An introduction to shape optimization, with applications in fluid mechanics

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Part I

Introduction

Introduction

- The main target of shape optimization is to provide a common and systematic framework for optimizing structures described by various possible physical or mechanical models.

- Its study has become increasingly popular in academics and industry, partly owing to the steady increase in the cost of raw materials, which has made it necessary to optimize mechanical parts from the early stages of design.

- Automatic techniques (implemented in industrial softwares) have started to replace the traditional trial-and-error methods used by engineers, but still leave room for many forthcoming developments.

Mathematical framework

A shape optimization problem writes as the minimization of a cost (or objective) function J of the domain Ω:

$$\min_{\Omega \in \mathcal{U}_{ad}} J(\Omega),$$

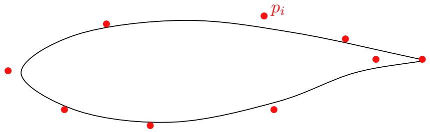
where $\mathcal{U}_{ad}$ is a set of admissible shapes (e.g. that satisfy constraints).

In most mechanical or physical applications, the relevant objective functions $J(\Omega)$ depend on Ω via a state u_Ω, which arises as the solution to a PDE posed on Ω (e.g. the linear elasticity system, or Stokes equations).

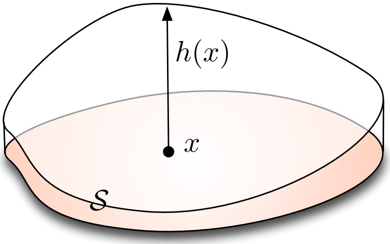
Various settings for shape optimization (I)

I. Parametric optimization

The considered shapes are described by means of a set of physical parameters $\{p_i\}_{i=1,\dots,N}$, typically thicknesses, curvature radii, etc...



Description of a wing by NURBS; the parameters of the representation are the control points p_i.



A plate with fixed cross-section $\mathcal{S}$ is parametrized by its thickness function $h : \Omega \to \mathbb{R}$.

Various settings for shape optimization (II)

- The parameters describing shapes are the only optimization variables, and the shape optimization problem rewrites:

$$\min_{\{p_i\} \in \mathcal{P}_{ad}} J(p_1, ..., p_N),$$

where $\mathcal{P}_{ad}$ is a set of admissible parameters.

- Parametric shape optimization is eased by the fact that it is straightforward to account for variations of a shape $\{p_i\}_{i=1,...,N}$:

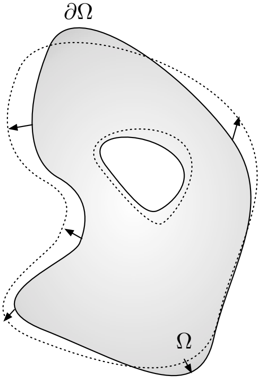
$$\{p_i\}_{i=1,...,N} \to \{p_i + \delta p_i\}_{i=1,...,N}.$$

- However, the variety of possible designs is severely restricted, and the use of such a method implies an a priori knowledge of the sought optimal design.

Various settings for shape optimization (III)

II. Geometric shape optimization

- The topology (i.e. the number of holes in $2d$) of the considered shapes is fixed.
- The boundary $\partial\Omega$ of the shapes Ω itself is the optimization variable.
- Geometric optimization allows more freedom than parametric optimization, since no a priori knowledge of the relevant regions of shapes to act on is required.



Optimization of a shape by performing 'free' perturbations of its boundary.

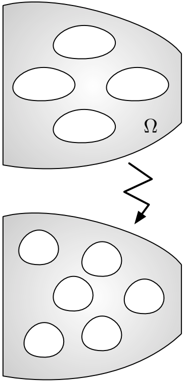
Various settings for shape optimization (IV)

III. Topology optimization

- In some applications, the suitable topology of shapes is unknown, and also subject to optimization.

- In this context, it is often preferred not to describe the boundaries of shapes, but to resort to different representations which allow for a more natural account of topological changes.

  For instance: Describing shapes Ω as density functions $\chi : D \to [0, 1]$.



Optimizing a shape by acting on its topology.

Various settings for shape optimization (V)

- A shape optimization process is a combination of:
  - A physical model, most often based on PDE (e.g. the linear elasticity equations, Stokes system, etc...) for describing the mechanical behavior of shapes,
  - A description of shapes and their variations (e.g. as sets of parameters, density functions, etc...),
  - A numerical description of shapes (e.g. by a mesh, a spline representation, etc...)
- These choices are strongly inter-dependent and influenced by the sought application.
- However very different in essence, all these different methods for shape optimization share a lot of common features.
- We are going to focus on geometric shape optimization methods.

Disclaimer

Disclaimer

- This course is very introductory, and by no means exhaustive, as well for theoretical as for numerical purposes.
- See the (non exhaustive) References section to go further.

Part II

Examples of shape optimization problems

Shape optimization in structure mechanics (I)

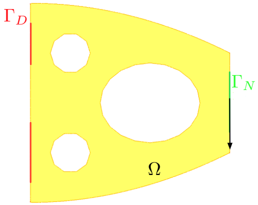
We consider a structure $\Omega \subset \mathbb{R}^d$, which is

- fixed on a part $\Gamma_D \subset \partial\Omega$ of its boundary,
- submitted to surface loads g, applied on $\Gamma_N \subset \partial\Omega$, $\Gamma_D \cap \Gamma_N = \emptyset$.

The displacement vector field $u_\Omega : \Omega \to \mathbb{R}^d$ is governed by the linear elasticity system:

$$\left\{ \begin{array}{rcll} -\mathrm{div}(Ae(u)) & = & 0 & \text{in } \Omega \\ u & = & 0 & \text{on } \Gamma_D \\ Ae(u)n & = & g & \text{on } \Gamma_N \\ Ae(u)n & = & 0 & \text{on } \Gamma := \partial\Omega \setminus (\Gamma_D \cup \Gamma_N) \end{array} \right.$$

where $e(u) = \frac{1}{2}(\nabla u^T + \nabla u)$ is the strain tensor field, and A is the Hooke's law of the material.



A 'Cantilever' beam

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The deformed cantilever

Shape optimization in structure mechanics (II)

Examples of objective functions:

- The work of the external loads g or compliance $C(\Omega)$ of domain Ω:

$$C(\Omega) = \int_\Omega Ae(u_\Omega) : e(u_\Omega) dx = \int_{\Gamma_N} g.u_\Omega \, ds$$

- A least-square discrepancy between the displacement u_Ω and a target displacement u_0 (useful when designing micro-mechanisms):

$$D(\Omega) = \left(\int_\Omega k(x) |u_\Omega - u_0|^\alpha dx \right)^{\frac{1}{\alpha}},$$

where α is a fixed parameter, and $k(x)$ is a weight factor.

Shape optimization in structure mechanics (III)

Examples of constraints:

- A constraint on the volume $\text{Vol}(\Omega) = \int_\Omega 1 \, dx$, or on the perimeter $P(\Omega) = \int_{\partial\Omega} 1 \, ds$ of shapes.
- A constraint on the total stress developped in shapes:

$$S(\Omega) = \int_\Omega ||\sigma(u_\Omega)||^2 \, dx,$$

  where $\sigma(u) = Ae(u)$ is the stress tensor.
- Geometric constraints, e.g. on the minimal and maximal thickness of shapes, on molding directions, etc... Such constraints play a crucial role when it comes to manufacturing shapes.

Shape optimization in fluid mechanics (I)

An incompressible fluid lies in a domain $\Omega \subset \mathbb{R}^d$.

- the flow u_{in} through the input boundary Γ_{in} is known.
- a pressure profile p_{out} is imposed on the exit boundary Γ_{out}.
- no slip boundary conditions are considered on the free boundary $\partial\Omega \setminus (\Gamma_{in} \cup \Gamma_{out})$.

The velocity $u_\Omega : \Omega \to \mathbb{R}^d$ and pressure $p_\Omega : \Omega \to \mathbb{R}$ of the fluid satisfy Stokes equations:

$$\left\{ \begin{array}{ll} -\mathrm{div}(D(u)) + \nabla p = f & \text{in } \Omega \\ \mathrm{div}(u) = 0 & \text{in } \Omega \\ u = u_{in} & \text{on } \Gamma_D \\ u = 0 & \text{on } \Gamma \\ \sigma(u)n = -p_{out} & \text{on } \Gamma_{out} \end{array} \right. ,$$

where $D(u) = \frac{1}{2}(\nabla u^T + \nabla u)$ is the symmetrized gradient of u.

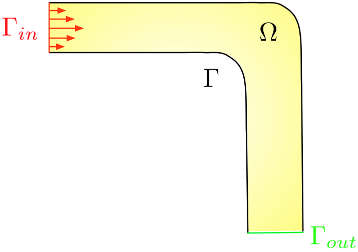
Shape optimization in fluid mechanics (II)

Model problem I: *Optimization of the shape of a pipe.*

- The shape subject to optimization is a pipe, connecting the (fixed) input area Γ_{in} and output area Γ_{out}.
- One is interested in minimizing the total work of the viscous forces inside the shape:

$$J(\Omega) = 2\mu \int_\Omega D(u_\Omega) : D(u_\Omega) \, dx.$$

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

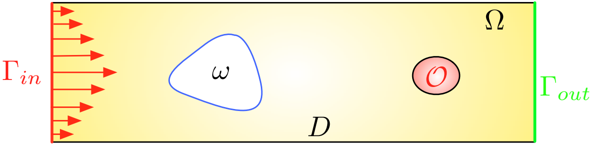


Shape optimization in fluid mechanics (III)

Model problem II: *Reconstruction of the shape of an obstacle.*

- An obstacle of unknown shape ω is immersed in a fixed domain D filled by the considered fluid.
- Given a mesure u_{meas} of the velocity u_Ω of the fluid inside a small observation area $\mathcal{O}$, one aims at reconstructing the shape of ω.
- The optimized domain is $\Omega := D \setminus \omega$, and only the part $\partial\omega$ of $\partial\Omega$ is optimized. One then minimizes the least-square criterion:

$$J(\Omega) = \int_{\mathcal{O}} |u_\Omega - u_{meas}|^2 \, dx.$$



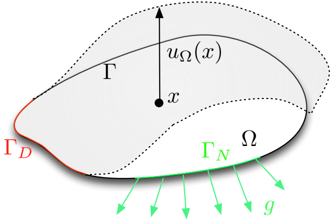
A simplified, academic example (I)

A membrane $\Omega \subset \mathbb{R}^d$ is:

- fixed on a part Γ_D of its boundary $\partial\Omega$.
- subject to traction loads g, applied on a part $\Gamma_N \subset \partial\Omega$, with $\Gamma_D \cap \Gamma_N = \emptyset$.

The vertical displacement $u_\Omega : \Omega \to \mathbb{R}$ of the membrane is solution to the Laplace equation:

$$\left\{ \begin{array}{rcll} -\Delta u & = & 0 & \text{in } \Omega \\ u & = & 0 & \text{on } \Gamma_D \\ \frac{\partial u}{\partial n} & = & g & \text{on } \Gamma_N \\ \frac{\partial u}{\partial n} & = & 0 & \text{on } \Gamma := \partial\Omega \setminus (\Gamma_D \cup \Gamma_N) \end{array} \right. .$$



The considered membrane

A simplified, academic example (II)

Examples of objective functions:

- Again, the compliance $C(\Omega)$ of the membrane Ω:

$$C(\Omega) = \int_\Omega |\nabla u_\Omega|^2 dx = \int_{\Gamma_N} g.u_\Omega \, ds.$$

- A least-square error between u_Ω and a target displacement u_0:

$$D(\Omega) = \left(\int_\Omega k(x) |u_\Omega - u_0|^\alpha dx \right)^{\frac{1}{\alpha}},$$

  where α is a fixed parameter, and $k(x)$ is a weight factor.

- The opposite of the first eigenvalue of the membrane:

$$-\lambda_1(\Omega), \text{where } \lambda_1(\Omega) = \min_{\substack{u \in H^1(\Omega) \\ u=0 \text{ on } \Gamma_D}} \frac{\displaystyle\int_\Omega |\nabla u|^2 \, dx}{\displaystyle\int_\Omega u^2 \, dx}.$$

More examples

- *Optimization of the shape of an airfoil:* reducing the drag acting on airplanes (even by a few percents) has been a tremendous challenge in aerodynamic industry for decades.

- *Optimization of the microstructure of composite materials:* in linear elasticity for instance, one is interested in the design of negative Poisson ratio materials, etc...

- *Optimization of the shape of wave guides* (e.g. optical fibers), in order to minimize the power loss of conducted electromagnetic waves.

- etc...

Why are those problems difficult?

- *From the modelling viewpoint:* difficulty to describe the physical problem at stake by a model which is relevant (thus complicated enough), yet tractable (i.e. simple enough).
- *From the theoretical viewpoint:* often, optimal shapes do not exist, and shape optimization problems enjoy at most local optima.
- *From both theoretical and numerical viewpoints:* the optimization variable is the domain! Hence the need for of a means to differentiate functions depending on the domain, and before that, to parametrize shapes and their variations.
- *On the numerical side:* difficulty to represent shapes and their evolutions.
- *On the numerical side:* shape optimization problems may be very sensitive and can be completely dominated by discretization errors.

Part III

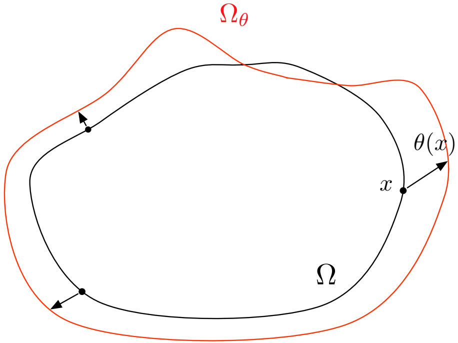
Shape derivatives of PDE-constrained functionals of the domain

Differentiation with respect to the domain: Hadamard's method

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

$$\Omega \mapsto \Omega_\theta := (I + \theta)(\Omega),$$

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



Lemma 1.

For $\theta \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ such that $||\theta||_{W^{1,\infty}(\mathbb{R}^d,\mathbb{R}^d)} < 1$, the application $(I + \theta)$ is a Lipschitz diffeomorphism.

Differentiation with respect to the domain: Hadamard's method

Definition 2.

Given a smooth domain Ω, a scalar function $\Omega \mapsto J(\Omega) \in \mathbb{R}$ is said to be shape differentiable at Ω if the function

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

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

$$\boxed{J(\Omega_\theta) = J(\Omega) + J'(\Omega)(\theta) + o\left(||\theta||_{W^{1,\infty}(\mathbb{R}^d,\mathbb{R}^d)}\right).}$$

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

Structure of shape derivatives (I)

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

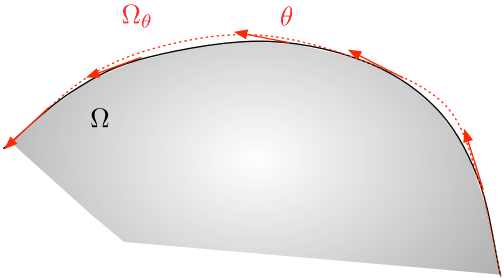


Figure : *At first order, a tangential vector field θ, (i.e. $\theta \cdot n = 0$) only results in a convection of the shape Ω, and it is expected that $J'(\Omega)(\theta) = 0$.*

Structure of shape derivatives (II)

Lemma 3.

Let Ω be a domain of class $\mathcal{C}^1$. Assume that the application

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

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 4.

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 form:

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

where $v_\Omega : \partial\Omega \to \mathbb{R}$ is a scalar field which 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 $t > 0$ yields:

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

First examples of shape derivatives

Theorem 5.

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

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

then J is shape differentiable at Ω and its shape derivative is:

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

First examples of shape derivatives

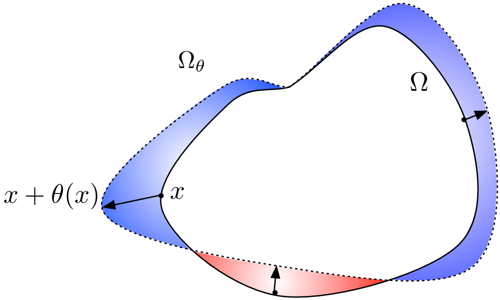


Figure : *Physical intuition: $J(\Omega_\theta)$ is obtained from $J(\Omega)$ by adding the blue area, where $\theta \cdot n > 0$, and removing the red area, where $\theta \cdot n < 0$. The process is 'weighted' by the integrand function f.*

First examples of shape derivatives

Remarks:

- This result is actually a particular case of the Transport (or Reynolds) theorem, used to derive the equations of conservation from conservation principles.

- It allows to calculate the shape derivative of the volume functional $\mathrm{Vol}(\Omega) = \int_\Omega 1\, dx$:

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

In particular, if $\mathrm{div}(\theta) = 0$, the volume does not vary (at first order) when Ω is perturbed by θ.

First examples of shape derivatives

Proof: The formula proceeds from a change of variables:

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

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

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

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

$$f \circ (I + \theta) = f + \nabla f \cdot \theta + o(\theta).$$

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

First examples of shape derivatives

Theorem 6.

Let $\Omega_0 \subset \mathbb{R}^d$ be a bounded, regular enough domain, and $g \in W^{2,1}(\mathbb{R}^d)$ be a fixed function. Consider the functional:

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

then J is shape differentiable at Ω_0 and its shape derivative is:

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

where κ stands for the mean curvature of $\partial\Omega$.

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

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

Towards more sophisticated examples

The examples of physical interest are those of PDE constrained shape optimization, i.e. one aims at minimizing functions which depend on Ω via the solution u_Ω of a PDE posed on Ω, for instance (in most of the forthcoming examples):

$$J(\Omega) = \int_\Omega j(u_\Omega)\,dx + \int_{\partial\Omega} k(u_\Omega)\,ds,$$

where u_Ω is e.g. the solution to the linear elasticity system posed on Ω, and j, k are given functions.

Doing so borrows methods from optimal control theory (adjoint techniques, etc...)

The framework

- Henceforth, we rely on the model of the Laplace equation: the state u_Ω is solution to the system

$$\begin{cases} -\Delta u = f & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \quad \text{(Dirichlet B.C)} \\ \frac{\partial u}{\partial n} = 0 & \text{on } \partial\Omega \quad \text{(Neumann B.C)} \end{cases}$$

  where $\int_\Omega f \, dx = 0$ in the Neumann case.

- The associated variational formulation reads:

$$\forall v \in H^1_0(\Omega)/H^1(\Omega), \ \int_\Omega \nabla u \cdot \nabla v \, dx - \int_\Omega fv \, dx = 0.$$

- We aim at calculating the shape derivative of $J(\Omega) = \int_\Omega j(u_\Omega) \, dx$, where $j : \mathbb{R} \to \mathbb{R}$ 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:

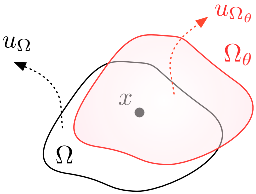
For a fixed $x \in \Omega$, $u'_\Omega(\theta)(x)$ is the derivative of the application

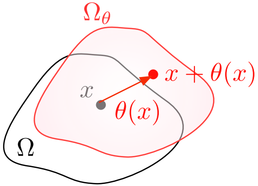
$$\theta \mapsto u_{\Omega_\theta}(x).$$

The Lagrangian point of view:

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

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





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 satsifies by u_Ω is clumsy:
even for θ 'small', $u_{\Omega_\theta}(x)$ may not make any sense if $x \in \partial\Omega$!

- The Lagrangian notion of shape derivative can be rigorously defined, and lends itself to mathematical analysis.

- The Eulerian derivative will be defined after the Lagrangian derivative, from the formal use of chain rule over the expression $u_{(I+\theta)(\Omega)} \circ (I + \theta)$:

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

Eulerian and Lagrangian derivatives (III)

Let $\Omega \mapsto u(\Omega) \in H^1(\Omega)$ be a function which to a domain, associates a function on the domain.

Definition 7.

The function $u : \Omega \mapsto u(\Omega)$ admits a material, or Lagrangian derivative $\dot{u}(\Omega)$ at a given domain Ω provided the transported function

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

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

Eulerian and Lagrangian derivatives (IV)

We are now in position to *define* the notion of Eulerian derivative.

Definition 8.

The function $u : \Omega \mapsto u(\Omega)$ admits 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 it admits a material derivative $\dot{u}(\Omega)(\theta)$ at Ω, and $\nabla u(\Omega) \cdot \theta \in H^1(\Omega)$.
One defines then:

$$u'(\Omega)(\theta) = \dot{u}(\Omega)(\theta) - \nabla u(\Omega).\theta \in W^{m,p}(\Omega). \tag{1}$$

Eulerian and Lagrangian derivatives (V)

Proposition 9.

Let $\Omega \subset \mathbb{R}^d$ be a smooth bounded domain, and suppose that $\Omega \mapsto u(\Omega)$ has a Lagrangian derivative $\dot{u(\Omega)}$ at Ω. If $j : \mathbb{R} \to \mathbb{R}$ is regular enough, the function $J(\Omega) = \int_\Omega j(u(\Omega))\, dx$ is then shape differentiable at Ω, and:

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

If $u(\Omega)$ has a Eulerian derivative $u'(\Omega)$ at Ω, one has the 'chain rule':

$$J'(\Omega)(\theta) = \underbrace{\int_{\partial\Omega} j(u(\Omega))\, \theta \cdot n \, ds}_{\substack{\text{Derivative of } \Omega \mapsto \int_\Omega j(u_\Omega) \\ \text{with respect to its first argument}}} + \underbrace{\int_\Omega j'(u(\Omega)) u'(\Omega)(\theta)\, dx}_{\substack{\text{Derivative of } \Omega \mapsto \int_\Omega j(u_\Omega) \\ \text{with respect to its second argument}}} .$$

Eulerian and Lagrangian derivatives (VI)

Let us return to our problem of calculating the shape derivative of:

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

The following result characterizes the Lagrangian derivative of $\Omega \mapsto u_\Omega$. Its proof can be adapted to many different PDE models:

Theorem 10.

Let $\Omega \subset \mathbb{R}^d$ be a smooth bounded domain. The application $\Omega \mapsto u_\Omega \in H^1_0(\Omega)$ admits 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:

$$\begin{cases} -\Delta Y = -\Delta(\theta \cdot \nabla u_\Omega) & \text{in } \Omega \\ Y = 0 & \text{on } \partial\Omega \end{cases}.$$

Eulerian and Lagrangian derivatives (VII)

Idea of the proof: The variational problem satisfied by u_{Ω_θ} is:

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

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

$$\forall v \in H^1_0(\Omega),\ \int_{\Omega} A(\theta)\nabla\overline{u}(\theta) \cdot \nabla v \, dx = \int_{\Omega_\theta} |\det(I + \nabla\theta)| fv \, dx,$$

where $A(\theta) := |\det(I + \nabla\theta)|\nabla\theta\,\nabla\theta^T$.

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.

Eulerian and Lagrangian derivatives (VIII)

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

- A use of the implicit function theorem provides the result.
- In particular, the transported function $\overline{u}(\theta)$ satisfies:

$$\forall v \in H^1_0(\Omega), \;\; \int_\Omega \nabla \overline{u}(\theta) \cdot \nabla v \, dx = \int_\Omega \nabla(\theta \cdot \nabla u_\Omega) \cdot \nabla v \, dx.$$

$\square$

Eulerian and Lagrangian derivatives (IX)

Remark: The Eulerian derivative of u_Ω can now be computed from its Lagrangian derivative. It satisfies:

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

or under variational form:

$$\forall v \in H_0^1(\Omega), \quad \int_\Omega \nabla u'_\Omega(\theta) \cdot \nabla v \, dx = \int_{\partial\Omega} \frac{\partial u_\Omega}{\partial n} v \, \theta \cdot n \, ds.$$

Using this formula in combination with:

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

will allow to express $J'(\Omega)(\theta)$ as a completely explicit expression of θ: this is the adjoint method from optimal control theory.

Eulerian and Lagrangian derivatives (X): the adjoint method

Idea: 'lift up' the term of $J'(\Omega)(\theta)$ which features the Eulerian derivative of u_Ω by introducing an adequate auxiliary problem.

- Let $p_\Omega \in H^1_0(\Omega)$ be defined as the solution to the problem:

$$\left\{ \begin{array}{cc} -\Delta p = -j'(u_\Omega) & \text{in } \Omega \\ p = 0 & \text{on } \partial\Omega \end{array} \right. .$$

- The variational formulation for p_Ω is:

$$\forall v \in H^1_0(\Omega), \;\; \int_\Omega \nabla p_\Omega \cdot \nabla v \, dx = -\int_\Omega j'(u_\Omega) \, v \, dx,$$

- ... to be compared with:

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

Eulerian and Lagrangian derivatives (XI): the adjoint method

$$\text{Thus, } J'(\Omega)(\theta) = \int_{\partial\Omega} j(u_\Omega)\,\theta\cdot n\,ds + \int_\Omega j'(u_\Omega)u'_\Omega(\theta)\,dx$$
$$= \int_{\partial\Omega} j(u_\Omega)\,\theta\cdot n\,ds - \int_\Omega \nabla p_\Omega\cdot\nabla u'_\Omega(\theta)\,dx \quad ,$$
$$= \int_{\partial\Omega} j(u_\Omega)\,\theta\cdot n\,ds - \int_{\partial\Omega} \frac{\partial p_\Omega}{\partial n}\frac{\partial u_\Omega}{\partial n}\theta\cdot n\,dx$$

where the variational problem for u'_Ω:

$$\forall v\in H_0^1(\Omega),\ \int_\Omega \nabla u'_\Omega(\theta)\cdot\nabla v\,dx = \int_{\partial\Omega}\frac{\partial u_\Omega}{\partial n}v\,\theta\cdot n\,ds.$$

was used in the last line, with test function $v = p_\Omega$.

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

Eulerian and Lagrangian derivatives: summary

- Mathematically speaking, it is the rigorous way to assess the differentiability of shape functionals.
- Several 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.
- This way of obtaining shape derivatives is very involved in terms of calculations.
- In practice, a formal method, which is much simpler, allows to calculate shape derivatives: Céa's method.

Céa's method

The philosophy of Céa's method comes from optimization theory:

Write the problem of minimizing $J(\Omega)$ as that of searching for the saddle points of a Lagrangian functional:

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

where the variables Ω, u, p are independent.

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

Céa's method: the Neumann case (I)

Consider the following Lagrangian functional:

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

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

One observes that, evaluating $\mathcal{L}$ with $v = u_\Omega$, it comes:

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

Céa's method: the Neumann case (II)

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:

- $\forall q \in H^1(\mathbb{R}^d), \;\; \dfrac{\partial \mathcal{L}}{\partial q}(\Omega, u, p)(q) = \displaystyle\int_\Omega \nabla u \cdot \nabla q \, dx - \int_\Omega fv \, dx = 0.$

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

Céa's method: the Neumann case (III)

Step 1: *Identification of u:*

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

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

$$\forall \psi \in \mathcal{C}_c^\infty(\Omega), \ \int_\Omega \nabla u \cdot \nabla \psi \, dx = 0 \Rightarrow \boxed{-\Delta u = f \text{ in } \Omega}.$$

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

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

Conclusion: $u = u_\Omega$.

Céa's method: the Neumann case (IV)

Step 2: *Identification of p:*

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

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

$$\forall \psi \in \mathcal{C}_c^\infty(\Omega), \int_\Omega \nabla p \cdot \nabla \psi \, dx + \int_\Omega j'(u)\psi \, dx = 0$$
$$\Rightarrow \boxed{-\Delta u = -j'(u_\Omega) \text{ in } \Omega}.$$

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

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

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

Céa's method: the Neumann case (V)

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

- We go back to the fact that:

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

- Differentiating with respect to Ω yields:

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

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

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

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

Céa's method: the Neumann case (VI)

This last (partial) derivative amounts to the shape derivative of a functional of the form:

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

where f is a fixed function.

Using Theorem 5, we end up with:

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

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

Céa's method: the Dirichlet case (I)

- We now consider the problem of derivating:

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

- **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 arises.
- We can no longer use the Lagrangian

$$\mathcal{L}(\Omega, v, q) = \int_\Omega j(v)\,dx + \int_\Omega \nabla v \cdot \nabla q\,dx - \int_\Omega fv\,dx,$$

since it would have to be defined for $v, q \in H^1_0(\Omega)$.
- In this case, the variables Ω, v, q would not be independent.

Céa's method: the Dirichlet case (II)

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

$$\mathcal{L}(\Omega, v, q, \mu) = \underbrace{\int_\Omega j(v)\, dx}_{\substack{\text{Objective function} \\ \text{where } u_\Omega \text{ is replaced by } v}} + \underbrace{\int_\Omega (-\Delta v - f) q\, dx}_{\substack{\text{penalization of the} \\ \text{`constraint'} -\Delta v = f}} + \underbrace{\int_{\partial\Omega} \mu v\, ds}_{\substack{\text{penalization of the} \\ \text{`constraint'} \ v=0 \text{ on } \partial\Omega}} .$$

By Green's formula, $\mathcal{L}$ rewrites:

$$\mathcal{L}(\Omega, v, q, \mu) = \int_\Omega j(v)\, dx + \int_\Omega \nabla v \cdot \nabla q\, dx - \int_\Omega fq\, dx + \int_{\partial\Omega} \left(\mu v - \frac{\partial v}{\partial n} q \right) ds.$$

Of course, evaluating $\mathcal{L}$ with $v = u_\Omega$, it comes:

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

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:

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

Céa's method: the Dirichlet case (IV)

Step 1: *Identification of u:*

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

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

$$\forall \psi \in \mathcal{C}^\infty_c(\Omega), \;\; \int_\Omega \nabla u \cdot \nabla \psi \, dx = 0 \Rightarrow \boxed{-\Delta u = f \text{ in } \Omega}.$$

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

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

Conclusion: $u = u_\Omega$.

Céa's method: the Dirichlet case (V)

Step 2: *Identification of p:*

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

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

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

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

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

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

Céa's method: the Dirichlet case (VI)

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** $\left\{ \begin{array}{cl} -\Delta p = -j'(u_\Omega) & \textbf{in } \Omega \\ p = 0 & \textbf{on } \partial\Omega \end{array} \right.$

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

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

Céa's method: the Dirichlet case (VII)

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

- We go back to the fact that:

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

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

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

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

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

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

Céa's method: the Dirichlet case (VIII)

Again, this (partial) derivative amounts to the shape derivative of a functional of the form:

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

where f is a fixed function.

Using Theorem 5 (and after some calculation), we end up with:

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

Part IV

Numerical aspects of shape optimization

The generic numerical algorithm

Gradient algorithm: Start from an initial shape Ω^0,

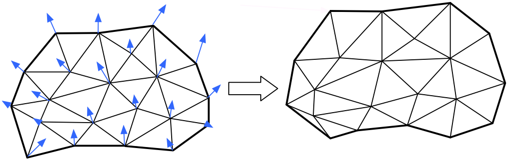
For $n = 0, \dots$ **convergence,**

1. Compute the state u_{Ω^n} (and possibly the adjoint p_{Ω^n}) of the considered PDE system on Ω^n.
2. Compute the shape gradient $J'(\Omega^n)$ thanks to the previous formula, and infer a descent direction θ^n for the cost functional.
3. Advect the shape Ω^n according to this displacement field for a small pseudo-time step τ^n, so as to get

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

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 the mesh $\mathcal{T}^n$ for computing u_{Ω^n} (and p_{Ω^n}) The descent direction θ^n is then calculated using the theoretical formula for the shape derivative of $J(\Omega)$.
- The shape advection step $\Omega^n \overset{(I+\tau^n\theta^n)}{\longmapsto} \Omega^{n+1}$ is performed by pushing the nodes of $\mathcal{T}^n$ along $\tau^n\theta^n$, to obtain the new mesh $\mathcal{T}^{n+1}$.



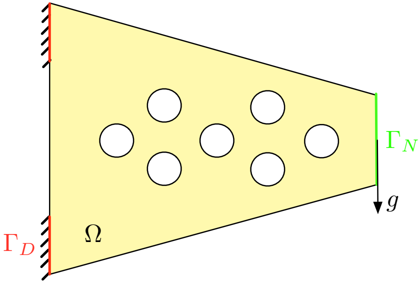
Deformation of a mesh by relocating its nodes to a prescribed final position.

Numerical examples (I)

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

$$C(\Omega) = \int_\Omega Ae(u_\Omega) : e(u_\Omega)\, dx.$$

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



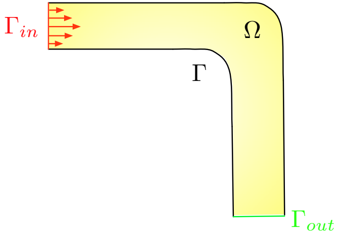
Minimization of the compliance of a cantilever (from [AlPan]; code available on [Allaire2]).

Numerical examples (II)

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

$$D(\Omega) = 2\mu \int_\Omega D(u_\Omega) : D(u_\Omega) \, dx.$$

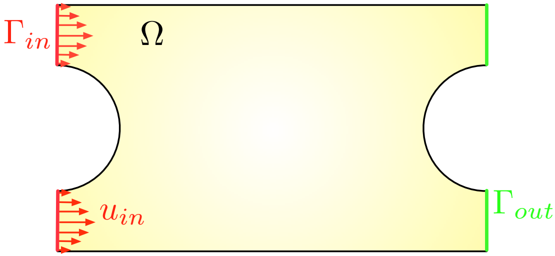
- A volume constraint is imposed by a *fixed* penalization of the function $D(\Omega)$ - i.e. the minimized function is $D(\Omega) + \ell \mathrm{Vol}(\Omega)$, where ℓ is a fixed Lagrange multiplier.



Minimization of the viscous dissipation inside a pipe.

Numerical examples (II)

- Still in fluid mechanics, minimization of the viscous dissipation $D(\Omega)$ in a double pipe.
- A volume constraint is imposed by a *fixed* penalization of the function $D(\Omega)$.

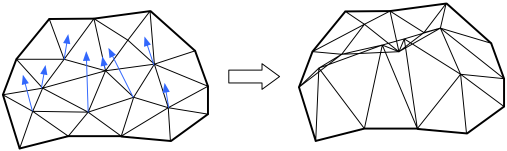


Minimization of the viscous dissipation inside a double pipe.

Numerical issues and difficulties (I)

I - The difficulty of mesh deformation:

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



Pushing nodes according to the velocity field may result in an invalid configuration.

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

Numerical issues and difficulties (II)

II - Velocity extension:

- A descent direction $\theta = -v_\Omega n$ from a shape Ω is inferred from the shape derivative of $J(\Omega)$:

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

- The new shape $(I + \theta)(\Omega)$ only depends on these values of θ on $\partial\Omega$.

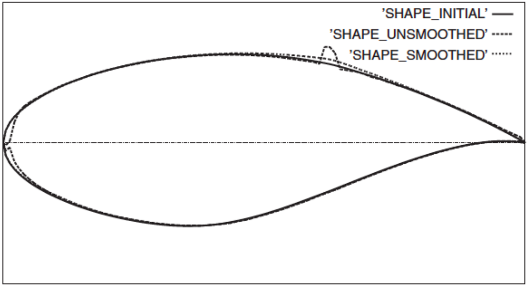
- For many reasons, in numerical practice, it is crucial to extend θ to Ω (or even $\mathbb{R}^d$) in a 'clever' way.
(for instance, deforming a mesh of Ω using a 'nice' vector field θ defined on the whole Ω may considerably ease the process)

- 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 (III)

III - Velocity regularization:

- Taking $\theta = -v_\Omega n$ on $\partial\Omega$ may produce a very irregular descent direction, 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.

Numerical issues and difficulties (IV)

A popular idea: extend AND regularize the velocity field

- Suppose we aim at extending the *scalar* field $v_\Omega : \partial\Omega \to \mathbb{R}$ 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. $\forall w \in H^1(\Omega)$,

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

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

Numerical issues and difficulties (IV)

- 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 allows:
  - to extend v_Ω to a large computational box D (an inner product over functions defined on D is used),
  - to extend the vector velocity $\theta = -v_\Omega n$ to Ω / D (an inner product over vector functions is used, e.g. that of linear elasticity).

Numerical issues: moral conclusion

The choice of a numerical method for shape optimization has to reach a tradeoff between numerical accuracy and robustness:

- The more accurate the representation of the boundaries of shapes, the more accurate the mechanical analyses performed on shapes (computation of u_{Ω^n}, p_{Ω^n}, etc...), and the more accurate the computation of descent directions.
- ... But the more tedious and error-prone the advection step between shapes $\Omega^n \mapsto \Omega^{n+1}$.

Part V

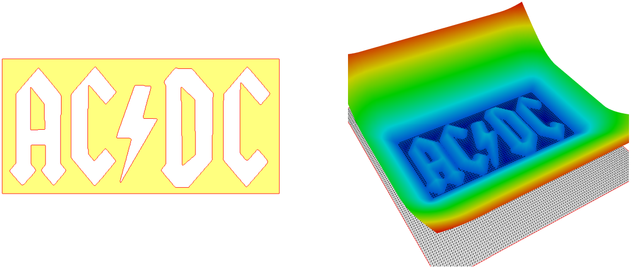
To go further: two popular methods

Other kinds of representation of shapes: the level set method (I)

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

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

Other kinds of representation of shapes: the level set method (II)

The motion of a domain $\Omega(t) \subset \mathbb{R}^d$ along a velocity field $v(t,x) \in \mathbb{R}^d$ is translated in terms of a 'level set function' $\phi(t,.)$ by the level set advection equation:

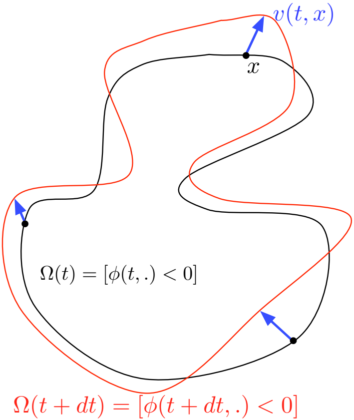
$$\boxed{\frac{\partial \phi}{\partial t}(t,x) + v(t,x).\nabla\phi(t,x) = 0}$$

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

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

the evolution equation rewrites as a Hamilton-Jacobi equation:

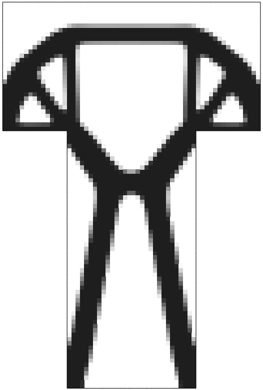
$$\boxed{\frac{\partial \phi}{\partial t}(t,x) + V(t,x)|\nabla\phi(t,x)| = 0}$$



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

- A fixed computational box D is meshed once and for all (e.g. with 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 has been calculated (as a scalar field defined at the nodes of the mesh), the advection step $\Omega^n \mapsto \Omega^{n+1} = (I + \tau^n\theta^n)(\Omega^n)$ is achieved by solving:

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



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

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

$\boxed{\textbf{Problem:}}$ Shapes are not meshed: how to solve a pde on a shape Ω?

$\boxed{\textbf{Solution:}}$ Approximate the PDE problem posed on Ω by a problem posed on the whole box D.

$\boxed{\textbf{Example:}}$ In the context of linear elasticity, the ersatz material approach consists in filling the void $D \setminus \Omega$ with a very 'soft' material, with Hooke's law εA, $\varepsilon \ll 1$.

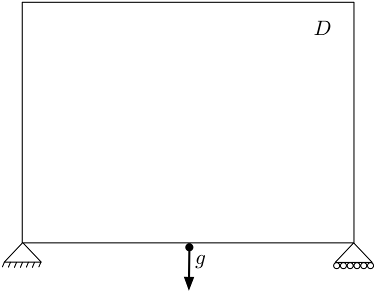
$$\left\{ \begin{array}{c} -\mathrm{div}(Ae(u)) = 0 \text{ in } \Omega \\ +B.C. \end{array} \right. \approx \left\{ \begin{array}{c} -\mathrm{div}(A_\Omega e(u)) = 0 \text{ in } D \\ A_\Omega = \mathbb{1}_\Omega A + (1 - \mathbb{1}_\Omega)\varepsilon A \\ +B.C. \end{array} \right.$$

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

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

In the context of linear elasticity, we are interested in the optimization of a bridge with respect to its compliance $C(\Omega)$.

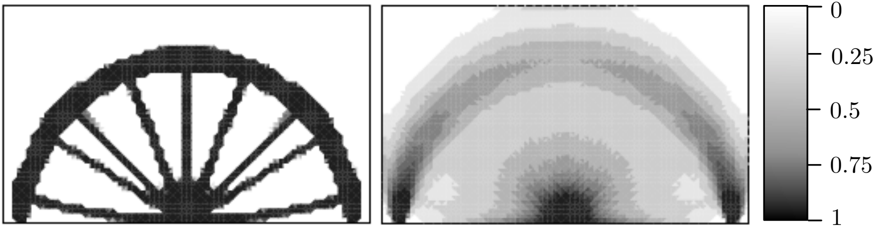
An equality constraint on the volume $\mathrm{Vol}(\Omega)$ of shapes is imposed.



Minimization of the compliance of a bridge using the level set method. (from [AlJouToa]; code available on [Allaire2])

Other kinds of representation of shapes: the SIMP method

- The SIMP method (Solid Isotropic Material Penalization) is a heuristic method for topology optimization derived from the mathematical theory of homogenization.
- It is very popular within the engineering community, and is already implemented in industrial softwares.
- It relies on a completely different point of view as regards the notion of shapes, as well on the theoretical side as on the numerical one.



(Left) 'Classical' 'black-and-white' shape, (right) shape represented by a density function (from [Allaire1])

The SIMP method: main ideas in the context of linear elasticity (I)

Problem formulation

In a fixed working domain D, find the optimal density $\rho : D \to [0,1]$ of a mixture of the considered elastic material and void.

Idea: The stiffness (i.e. the Hooke's law) $A(\rho)$ of the total structure D is proportional to a power of the density ρ via an empiric law:

$$A(\rho) = \rho^p A, \text{ where } A \text{ is the Hooke's law of the material.}$$

In numerical practice, one takes $p \geq 3$, so as to penalize the intermediate densities $\rho \neq 0, 1$ which correspond to greyscale patterns and are difficult to interprete in terms of 'classical' black-and-white designs.

The SIMP method: main ideas in the context of linear elasticity (II)

- The displacement u_ρ of D is solution to the linear elasticity system:

$$\left\{ \begin{array}{rcll} -\text{div}(A(\rho)e(u)) & = & 0 & \text{in } D \\ u & = & 0 & \text{on } \Gamma_D \\ A(\rho)e(u)n & = & g & \text{on } \Gamma_N \\ A(\rho)e(u)n & = & 0 & \text{on } \Gamma := \partial D \setminus (\Gamma_D \cup \Gamma_N) \end{array} \right. .$$

- **Example:** The compliance minimization problem is formulated as:

$$\min_{\rho \in \mathcal{D}_{ad}} J(\rho), \;\; J(\rho) = \int_D A(\rho)e(u_\rho) : e(u_\rho)\, dx,$$

where $\mathcal{D}_{ad}$ is a set of admissible density functions.

- The derivative $J'(\rho)$ of J can be computed using the techniques presented in this course (Céa's method).

The SIMP method: main ideas in the context of linear elasticity (III)

In the context of linear elasticity, one minimizes the compliance $C(\Omega)$ of a cantilever beam.

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

Minimization of the compliance of a cantilever using the SIMP method. (from [Sigmund]; code available on [DTU])

The SIMP method: pros and cons

Assets:

- Easy to analyze from the mathematical viewpoint: the problem is almost reduced to a parametric shape optimization framework.
- Simple and robust implementation: no mesh deformation is necessary, and the update of a 'shape' ρ^n of the process to the next one ρ^{n+1} is performed via the simple operation:

$$\rho^{n+1} = \rho^n - \tau^n J'(\rho^n).$$

Drawbacks:

- The method is heuristic, and may entail uncontrolled approximation of the real physical model.
- The geometry of shapes is lost; it may be awkward to formulate in this context constraints on the curvature, thickness of shapes, etc...

A first taste of the SIMP method in fluid mechanics

- One optimizes a density function $\rho : D \to [0,1]$ over a domain D:
  - $\rho(x) = 0$ indicates that no fluid occupies the area around $x \in D$.
  - $\rho(x) = 1$ indicates that only fluid occupies this area.
- The approximate Stokes system on the total domain D is:

$$\left\{ \begin{array}{cl} -\mathrm{div}(D(u)) + \alpha(\rho) u + \nabla p = f & \text{in } D \\ \mathrm{div}(u) = 0 & \text{in } D \\ + \text{ boundary conditions} & \end{array} \right. .$$

- The coefficient $\alpha(\rho)$ incorporates a solid part to the model by using a heuristic penalization inspired by the homogenization theory:

$$\alpha(\rho) \approx 0 \text{ in the fluid phase, } \alpha(\rho) \approx \infty \text{ in the solid phase.}$$

  In practice, one uses a penalization of the form:

$$\alpha(\rho) = \alpha_{max} + (\alpha_{min} - \alpha_{max}) \rho \frac{1+q}{\rho + q}, \quad q, \alpha_{min}, \alpha_{max} \text{ parameters.}$$

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- [BorPet] T. Borrvall and J. Petersson, *Topology optimization of fluids in Stokes flow*, Int. J. Numer. Methods in Fluids, Volume 41, (2003), pp. 77–107.

Online resources I

- [Allaire2] *Grégoire Allaire's web page*, http://www.cmap.polytechnique.fr/ allaire/.
- [Allaire3] G. Allaire, *Conception optimale de structures*, slides of the course (in English), available on the webpage of the author.
- [DTU] *Web page of the Topopt group at DTU*, http://www.topopt.dtu.dk.
- [FreeFem++] O. Pironneau, F. Hecht, A. Le Hyaric, *FreeFem++ version 2.15-1*, http://www.freefem.org/ff++/.