{Id}+\theta)(\Omega)$ 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 $\mathcal{C}^2$, and let $g \in W^{2,1}(\mathbb{R}^d)$ be a fixed function. Consider the functional:

$$J(\Omega) = \int_{\partial\Omega} g(x)\, \mathrm{d}s;$$

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:

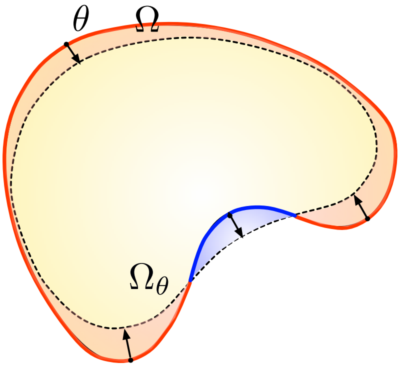
$$J'(\Omega)(\theta) = \int_{\partial\Omega} \left(\frac{\partial g}{\partial n} + \kappa g \right) (\theta \cdot n)\, \mathrm{d}s,$$

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

Example: The shape derivative of the perimeter $\mathrm{Per}(\Omega) = \int_{\partial\Omega} 1\, \mathrm{d}s$ is:

$$\mathrm{Per}'(\Omega)(\theta) = \int_{\partial\Omega} \kappa\, (\theta \cdot n)\, \mathrm{d}s.$$

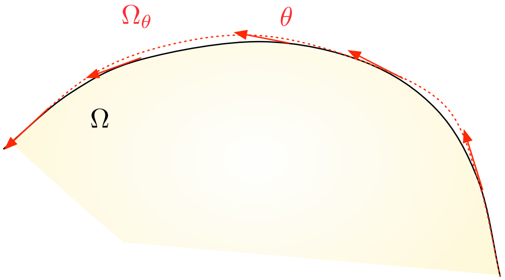
First examples of shape derivatives (VI)



Intuition: $\theta = -\kappa n$ *is a descent direction for* $\mathrm{Per}(\Omega)$*: 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 $\mathcal{C}^1$. Assume that the mapping

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

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

Corollary 5.

Under the same hypotheses, if $\theta_1, \theta_2 \in \mathcal{C}^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ 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:

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

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

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

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

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

Part III

Geometric optimization problems

Shape derivatives of PDE constrained functionals

- Hitherto, we have studied the shape derivatives of functionals of the form
$$F_1(\Omega) = \int_\Omega f(x)\,\mathrm{d}x, \text{ and } F_2(\Omega) = \int_{\partial\Omega} g(x)\,\mathrm{d}s,$$
where $f, g : \mathbb{R}^d \to \mathbb{R}$ are given, smooth enough functions.

- We now intend to consider functions of the form
$$J_1(\Omega) = \int_\Omega j(u_\Omega(x))\,\mathrm{d}x, \text{ or } J_2(\Omega) = \int_{\partial\Omega} k(u_\Omega(x))\,\mathrm{d}s,$$
where $j, k : \mathbb{R} \to \mathbb{R}$ are given, smooth enough functions, and $u_\Omega : \Omega \to \mathbb{R}$ 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 $f : \mathbb{R}^d \to \mathbb{R}$.

- The associated variational formulation reads:

$$\forall v \in H^1_0(\Omega), \ \int_\Omega \nabla u_\Omega \cdot \nabla v \, \mathrm{d}x = \int_\Omega fv \, \mathrm{d}x.$$

- In this setting:

  1. We calculate the "derivative" of the state $\Omega \mapsto u_\Omega$ in a sense to be defined.
  2. We infer the shape derivative of a shape functional of the form:

$$J(\Omega) = \int_\Omega j(u_\Omega) \, \mathrm{d}x,$$

  where $j : \mathbb{R} \to \mathbb{R}$ is a "smooth enough" function.

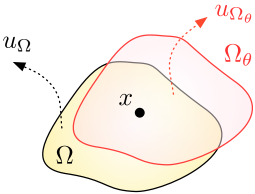
- The rigorous way to address this problem requires a notion of differentiation of functions $\Omega \mapsto u_\Omega$, which to a domain Ω associates a function defined on Ω.

- 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

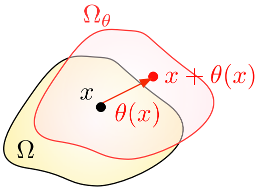
$$\theta \mapsto u_{\Omega_\theta}(x).$$



The Lagrangian point of view:

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

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



Eulerian and Lagrangian derivatives (II)

- 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:

  1. Defining properly the Lagrangian derivative $\mathring{u}_\Omega(\theta)$;
  2. Defining the Eulerian derivative $u'_\Omega(\theta)$ 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 $u_{(\mathrm{Id}+\theta)(\Omega)} \circ (\mathrm{Id} + \theta)$:

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

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* $\mathring{u}_\Omega(\theta) \in H^1(\Omega)$ *at a particular domain* Ω *provided the transported function*

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

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* $\mathring{u}_\Omega(\theta)$ *at* Ω*;*
2. *the quantity* $\nabla u_\Omega \cdot \theta$ *belongs to* $H^1(\Omega)$*.*

One defines then:

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

Eulerian and Lagrangian derivatives (V)

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 $\mathring{u}_\Omega$ at Ω. If $j : \mathbb{R} \to \mathbb{R}$ is regular enough, the function

$$J(\Omega) = \int_\Omega j(u_\Omega)\,\mathrm{d}x$$

is then shape differentiable at Ω, and:

$$\forall \theta \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d), \;\; J'(\Omega)(\theta) = \int_\Omega \left(j'(u_\Omega)\mathring{u}_\Omega(\theta) + (\mathrm{div}\theta) j(u_\Omega) \right)\,\mathrm{d}x.$$

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

$$J'(\Omega)(\theta) = \underbrace{\int_{\partial\Omega} j(u_\Omega)\,\theta\cdot n\,\mathrm{d}s}_{\substack{\textbf{Derivative of the partial mapping} \\ \Omega \mapsto \int_\Omega j(u_\Omega)}} + \underbrace{\int_\Omega j'(u_\Omega)u'_\Omega(\theta)\,\mathrm{d}x}_{\substack{\textbf{Derivative of the partial mapping} \\ \Omega \mapsto \int_\Omega j(u_\Omega)}}.$$

Eulerian and Lagrangian derivatives (VI)

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

$$J(\Omega_\theta) = \int_{(\mathrm{Id}+\theta)(\Omega)} j(u_{\Omega_\theta})\,\mathrm{d}x = \int_\Omega |\det(\mathrm{I} + \nabla\theta)| j(\overline{u}(\theta))\,\mathrm{d}x.$$

- The mapping $\theta \mapsto |\det(\mathrm{I} + \nabla\theta)|$ is Fréchet differentiable at $\theta = 0$ and
$$|\det(\mathrm{I} + \nabla\theta)| = 1 + \mathrm{div}\theta + \mathrm{o}(\theta);$$
- The mapping $\theta \mapsto \overline{u}(\theta)$ is Fréchet differentiable at $\theta = 0$ and
$$\overline{u}(\theta) = u_\Omega + \mathring{u}_\Omega(\theta) + \mathrm{o}(\theta);$$

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

$$J'(\Omega)(\theta) = \int_\Omega \left((\mathrm{div}\theta) j(u_\Omega) + j'(u_\Omega)\mathring{u}_\Omega(\theta)\right)\mathrm{d}x.$$

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:

$$J'(\Omega)(\theta) = \int_{\partial\Omega} j(u_\Omega)\,\theta\cdot n\,\mathrm{d}s + \int_\Omega j'(u_\Omega) u'_\Omega(\theta)\,\mathrm{d}x.$$

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 $\Omega \mapsto u_\Omega \in H^1_0(\Omega)$ has a Lagrangian derivative $\mathring{u}_\Omega(\theta)$, and for any $\theta \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$, $\mathring{u}_\Omega(\theta) \in H^1_0(\Omega)$ is the unique solution to the variational problem:

$$\forall v \in H^1_0(\Omega), \ \int_\Omega \nabla(\mathring{u}_\Omega(\theta)) \cdot \nabla v \, dx = \int_\Omega \text{div}(f\theta) v \, dx - \int_\Omega (\text{div}(\theta)\text{I} - \nabla\theta - \nabla\theta^T)\nabla u_\Omega \cdot \nabla v \, dx,$$

or, under classical form:

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

Eulerian and Lagrangian derivatives (VIII)

Idea of the proof:

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

$$\forall v \in H^1_0(\Omega_\theta), \int_{\Omega_\theta} \nabla u_{\Omega_\theta} \cdot \nabla v \, \mathrm{d}x = \int_{\Omega_\theta} fv \, \mathrm{d}x.$$

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

$$\forall v \in H^1_0(\Omega), \int_\Omega A(\theta)\nabla\overline{u}(\theta) \cdot \nabla v \, \mathrm{d}x = \int_\Omega |\det(\mathrm{I} + \nabla\theta)|(f \circ (\mathrm{Id} + \theta))v \, \mathrm{d}x,$$

where

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

- This variational problem features a fixed domain and a fixed function space $H^1_0(\Omega)$, and only the coefficients of the formulation depend on θ.

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

Eulerian and Lagrangian derivatives (IX)

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

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

for appropriate definitions of the operators:

  - $\mathcal{F} : W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d) \times H^1_0(\Omega) \to H^{-1}(\Omega)$,
  - $\mathcal{G} : W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d) \to H^{-1}(\Omega)$.

- The implicit function theorem shows that $\theta \mapsto \overline{u}(\theta)$ is differentiable at $\theta = 0$.

- The Lagrangian derivative $\mathring{u}_\Omega(\theta)$ of the transported mapping $\overline{u}(\theta)$ can now be computed by taking derivatives inside the variational formula:

$$\forall v \in H^1_0(\Omega), \int_\Omega \nabla \mathring{u}_\Omega(\theta) \cdot \nabla v \, \mathrm{d}x = \int_\Omega \mathrm{div}(f\theta) v \, \mathrm{d}x - \int_\Omega (\mathrm{div}(\theta)\mathrm{I} - \nabla\theta - \nabla\theta^T)\nabla u_\Omega \cdot \nabla v \, \mathrm{d}x.$$

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:

$$\boxed{J'(\Omega)(\theta) = \int_\Omega \left(j'(u_\Omega)\mathring{u}_\Omega(\theta) + (\mathrm{div}\theta) j(u_\Omega) \right) \, \mathrm{d}x,}$$

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

$$\boxed{J'(\Omega)(\theta) = \int_{\partial\Omega} j(u_\Omega)\, \theta \cdot n \, \mathrm{d}s + \int_\Omega j'(u_\Omega) u'_\Omega(\theta) \, \mathrm{d}x.}$$

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

Eulerian and Lagrangian derivatives (XI): the adjoint method

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):

$$J'(\Omega)(\theta) = \int_\Omega (\text{div}\theta) j(u_\Omega)\,\text{d}x + \int_\Omega (\text{div}(\theta)\text{I} - \nabla\theta - \nabla\theta^T)\nabla u_\Omega \cdot \nabla p_\Omega \,\text{d}x - \int_\Omega \text{div}(f\theta) p_\Omega \,\text{d}x,$$

where the adjoint state $p_\Omega \in H^1_0(\Omega)$ 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:

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

Proof of the volume form.

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

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

- Here, the Lagrangian derivative $\mathring{u}_\Omega(\theta) \in H^1_0(\Omega)$ solves:

$$\forall v \in H^1_0(\Omega), \; \int_\Omega \nabla \mathring{u}_\Omega(\theta) \cdot \nabla v \, \text{d}x = \int_\Omega \text{div}(f\theta) v \, \text{d}x - \int_\Omega (\text{div}(\theta)\text{I} - \nabla\theta - \nabla\theta^T)\nabla u_\Omega \cdot \nabla v \, \text{d}x.$$

- This is to be compared with the variational formulation for p_Ω:

$$\forall v \in H^1_0(\Omega), \; \int_\Omega \nabla p_\Omega \cdot \nabla v \, \text{d}x = -\int_\Omega j'(u_\Omega) v \, \text{d}x.$$

- Thus,

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

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

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

$$J'(\Omega)(\theta) = \int_\Omega (\text{div}\theta) j(u_\Omega)\,\mathrm{d}x + \int_\Omega (\text{div}(\theta)\mathrm{I} - \nabla\theta - \nabla\theta^T)\nabla u_\Omega \cdot \nabla p_\Omega\,\mathrm{d}x$$
$$- \int_\Omega \text{div}(f\theta) p_\Omega\,\mathrm{d}x.$$

Eulerian and Lagrangian derivatives (XIV): the adjoint method

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:

$$J'(\Omega)(\theta) = \int_{\partial\Omega} v_\Omega \theta \cdot n \, \mathrm{d}s + \int_{\partial\Omega} t_\Omega \cdot \theta_{\partial\Omega} \, \mathrm{d}s + \int_\Omega S_\Omega \cdot \theta \, \mathrm{d}x,$$

  where:

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

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

  - $S_\Omega : \Omega \to \mathbb{R}^d$ 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:

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

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.

$\Rightarrow$ 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.

$\Rightarrow$ A descent direction θ for $J(\Omega)$ is immediately revealed.

Eulerian and Lagrangian derivatives: summary

- 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.

Part III

Geometric optimization problems

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:*

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

  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.

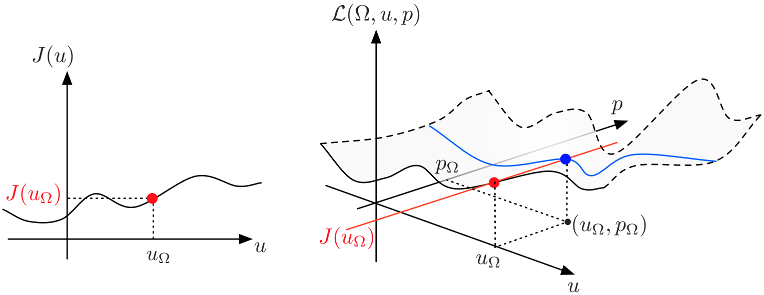
This method is formal: in particular, it assumes that we already know that $\Omega \mapsto u_\Omega$ is differentiable.

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:

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

We first consider the case of Neumann boundary conditions:

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

where the $+u$ 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:

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

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

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

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

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:

- $\forall \widehat{p} \in H^1(\mathbb{R}^d), \;\; \dfrac{\partial \mathcal{L}}{\partial p}(\Omega, u, p)(\widehat{p}) =$
$$\int_\Omega \nabla u \cdot \nabla \widehat{p}\, \mathrm{d}x + \int_\Omega u \widehat{p}\, \mathrm{d}x - \int_\Omega f \widehat{p}\, \mathrm{d}x = 0.$$

- $\forall \widehat{u} \in H^1(\mathbb{R}^d), \;\; \dfrac{\partial \mathcal{L}}{\partial u}(\Omega, u, p)(\widehat{u}) =$
$$\int_\Omega j'(u) \widehat{u}\, \mathrm{d}x + \int_\Omega \nabla \widehat{u} \cdot \nabla p\, \mathrm{d}x + \int_\Omega \widehat{u} p\, \mathrm{d}x = 0.$$

Céa's method: the Neumann case (III)

Step 1: *Identification of u:*

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

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

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

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

$$\int_{\partial\Omega} \frac{\partial u}{\partial n} \psi \,\mathrm{d}s = 0 \Rightarrow \boxed{\tfrac{\partial u}{\partial n} = 0 \text{ on } \partial\Omega}.$$

Conclusion: $u = u_\Omega$.

Céa's method: the Neumann case (IV)

Step 2: *Identification of p:*

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

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

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

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

$$\int_{\partial\Omega} \frac{\partial p}{\partial n} \psi \,\mathrm{d}s = 0 \Rightarrow \boxed{\frac{\partial p}{\partial n} = 0 \text{ on } \partial\Omega.}$$

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

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

- We go back to the fact that:

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

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

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

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:

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

where f is a fixed function.

Using Theorem 2, we end up with:

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

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

Céa's method: the Dirichlet case (I)

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

$$J(\Omega) = \int_\Omega j(u_\Omega)\,\mathrm{d}x, \text{ where } \left\{ \begin{array}{cl} -\Delta u = f & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega. \end{array} \right. .$$

- **Warning:** When the state u_Ω satisfies essential boundary conditions, i.e. boundary conditions that are tied to the definition space of functions (here, $H^1_0(\Omega)$), an additional difficulty generally arises.

- It is no longer possible to rely on the Lagrangian

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

since it would have to be defined for $u, p \in H^1_0(\Omega)$.

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

Solution: Add an extra variable $\mu \in H^1(\mathbb{R}^d)$ to the Lagrangian to penalize the boundary condition: for all $u, p, \lambda \in H^1(\mathbb{R}^d)$;

$$\mathcal{L}(\Omega, u, p, \lambda) = \underbrace{\int_\Omega j(u)\,\mathrm{d}x}_{\substack{\text{Objective function} \\ \text{where } u_\Omega \text{ is replaced by } u}} + \underbrace{\int_\Omega (-\Delta u - f)p\,\mathrm{d}x}_{\substack{\text{penalization of the} \\ \text{“constraint”} -\Delta u = f}} + \underbrace{\int_{\partial\Omega} \lambda u\,\mathrm{d}s}_{\substack{\text{penalization of the} \\ \text{“constraint”} \ u=0 \text{ on } \partial\Omega}} .$$

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

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

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

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

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:

- $\forall \widehat{p} \in H^1(\mathbb{R}^d), \;\; \dfrac{\partial \mathcal{L}}{\partial p}(\Omega, u, p, \lambda)(\widehat{p}) = \displaystyle\int_\Omega \nabla u \cdot \nabla \widehat{p} \, \mathrm{d}x - \int_\Omega f \widehat{p} \, \mathrm{d}x + \int_{\partial\Omega} \frac{\partial u}{\partial n} \widehat{p} \, \mathrm{d}s = 0.$

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

- $\forall \widehat{\lambda} \in H^1(\mathbb{R}^d), \;\; \dfrac{\partial \mathcal{L}}{\partial \lambda}(\Omega, u, p, \lambda)(\widehat{\lambda}) = \displaystyle\int_{\partial\Omega} \widehat{\lambda} u \, \mathrm{d}s = 0.$

Step 1: *Identification of* u*:*

$$\forall q \in H^1(\mathbb{R}^d), \;\; \int_\Omega \nabla u \cdot \nabla q \, \mathrm{d}x - \int_\Omega fq \, \mathrm{d}x + \int_{\partial\Omega} \frac{\partial u}{\partial n} q \, \mathrm{d}s = 0.$$

- Taking q as any $\mathcal{C}^\infty$ function ψ with compact support in Ω, we obtain:

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

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

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

Conclusion: $u = u_\Omega$.

Step 2: *Identification of p:*

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

- Taking v as any $\mathcal{C}^\infty$ function ψ with compact support in Ω, we see that:

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

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

- Now taking v as a $\mathcal{C}^\infty$ function ψ and using Green's formula, we obtain:

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

Step 2 (continued):

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

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

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 $\frac{\partial \psi}{\partial n} = 0$:

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

Céa's method: the Dirichlet case (VII)

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

- We return to the fact that:

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

- 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:

$$\Omega \mapsto \int_\Omega f(x)\,\mathrm{d}x, \text{ or } \Omega \mapsto \int_{\partial\Omega} g(x)\,\mathrm{d}s,$$

where f and g are fixed functions.

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

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

Part III

Geometric optimization problems

The generic numerical algorithm

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

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

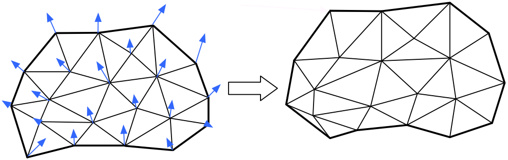
One possible implementation

- 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:

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

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

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



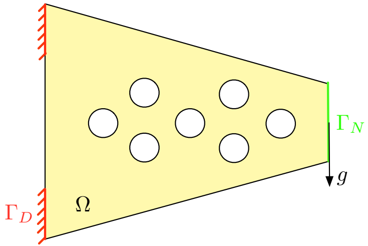
Deformation of a mesh by relocating its nodes to a prescribed final position.

Numerical examples (I)

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

$$C(\Omega) = \int_{\Omega} Ae(u_{\Omega}) : e(u_{\Omega}) \, \mathrm{d}x.$$

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

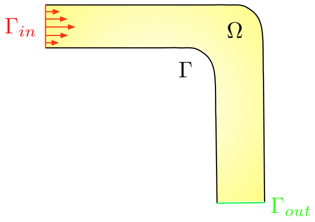


Numerical examples (II)

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

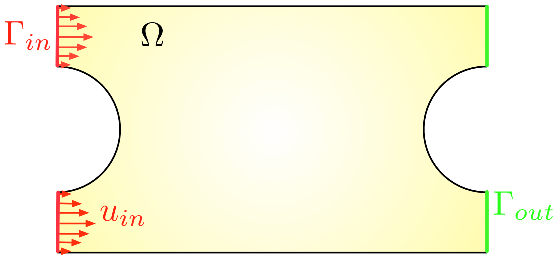
$$D(\Omega) = 2\nu \int_\Omega D(u_\Omega) : D(u_\Omega)\, \mathrm{d}x.$$

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



Numerical examples (III)

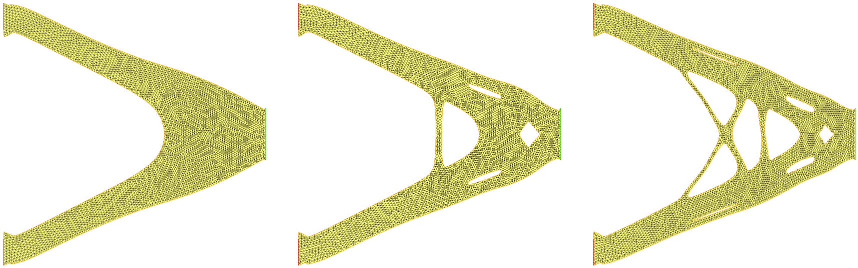
- Still in fluid mechanics, the viscous dissipation $D(\Omega)$ of a double pipe system is minimized.
- A volume constraint is imposed.



Numerical issues and difficulties (I)

I - Existence of many local minimizers:

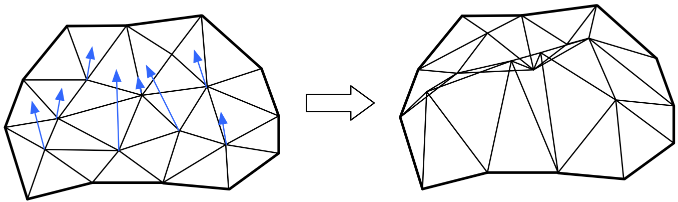
- In "most" shape optimization problems, no "true" global minimizer exists: the latter would have to be searched as a homogenized design;
- However, there exist many local minimizers;
- In practice, shape optimization algorithms are very sensitive to the initial design, to the size of the computational 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 $\Omega^n \mapsto (\mathrm{Id} + \theta^n)(\Omega^n) = \Omega^{n+1}$ 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 $(\mathrm{Id} + \theta)(\Omega)$ 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.

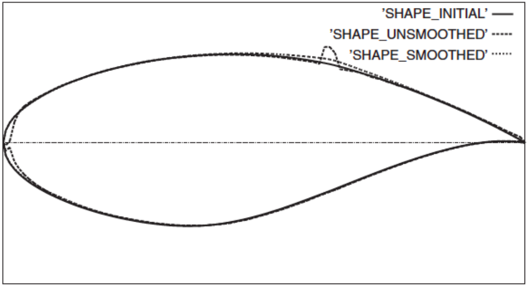
  (for instance, deforming a mesh of Ω using a "nice" vector field θ defined on the whole Ω may considerably ease the process)

- The "natural" extension of the formula $\theta = -v_\Omega n$, which is only legitimate on $\partial\Omega$ may not be a "good" choice.

Numerical issues and difficulties (IV)

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.

Part III

Geometric optimization problems

The Hilbertian method (I)

- Like in the parametric optimization context, the Hilbertian method allows to **extend AND regularize the velocity field** at the same time.
- Suppose we aim at extending the *scalar* field $v_\Omega : \partial\Omega \to \mathbb{R}$ into $V : \Omega \to \mathbb{R}$.
- **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 for the extended / regularized scalar field V as:

$$\text{Find } V \in H^1(\Omega) \text{ s.t. } \forall w \in H^1(\Omega), \quad a(V,w) = J'(\Omega)(wn),$$

where $a(V,w) := \alpha^2 \int_\Omega \nabla V \cdot \nabla w \,\mathrm{d}x + \int_\Omega V w \,\mathrm{d}x$, and $J'(\Omega)(wn) = \int_{\partial\Omega} v_\Omega w \,\mathrm{d}s$.

- The vector field $-Vn$ is still a descent direction for $J(\Omega)$, since

$$\text{For "small" } \tau > 0, \quad J((\mathrm{Id} - \tau Vn)(\Omega)) \approx J(\Omega) - \tau \underbrace{J'(\Omega)(Vn)}_{=a(V,V)>0}.$$

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

The Hilbertian method (II)

- 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:

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

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

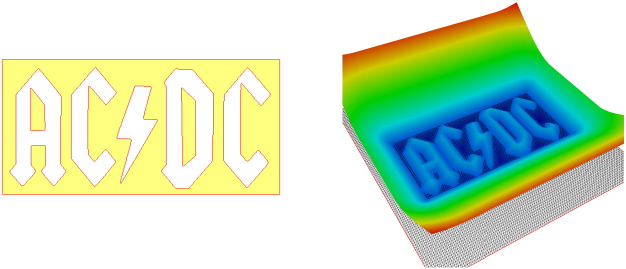
Part III

Geometric optimization problems

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 $\phi : \mathbb{R}^d \to \mathbb{R}$ such that:

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



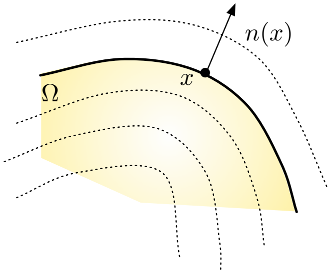
A domain $\Omega \subset \mathbb{R}^2$ (left), some level sets of an associated level set function (right).

Level set functions and geometry (I)

If $\phi : \mathbb{R}^d \to \mathbb{R}$ is a level set function of class $\mathcal{C}^2$ 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:

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



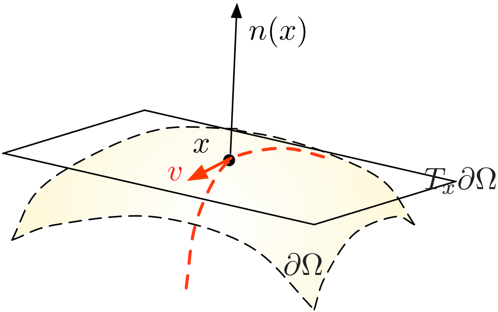
Normal vector to a domain Ω; some isolines of the function ϕ are dotted.

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

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

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

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



$\mathrm{II}_x(v,v)$ *is the curvature of a curve drawn on* $\partial\Omega$ *with tangent vector* v *at* x.

- 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 th level set advection equation:

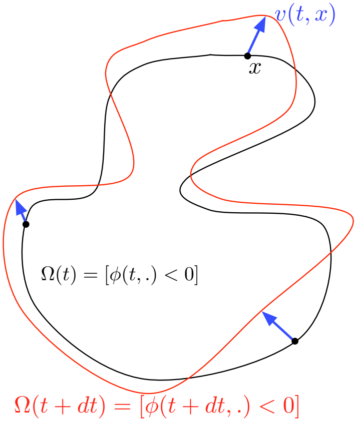
$$\frac{\partial \phi}{\partial t}(t,x) + v(t,x).\nabla\phi(t,x) = 0$$

- 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:

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



Part III

Geometric optimization problems

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

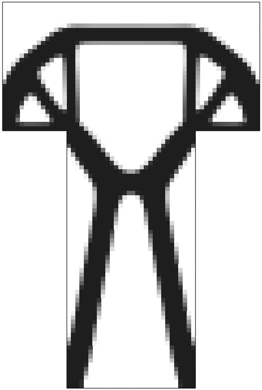
$$\Omega^n \mapsto \Omega^{n+1} = (\mathrm{Id} + \tau^n \theta^n)(\Omega^n)$$

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])

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

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

$\Rightarrow$ 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 $u_\Omega : \Omega \to \mathbb{R}^d$ by that $u_{\Omega,\varepsilon} : D \to \mathbb{R}^d$ of the total domain D when the void $D \setminus \overline{\Omega}$ is filled with a very 'soft' material:

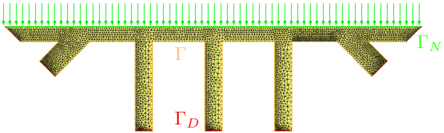
$$\left\{ \begin{array}{cl} -\text{div}(Ae(u_\Omega)) = 0 & \text{in } \Omega, \\ u_\Omega = 0 & \text{on } \Gamma_D, \\ Ae(u_\Omega)n = g & \text{on } \Gamma_N, \\ Ae(u_\Omega)n = 0 & \text{on } \Gamma. \end{array} \right. \approx \left\{ \begin{array}{cl} -\text{div}(A_\varepsilon e(u_{\Omega,\varepsilon})) = 0 & \text{in } D, \\ u_{\Omega,\varepsilon} = 0 & \text{on } \Gamma_D, \\ A_\varepsilon e(u_{\Omega,\varepsilon})n = g & \text{on } \Gamma_N, \\ Ae(u_{\Omega,\varepsilon})n = 0 & \text{on } \partial D \setminus (\Gamma_D \cup \Gamma_N), \end{array} \right.$$

(Problem posed on Ω) *(Problem posed on D)*

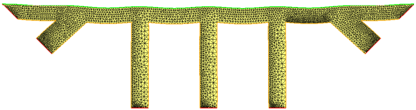
where the approximate Hooke's tensor A_ε reads:

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

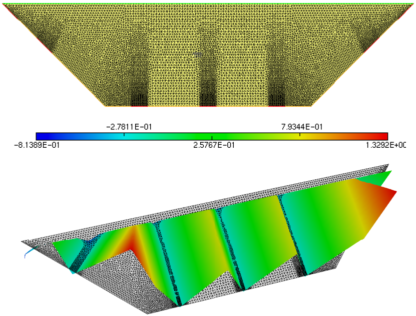
The ersatz material approximation in linearized elasticity (II)



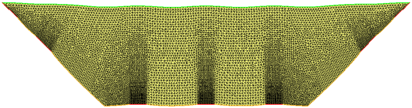
Physical situation of a bridge



Deformed configuration of the bridge



Implicit definition of the bridge on a mesh of D



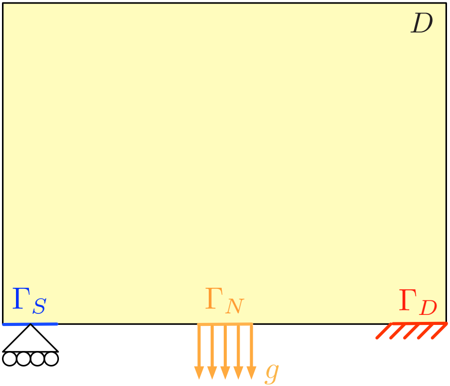
Deformed configuration of the domain D

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

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

$$C(\Omega) = \int_\Omega Ae(u_\Omega) : e(u_\Omega)\,\mathrm{d}x.$$

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

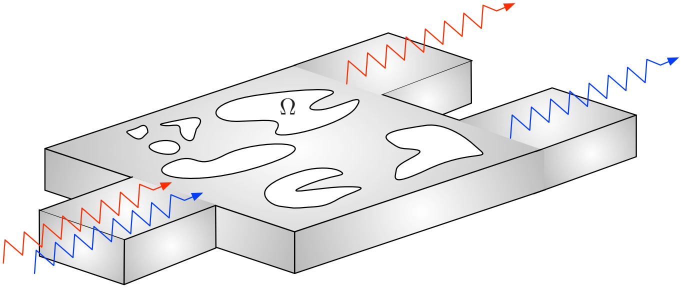


Part III

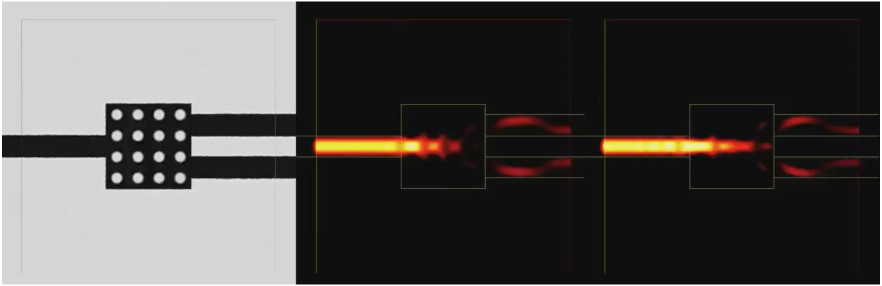
Geometric optimization problems

An example in electromagnetism (I)

- Light waves are usually conveyed through wave guides.
- The attached electric and magnetic fields are governed by Maxwell's equations.
- Demultiplexers are nanophotonic devices in charge of directing the incoming wave to different output wave guides, depending on its wave length.
- We aim to optimize the shape Ω of air inclusions in the Si core with the aim to realize this behavior.



An example in electromagnetism (II)



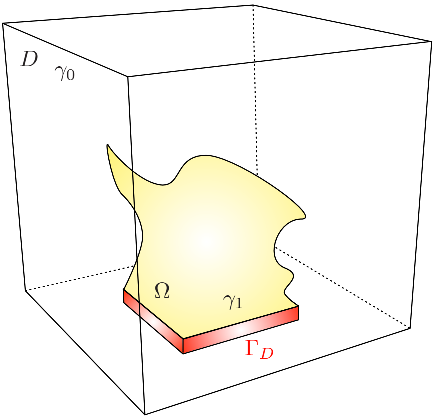
Optimization of the shape of a demultiplexer.

Optimization of the shape of a heat diffuser (I)

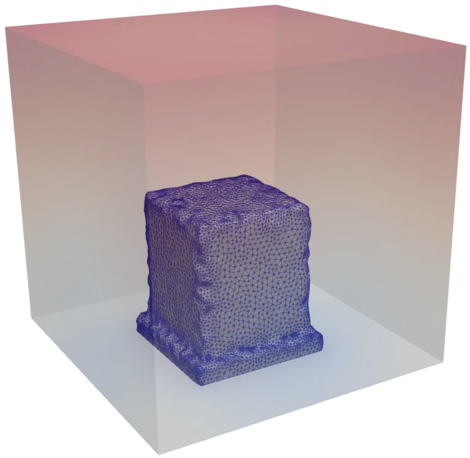
- A thermal chamber D is divided into
  - A phase Ω with high conductivity γ_1
  - A phase $D \setminus \overline{\Omega}$ with low conductivity γ_0.
- A temperature $T_0 = 0$ is imposed on Γ_D and the remaining boundary $\partial D \setminus \overline{\Gamma_D}$ is insulated from the outside.
- A heat source is acting inside D.
- The temperature u_Ω inside D is solution to the two-phase Laplace equation.
- The average temperature inside D,

$$J(\Omega) = \frac{1}{|D|} \int_D u_\Omega \, dx$$

is minimized under a volume constraint.



Optimization of the shape of a heat diffuser (II)



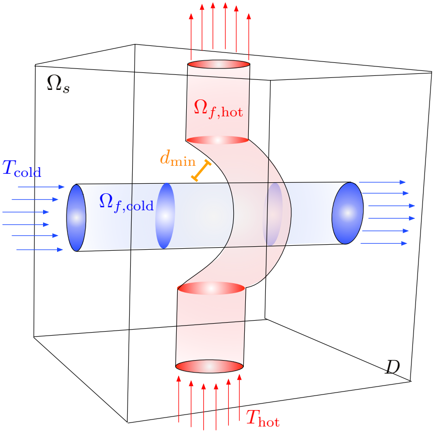
Optimization of the shape of a heat diffuser.

Optimization of the shape of a heat exchanger (I)

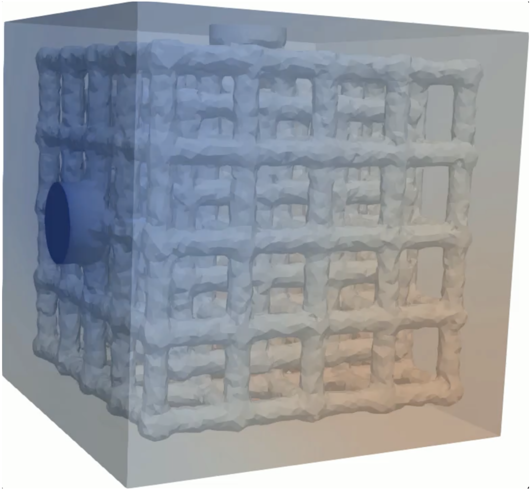
- A thermal chamber D is divided into
  - A phase $\Omega_{f,\text{hot}}$ conveying a hot fluid;
  - A phase $\Omega_{f,\text{cold}}$ conveying a cold fluid;
  - A solid phase Ω_s.
- The Navier-Stokes equations are satisfied in $\Omega_{f,\text{hot}}$, $\Omega_{f,\text{cold}}$.
- The stationary heat equation accounts for the temperature diffusion within D.
- The heat transferred from $\Omega_{f,\text{hot}}$ to $\Omega_{f,\text{cold}}$ is maximized.
- A constraint is imposed on the minimal distance between $\Omega_{f,\text{hot}}$ and $\Omega_{f,\text{cold}}$:

$$d(\Omega_{f,\text{hot}}, \Omega_{f,\text{cold}}) \geq d_{\text{min}}.$$

- Volume and pressure drop constraints are added on $\Omega_{f,\text{hot}}$, $\Omega_{f,\text{cold}}$.



Optimization of the shape of a heat exchanger (II)



Optimization of the shape of a heat exchanger.

Technical appendix

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 $\theta : \mathbb{R}^d \to \mathbb{R}^d$, i.e. there exists $C > 0$ such that:*

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

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

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

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

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

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 $\varphi : \Omega \to \mathbb{R}^d$ 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:

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

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

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

$$\int_{\varphi(\Gamma)} g \, \mathrm{d}s = \int_\Gamma |\mathrm{Com}(\nabla\varphi)n| g \circ \varphi \, \mathrm{d}s,$$

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

Remark: The integrand

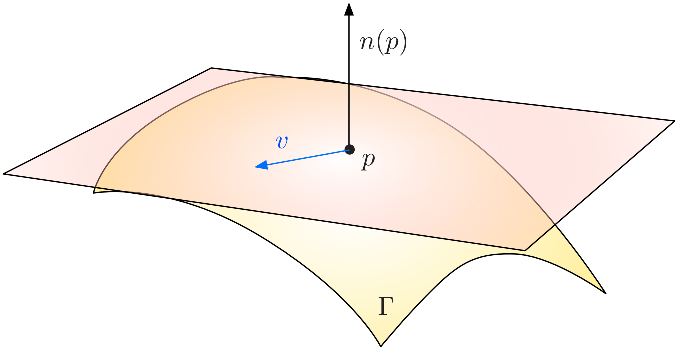
$$|\mathrm{Com}(\nabla\varphi)n| = |\det(\nabla\varphi)||\nabla\varphi^{-T} n|$$

is sometimes called the tangential Jacobian of the diffeomorphism φ.

Surfaces and curvature (I)

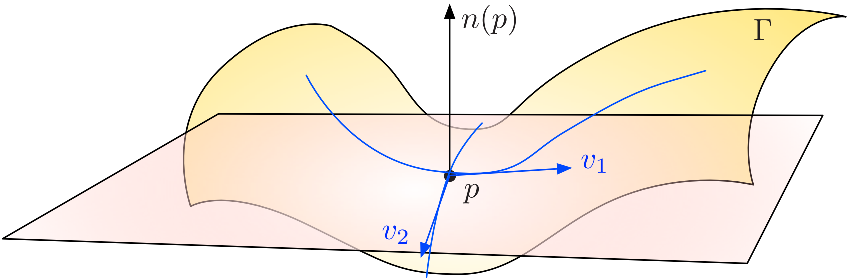
At first order, in the neighborhood of a point $p \in \Gamma$, a surface Γ behaves like a plane, the tangent plane,

- 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 $\kappa(p) = \kappa_1(p) + \kappa_2(p)$.



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 $\mathcal{F} : \mathcal{V} \times U \to F$ 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:

The differential $\mathrm{d}_u \mathcal{F}(\theta_0, u_0) : E \to F$ is a linear isomorphism.

Then there exist open neighborhoods $\mathcal{V}' \subset \mathcal{V}$ of θ_0 in Θ and $U' \subset U$ of u_0 in E, and a mapping $g : \mathcal{V}' \to U'$ 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 $u \in U'$, 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:
>
> $$f \in H^k(\Omega) \Rightarrow u \in H^{k+2}(\Omega), \text{ and } ||u||_{H^{k+2}(\Omega)} \leq C||f||_{H^k(\Omega)}.$$

A model example of elliptic regularity

Theorem 12.

Let $\Omega \subset \mathbb{R}^d$ be a bounded domain of class $\mathcal{C}^{k+2}$, and let $f \in H^k(\Omega)$. Then, the unique solution $u \in H^1_0(\Omega)$ 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 [Bre], §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 $\chi \in \mathcal{C}_c^\infty(\Omega)$,

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

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 $\mathcal{O}$ containing x_0 such that for any cutoff function $\chi \in \mathcal{C}_c^\infty(\mathbb{R}^d)$ with compact support inside $\overline{\mathcal{O}}$,

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

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

Proof of 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 $H^1_0(\Omega)$ to the problem:

$$\forall v \in H^1_0(\Omega), \int_\Omega \nabla(\chi u)\cdot\nabla v \,\mathrm{d}x = \int_\Omega gv\,\mathrm{d}x. \quad \text{(VF)}$$

- Intuitively, because $g \in L^2(\Omega)$ and $\mathrm{supp}(g)$ 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

$$\forall v \in H^1_0(\Omega), \int_\Omega \nabla w_i\cdot\nabla v\,\mathrm{d}x = \left\langle \frac{\partial g}{\partial x_i}, v\right\rangle_{H^{-1}(\Omega),H^1_0(\Omega)},$$

obtained by formally taking derivatives in (SF) or (VF), has a unique solution $w_i \in H^1_0(\Omega)$, 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 $u : \Omega \to \mathbb{R}$, 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:*
$$\forall i = 1, \ldots, d, \ \forall \varphi \in \mathcal{C}_c^\infty(\Omega), \ \left| \int_\Omega u \frac{\partial \varphi}{\partial x_i} \, \mathrm{d}x \right| \leq C ||\varphi||_{L^2(\Omega)}.$$
3. *There exists* $C > 0$ *such that for any open subset* $\omega \Subset \Omega$, *and any vector* $h \in \mathbb{R}^d$ *with* $|h| < \mathrm{dist}(\omega, \partial\Omega)$,
$$||D_h u||_{L^2(\omega)} \leq C.$$

In addition, one may take $C = ||\nabla u||_{L^2(\Omega)^2}$ *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 $\mathrm{supp}(\chi u)$ is a compact of Ω; this yields:

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

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

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

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

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

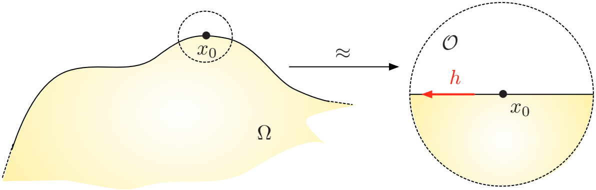
  and so:

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

- 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 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:

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

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

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

Proof of Step (iii).

- By compactness of $\overline{\Omega}$, 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:

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

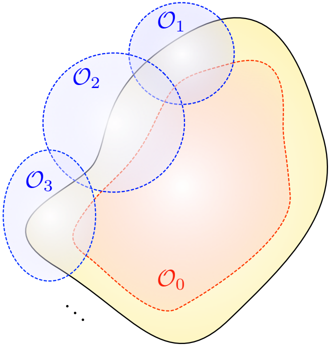
- Let $\{\theta_i\}_{i=0,\dots,N}$ be a partition of unity associated to the covering $\{\mathcal{O}_i\}_{i=0,\dots,N}$, i.e.

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

- Then:

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

$\square$



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 $p \to \infty$.

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