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An introduction to shape and topology optimization

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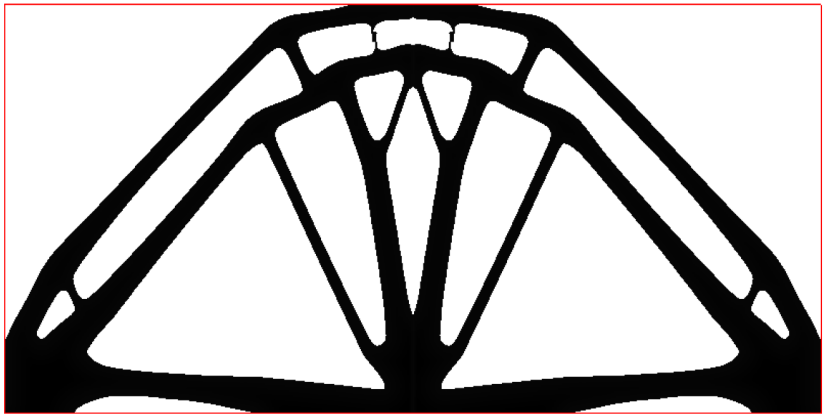
Thanks: *P. Frey, Y. Privat.*

$15^{\text{th}} - 17^{\text{th}}$ October, 2018

Foreword

- Shape optimization is about the minimization of an objective function $J(\Omega)$, depending on a shape Ω of $\mathbb{R}^2$ or $\mathbb{R}^3$, under certain constraints.
- Such problems have come up early in the history of sciences, and they are ubiquitous in nature.
- Nowadays, they arouse a tremendous enhusiasm in engineering.
- They are at the interface between mathematics, physics, mechanical engineering and computer science.
- Shape optimization is a burning field of research!



Contents (I)

- The present course is composed of
  - 6 hours of lectures, covering the main theoretical aspects;
  - A hands-on session of 6 hours, dedicated to the numerical implementation of basic shape and topology optimization algorithms in `FreeFem++`.

- All the material from the course (slides of the lectures, subjects and solution programs for the hands-on session) is available on the `GitHub` repository:

  `https://github.com/dapogny/GDR-MOA-Course`

- Feel free to contact me for any comment, suggestion or question:

  `charles.dapogny[AT]univ-grenoble-alpes.fr`

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Part I

Some selected milestones in shape optimization

- Dido's problem and the isoperimetric inequality
- Shape optimization in architecture
- Towards 'modern' shape and topology optimization

Dido's problem (I)

- Dido's problem is reported in the myth of the foundation of Carthage by Phœnician princess Dido, in 814 B.C. (cf. Virgil's *Aeneid*, $\approx$ 100 B.C.).

- Dido fled Tyr (actual Lebanon) after her husband got murdered by her brother Pygmalion.

- Accompanied by here fellows, she landed on the Tunisian shore, where she required a land from local king Jarbas...

- *... They came to this spot, where to-day you can behold the mighty Battlements and the rising citadel of New Carthage,*
  And purchased a site, which was named 'Bull's Hide' after the bargain
  By which they should get as much land as they could enclose with a bull's hide...

  [Virgil, Aeneid]

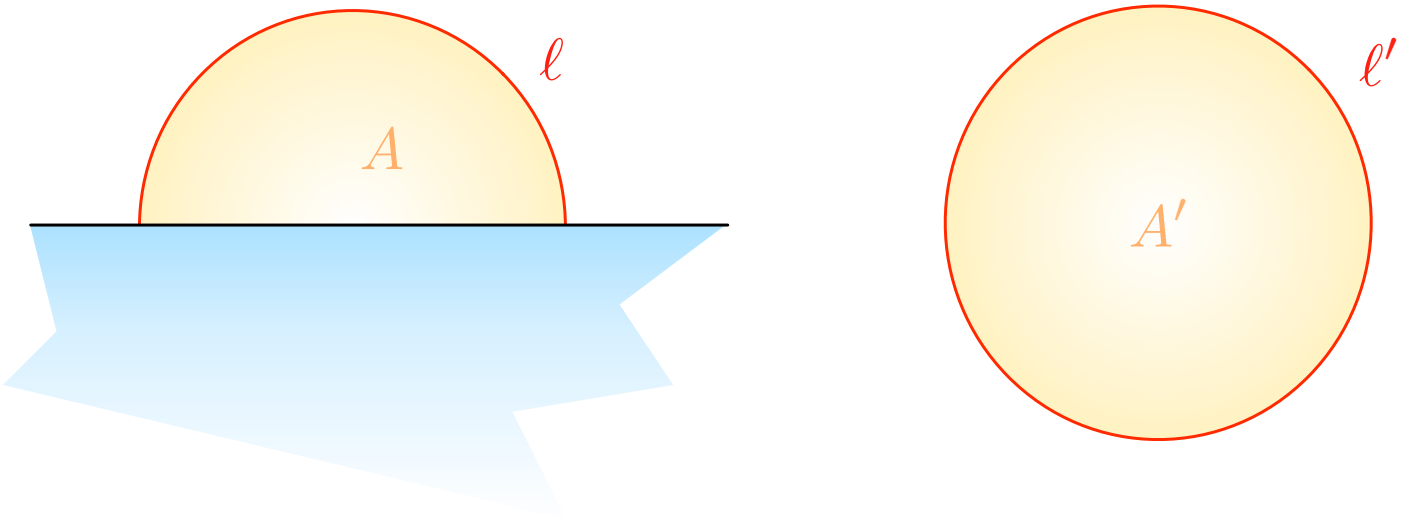
Dido's problem (II)

W. Turner: 'Dido Building Carthage' or 'The Rise of the Carthaginian Empire' (1815).

Dido's problem (III)

Using modern terminology:

How to surround the largest possible area A with a given contour length ℓ?



(Left) The solution to Dido's problem in the case where the surrounded domain is limited by the sea; (right) an 'unconstrained' version of Dido's problem.

The isoperimetric inequality (I)

- Incidentally, Queen Dido had just discovered the isoperimetric inequality:

> Let $\Omega \subset \mathbb{R}^2$ be a domain with 'smooth enough' boundary $\partial\Omega$. Let A be the area covered by Ω, and ℓ be the length of $\partial\Omega$. Then,
>
> $$4\pi A \leq \ell^2,$$
>
> where equality holds if and only if Ω is a disk.

- Equivalently,

> Among all domains $\Omega \subset \mathbb{R}^2$ with prescribed area, that with minimum perimeter is the disk.

- Other versions of this problem exist.

  Example: One may impose that the boundary of Ω should contain a non optimizable region (a segment).

The isoperimetric inequality (II)

- This fact was first proved in 1838 by J. Steiner, ... but the proof was false! Actually, J. Steiner proved that, assuming that an optimal shape exist... it should then be a disk.

- However, many shape optimization problems do not have a solution, for deep mathematical and physical reasons.

- Only in 1860 did K. Weierstrass complete the proof of the isoperimetric inequality in two dimensions.

- The isoperimetric inequality holds in more general contexts, for instance in three space dimensions (H. Schwarz, 1884):

Among all domains $\Omega \subset \mathbb{R}^3$ with prescribed volume, that with minimum surface is the ball.

Another occurrence of the isoperimetric inequality

Medieval cities often have a circular shape so as to minimize the perimeter of the necessary fortifications around a given population (i.e. their area).

Map of Paris during the Dark Ages.

Part I

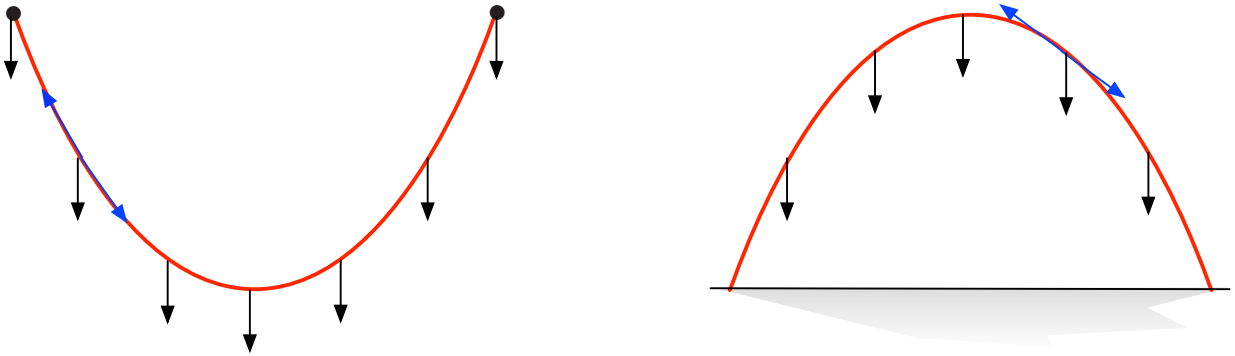
Some selected milestones in shape optimization

- Dido's problem and the isoperimetric inequality
- Shape optimization in architecture
- Towards 'modern' shape and topology optimization

The quest of architects for optimal design (I)

- Structural optimization has long been a central concern in architectural design.
- One crucial step towards modern design: the Hooke's theorem (1675)

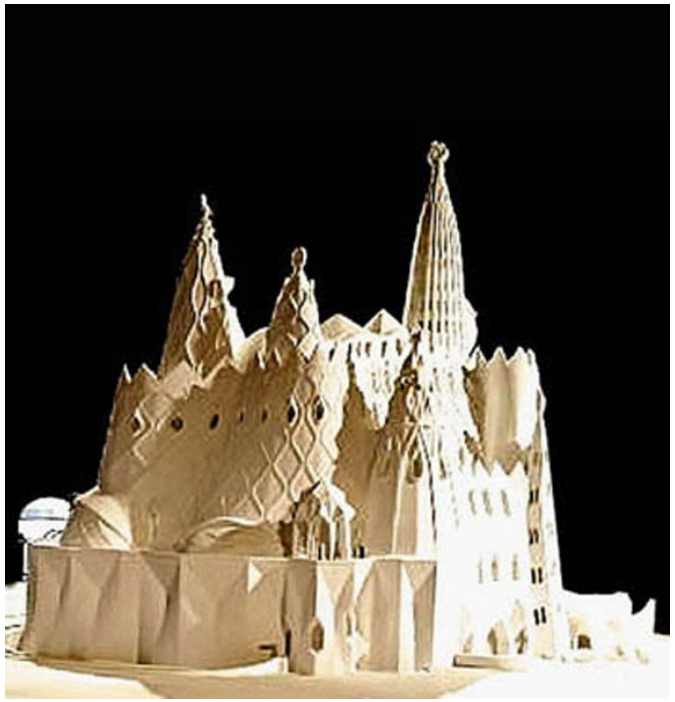
"As hangs the flexible chain, so but inverted will stand the rigid arch."



(Left) A chain hanging in equilibrium under the action of gravity and tension forces; (right) an arch standing in equilibrium under gravity and compression forces.

The quest of architects for optimal design (II)

- A. Gaudi sketched the plans of the church of the Colònia Güell (1889-1914) by relying on a funicular model so as to determine a stable assembly of columns and vaults.

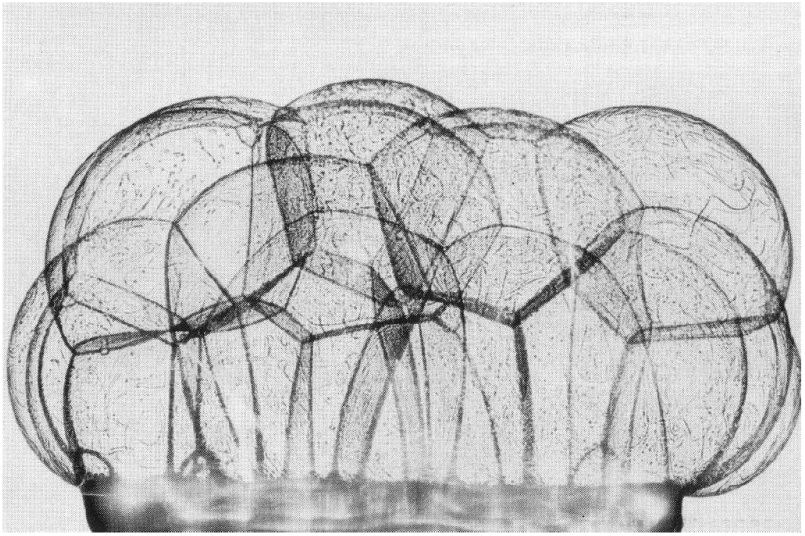


(Left) Gaudi's experimental device, (right) model of the Colònia Güell ***(Photo credits: http://www.gaudidesigner.com)***.

The quest of architects for optimal design (III)

Since then, optimal design concepts have attracted the attention of world-renowned architects: Heinz Isler, Gustave Eiffel, Frei Otto, etc.

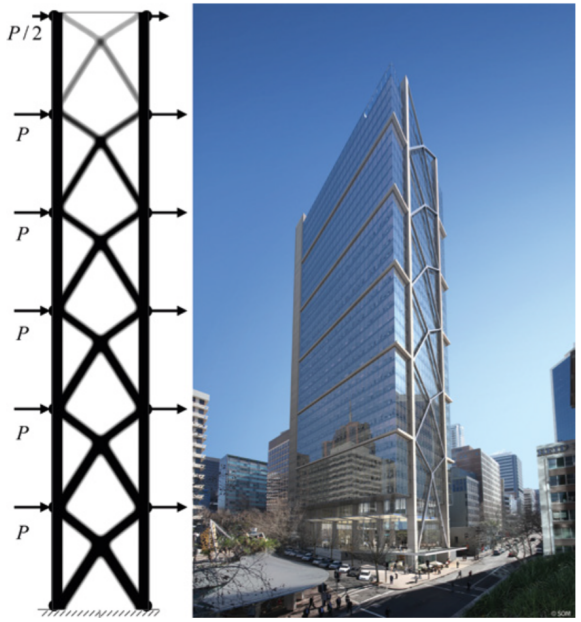
- They allow to model complex geometric criteria, related to the æstethics, the constructibility, and the mechanical performance of structures.
- Optimized shapes with respect to mechanical considerations have often 'elegant' outlines: their organic nature is very appreciated by architects.



(Left) A soap-film structure, coined by Frei Otto, (right) interior view of the Manheim Garden festival.

The quest of architects for optimal design (IV)

- Nowadays, modern structural optimization techniques are currently employed for the design of large-scale buildings.



(Left) Entrance of the Qatar National Convention Center, in Doha [Sasaki et al]. (Right) Sketch of a 288m high skyscraper in Australia by Skidmore, Owings & Merrill.

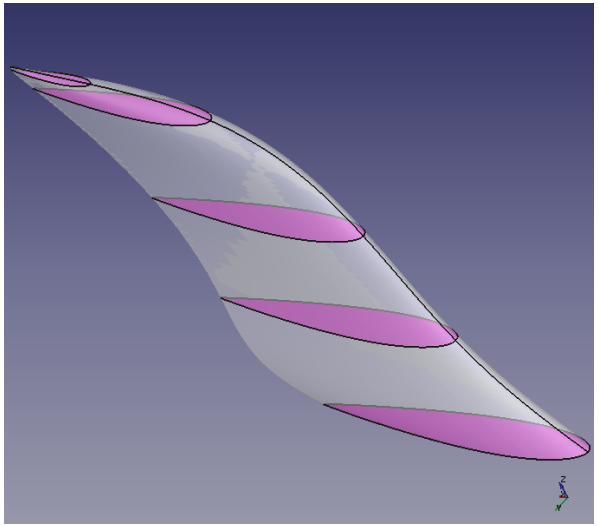
Part I

Some selected milestones in shape optimization

- Dido's problem and the isoperimetric inequality
- Shape optimization in architecture
- Towards 'modern' shape and topology optimization

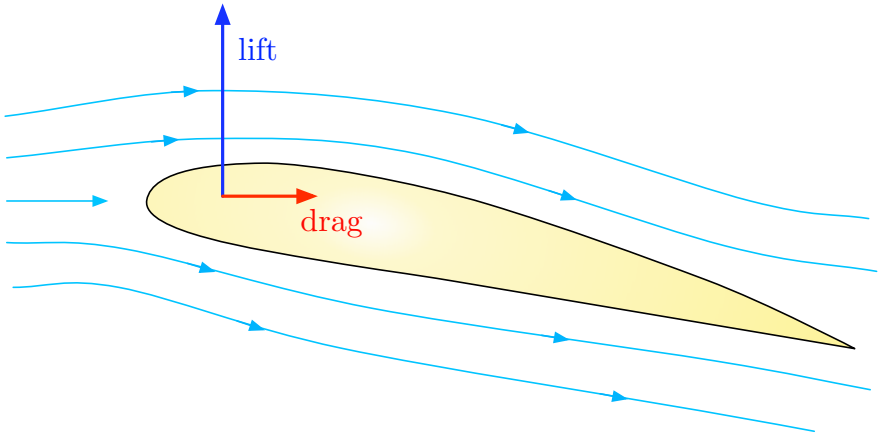
Towards 'modern' shape and topology optimization (I)

- More advanced shape optimization methods have emerged from the 1960's, mainly due to
  - The development of efficient numerical tools for analyzing complex physical phenomena (notably the finite element method);
  - The increase in computational power.



Sketch of the wing of an aircraft

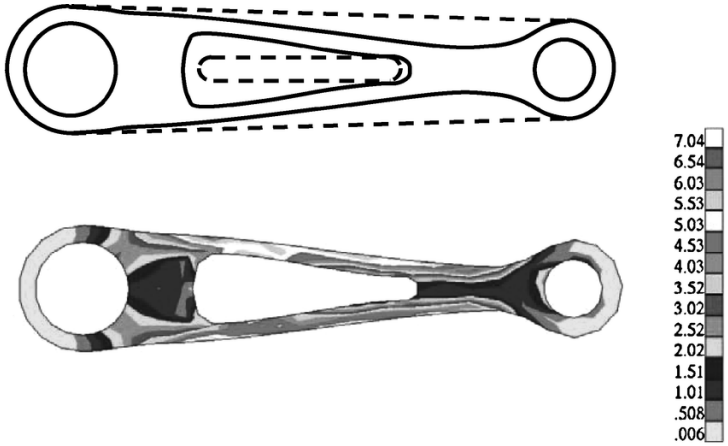
- One of the first fields involved is aeronautics, where engineers were motivated to optimize airfoils so as to
  - Minimize the drag of aircrafts;
  - Increase their lift.



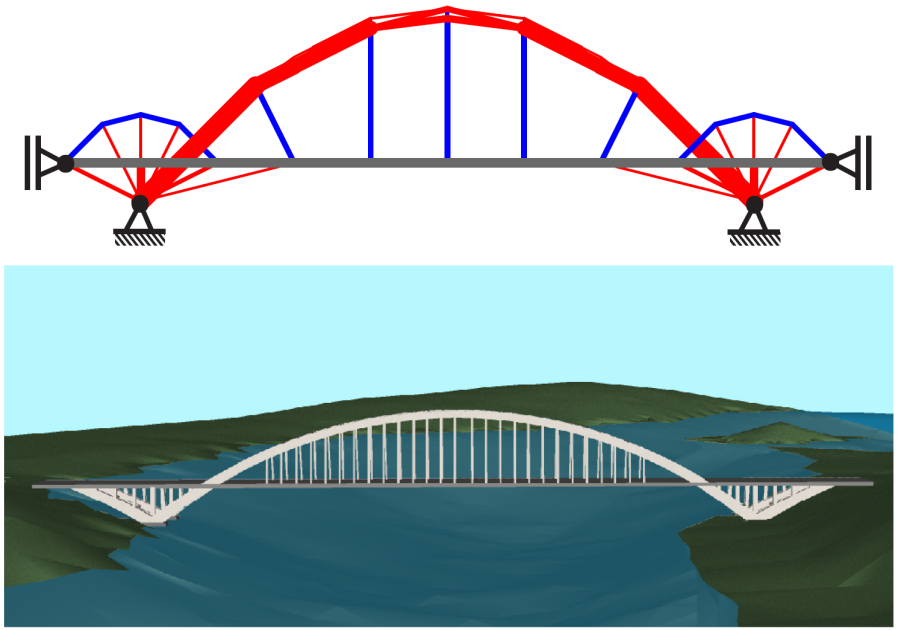
An airfoil subjected to the reaction of air

Towards 'modern' shape and topology optimization (II)

Concurrently, such computer-aided methods have aroused a great enthusiasm in civil and mechanical engineering.



Optimization of a torque arm ***(from*** *[KiWan]****)***

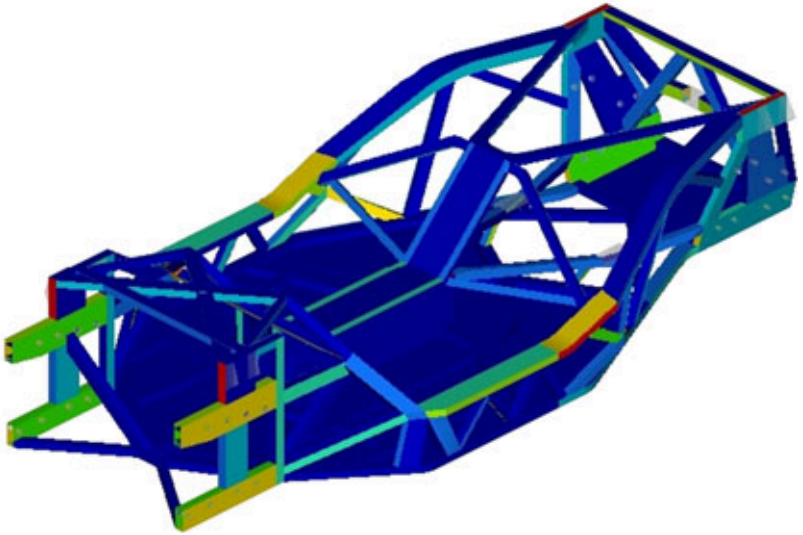


Optimization of an arch bridge ***(from*** *[ZhaMa]****)***

Towards 'modern' shape and topology optimization (III)

- Since then, much headway has been made in the mathematical and algorithmic practice of shape and topology optimization.
- Nowadays, shape and topology optimization techniques are consistently used in industry in a wide variety of situations.
- Several industrial softwares are available: `OptiStruct`, `Ansys`, `Tosca`, etc.

Optimization of a hip prosthesis ***(Photo credits:*** *[Al]****)***



Optimization of an automotive chassis

(from *[CaBa]****)***

Part II

Generalities about shape optimization problems and examples

- What is a shape optimization problem?
- Examples of model problems
- A refresher about the finite element method

What is a shape optimization problem? (I)

- A typical shape optimization problem arises under the form:

$$\boxed{\min_{\Omega \in \mathcal{U}_{ad}} J(\Omega), \text{ s.t. } C(\Omega) \leq 0,}$$

where

  - Ω is the shape, or the design variable;
  - $J(\Omega)$ is an objective function to be minimized;
  - $C(\Omega)$ is a constraint function;
  - $\mathcal{U}_{ad}$ is a set of admissible shapes;

- In mechanical or physical applications, $J(\Omega)$ and $C(\Omega)$ often depend on Ω via a state u_Ω, solution to a PDE posed on Ω (e.g. the linear elasticity system, or Stokes equations).

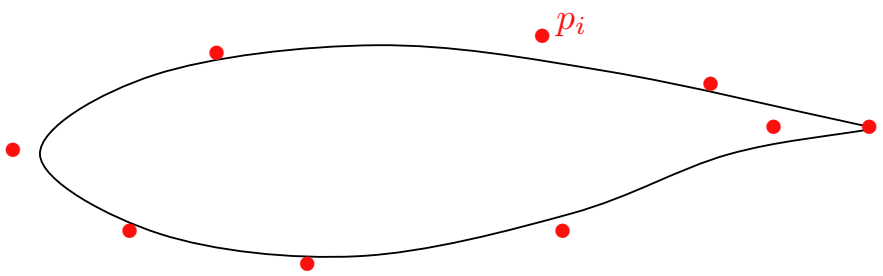
What is a shape optimization problem? (II)

- A shape optimization process is the 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 mathematical 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 they are often guided by the particular application.
- Roughly speaking, shape and topology optimization problems fall intro three main categories: parametric, geometric and topology optimization.
- This classification is quite arbitrary; it mainly reflects a point of view about what is important in the problem. The associated mathematical and numerical methods share a lot of common features.

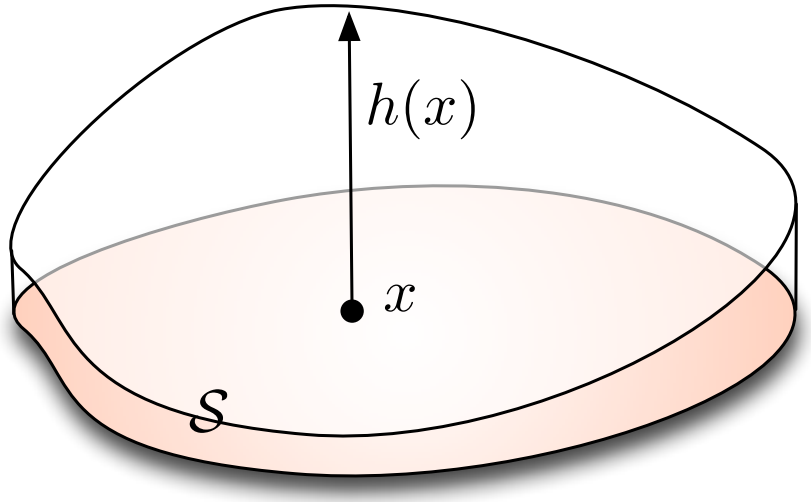
Various settings for shape optimization (I)

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 $h : \mathcal{S} \to \mathbb{R}$.

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 $\{p_i\}_{i=1,\dots,N}$:

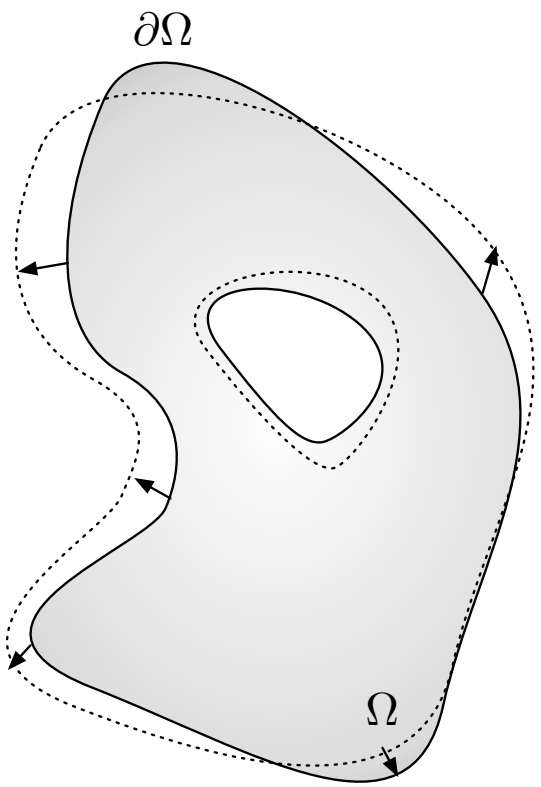
$$\{p_i\}_{i=1,\dots,N} \to \{p_i + \delta p_i\}_{i=1,\dots,N}\,.$$

- 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 of shapes is fixed (i.e. their number of holes in 2d).
- The whole boundary $\partial\Omega$ of shapes Ω 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 Ω via 'free' perturbations of the boundary $\partial\Omega$.

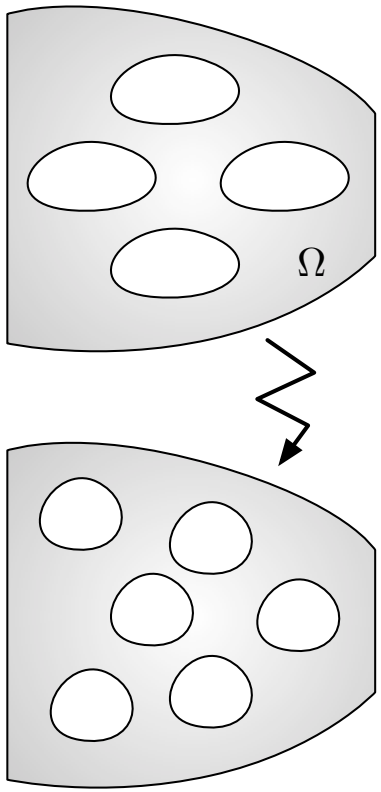
Various settings for shape optimization (IV)

III. Topology optimization

- In many applications, the suitable topology of shapes is unknown, and it is 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.

Example Describing shapes Ω as density functions $h : D \to [0, 1]$.



Optimizing a shape by acting on its topology.

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

Generalities about shape optimization problems and examples

- What is a shape optimization problem?
- Examples of model problems
- A refresher about the finite element method

A simplified, academic example (I)

A cavity $D \subset \mathbb{R}^d$ is filled with a material with thermal conductivity $h : D \to \mathbb{R}$.

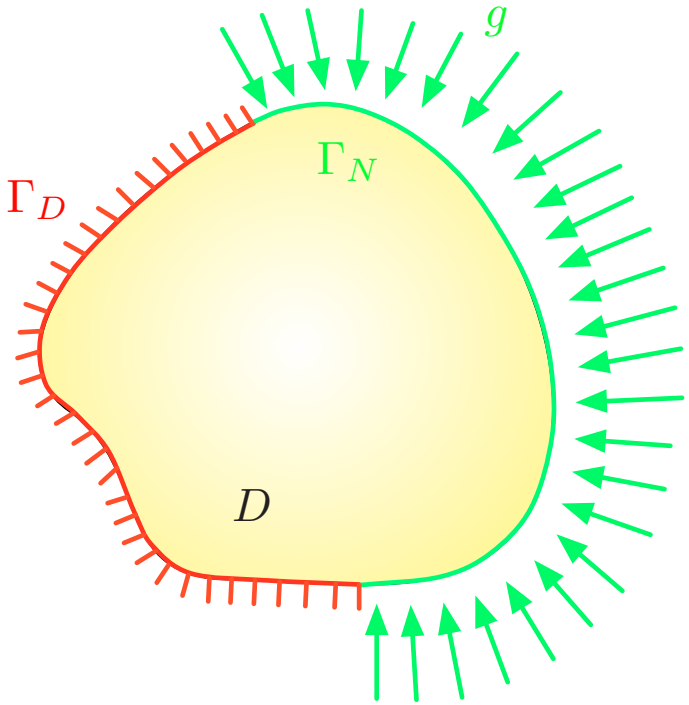
- A region $\Gamma_D \subset \partial D$ is kept at temperature 0.
- A heat flux g is applied on $\Gamma_N := \partial D \setminus \overline{\Gamma_D}$.
- A heat source or sink $f : D \to \mathbb{R}$ is acting inside D.

The temperature $u_h : D \to \mathbb{R}$ within the cavity is solution to the conductivity equation:

$$\left\{ \begin{array}{rcll} -\mathrm{div}(h\nabla u_h) & = & f & \text{in } D, \\ u_h & = & 0 & \text{on } \Gamma_D, \\ h\frac{\partial u_h}{\partial n} & = & g & \text{on } \Gamma_N. \end{array} \right. .$$

Parametric optimization problem: the design variable is the conductivity distribution $h \in \mathcal{U}_{\mathrm{ad}}$, where

$$\mathcal{U}_{\mathrm{ad}} = \{h \in L^\infty(D),\ \alpha \leq h(x) \leq \beta,\ x \in D\}.$$



The considered cavity

A simplified, academic example (II)

Examples of objective functions:

- The compliance $C(h)$ of the cavity D:

$$C(h) = \int_D h|\nabla u_h|^2 dx = \int_{\Gamma_N} g u_h \, ds,$$

as a measure of the heat power inside D, or of the work of the heat flux on D.

- A least-square error between u_h and a target temperature u_0:

$$D(h) = \left(\int_D k(x)|u_h - u_0|^\alpha dx \right)^{\frac{1}{\alpha}},$$

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

- The opposite of the first eigenvalue of the cavity:

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

which characterizes the decay rate of the heat inside D in the transient version of the conductivity equation.

A simplified, academic example (III)

This problem has a geometric optimization variant: the conductivity inside D equals

- A high value β inside a region $\Omega \subset D$;
- A low value α inside $D \setminus \overline{\Omega}$;

that is:

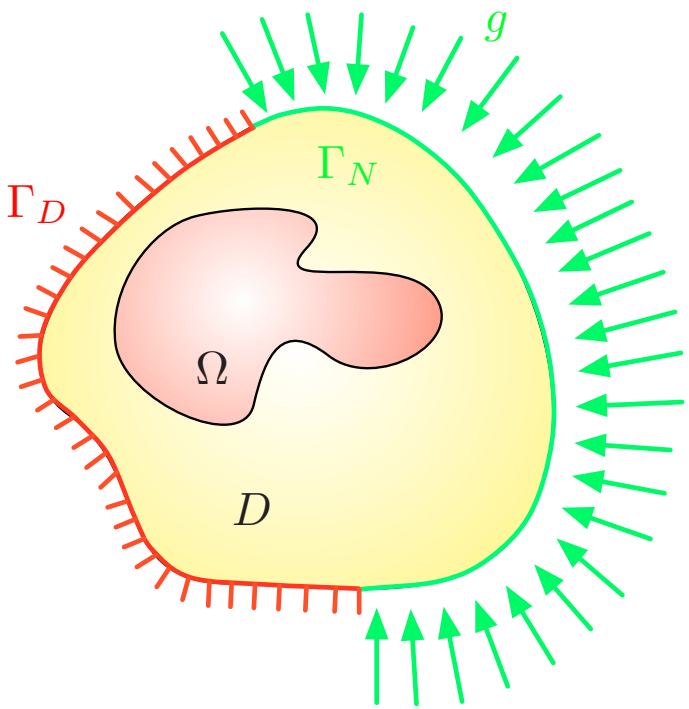
$$h_\Omega = \alpha + \chi_\Omega(\beta - \alpha),$$

where χ_Ω is the characteristic function of Ω.

The temperature $u_\Omega : D \to \mathbb{R}$ is solution to the conductivity equation:

$$\left\{ \begin{array}{rcll} -\mathrm{div}(h_\Omega \nabla u_\Omega) & = & f & \text{in } D, \\ u_\Omega & = & 0 & \text{on } \Gamma_D, \\ h_\Omega \frac{\partial u_\Omega}{\partial n} & = & g & \text{on } \Gamma_N. \end{array} \right. .$$

Geometric optimization problem: the design variable is the geometry Ω of the good conducting phase.



The two-phase conductivity setting

Shape optimization in structure mechanics (I)

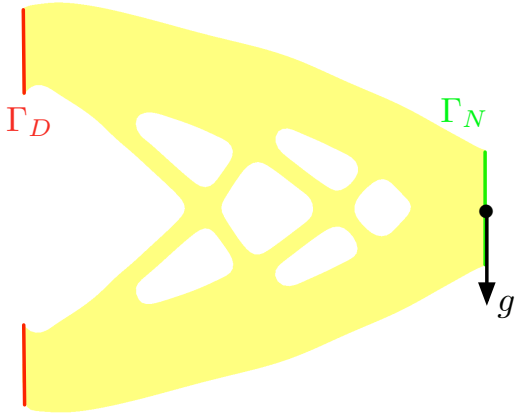
We consider a structure $\Omega \subset \mathbb{R}^d$, that is, a bounded domain which is

- 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

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 $\mathrm{Vol}(\Omega)$, or on the perimeter $\mathrm{Per}(\Omega)$ of shapes.

$$\mathrm{Vol}(\Omega) = \int_\Omega dx, \;\; \mathrm{Per}(\Omega) = \int_{\partial\Omega} ds.$$

- 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.
  - Constraints on the minimal and maximum thickness of shapes;
  - Constraints on their curvature radii;

  such constraints are often imposed by the manufacturing process.

Shape optimization in fluid mechanics (I)

An incompressible fluid with kinematic viscosity ν occupies 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 $\partial\Omega \setminus (\Gamma_{\text{in}} \cup \Gamma_{\text{out}})$.

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

$$\begin{cases} -2\nu \mathrm{div}(D(u)) + \nabla p = f & \text{in } \Omega \\ \mathrm{div}(u) = 0 & \text{in } \Omega \\ u = u_{\text{in}} & \text{on } \Gamma_{\text{in}} \\ u = 0 & \text{on } \Gamma \\ \sigma(u)n = -p_{\text{out}} & \text{on } \Gamma_{\text{out}} \end{cases},$$

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

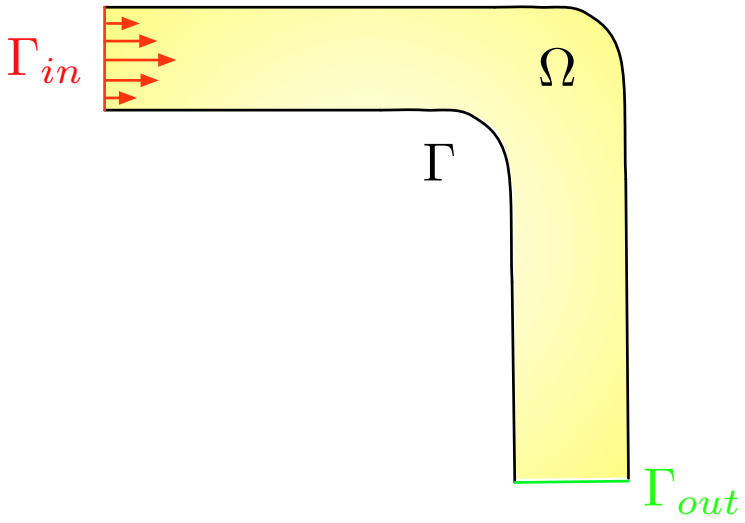
Shape optimization in fluid mechanics (II)

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:

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

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

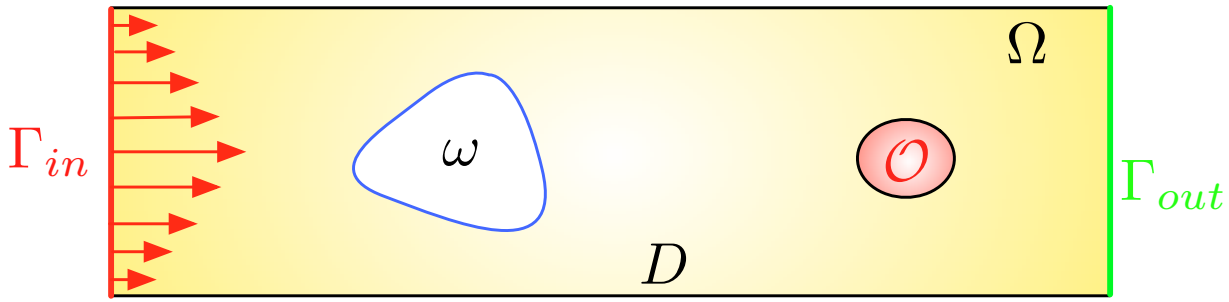


Shape optimization in fluid mechanics (III)

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 $\Omega := D \setminus \overline{\omega}$, and only the part $\partial\omega$ of $\partial\Omega$ is optimized. One then minimizes the least-square criterion:

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



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, 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 shape optimization 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 II

Generalities about shape optimization problems and examples

- What is a shape optimization problem?
- Examples of model problems
- A refresher about the finite element method

The finite element method: variational formulations (I)

- As a model problem, we consider the Laplace equation:

$$\text{Search for } u \in H_0^1(D) \text{ s.t. } \begin{cases} -\Delta u = f & \text{in } D, \\ u = 0 & \text{on } \partial D, \end{cases}$$

where $f \in L^2(D)$ is a given source.

- The associated variational formulation reads:

$$\boxed{\text{Search for } u \in V \text{ s.t. } \forall v \in V, \;\; a(u,v) = \ell(v),}$$

where

  - The Hilbert space V is the Sobolev space $H_0^1(D)$;
  - $a(\cdot,\cdot)$ is the bilinear form on V given by: $a(u,v) = \displaystyle\int_D \nabla u \cdot \nabla v \, dx$;
  - $\ell(\cdot)$ is the linear form on V defined by: $\ell(v) = \displaystyle\int_D fv \, dx$.

- The above variational problem has a unique solution $u \in V$ owing to the Lax-Milgram theorem.

The finite element method: variational formulations (II)

- The finite element method advocates to search for an approximation u_h to h inside a finite-dimensional subspace $V_h \subset V$.

- The exact variational problem is replaced by:

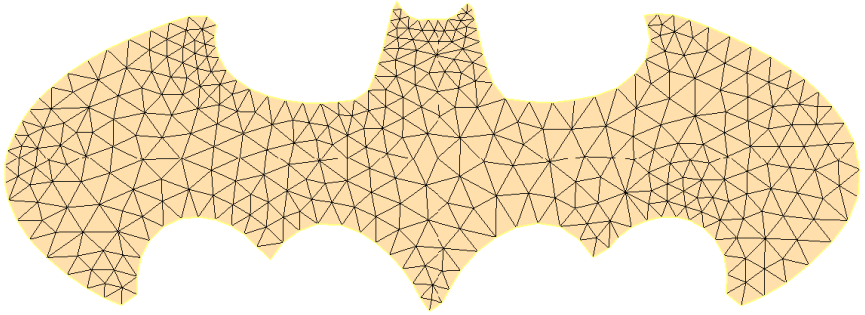
$$\boxed{\text{Search for } u_h \in V_h \text{ s.t. } \forall v_h \in V_h,\ a(u_h, v_h) = \ell(v_h),}$$

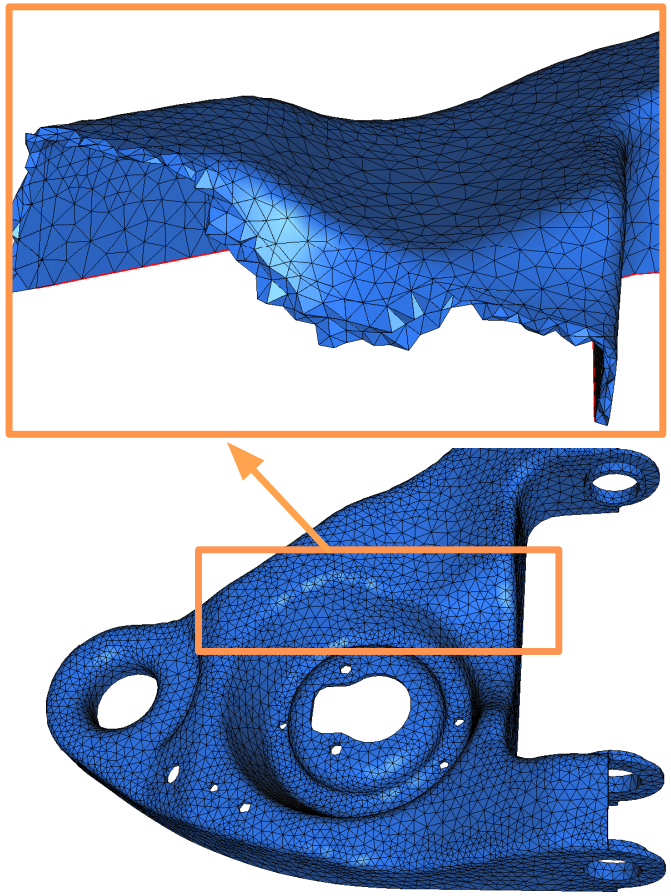
  which is also well-posed owing to the Lax-Milgram theorem.

- The subscript h refers to the sharpness of the approximation: as $h \to 0$, it is expected that $V_h \approx V$ and $u_h \approx u$.

Construction of the finite element space V_h (I)

- The domain D is discretized by means of a mesh $\mathcal{T}_h$, i.e. a covering by triangles in 2d, tetrahedra in 3d.
- The parameter h is the typical size of an element in the mesh.





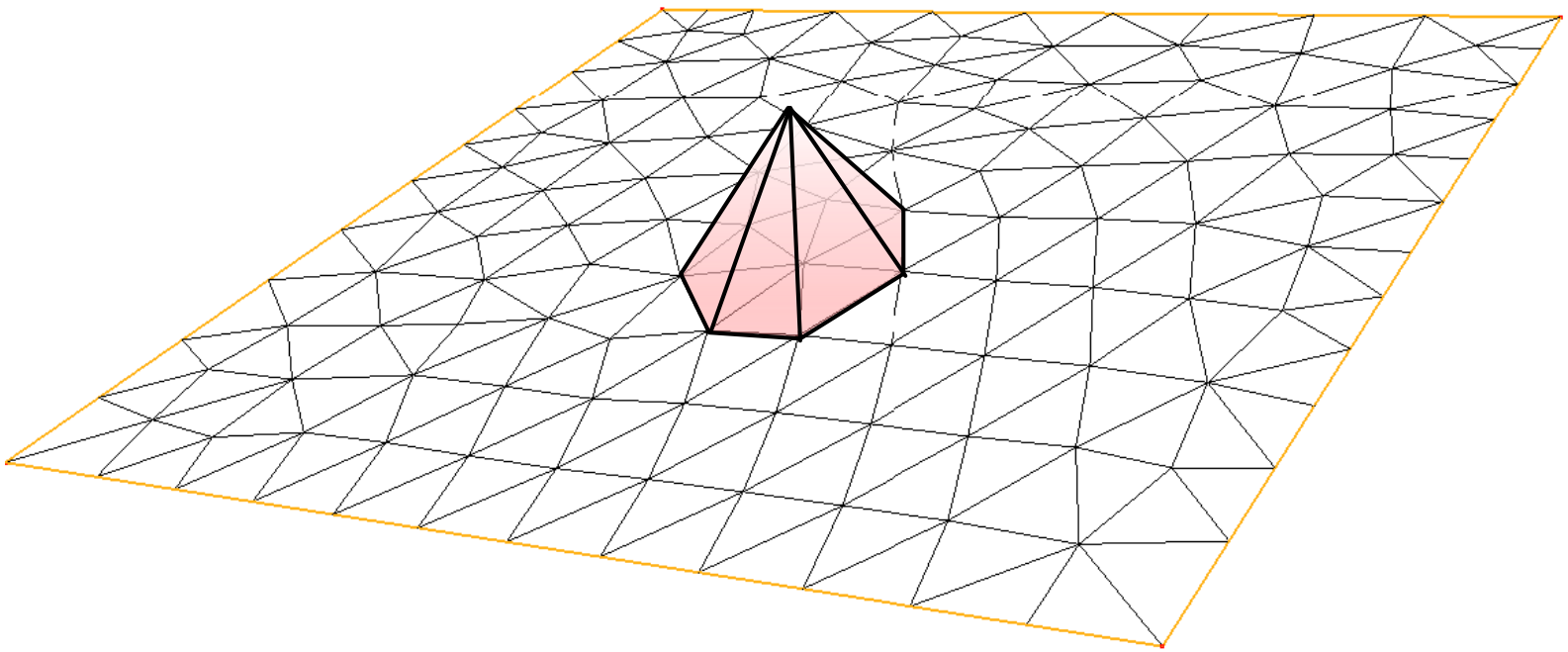
Construction of the finite element space V_h (II)

A basis $\{\varphi_1, ..., \varphi_{N_h}\}$ of finite element functions is introduced on the mesh $\mathcal{T}_h$.

Example:

- N_h is the number of vertices $a_1, ..., a_{N_h}$ of the mesh:
- For $i = 1, ..., N_h$, φ_i is affine in restriction to each triangle $T \in \mathcal{T}_h$ and

$$\varphi_i(a_i) = 1 \text{ and } \varphi_i(a_j) = 0 \text{ for } j \neq i.$$



The finite element method in a nutshell (I)

Introducing the (sought) decomposition of the (sought) function u_h on this basis:

$$u_h = \sum_{i=1}^{N_h} u_i \varphi_i,$$

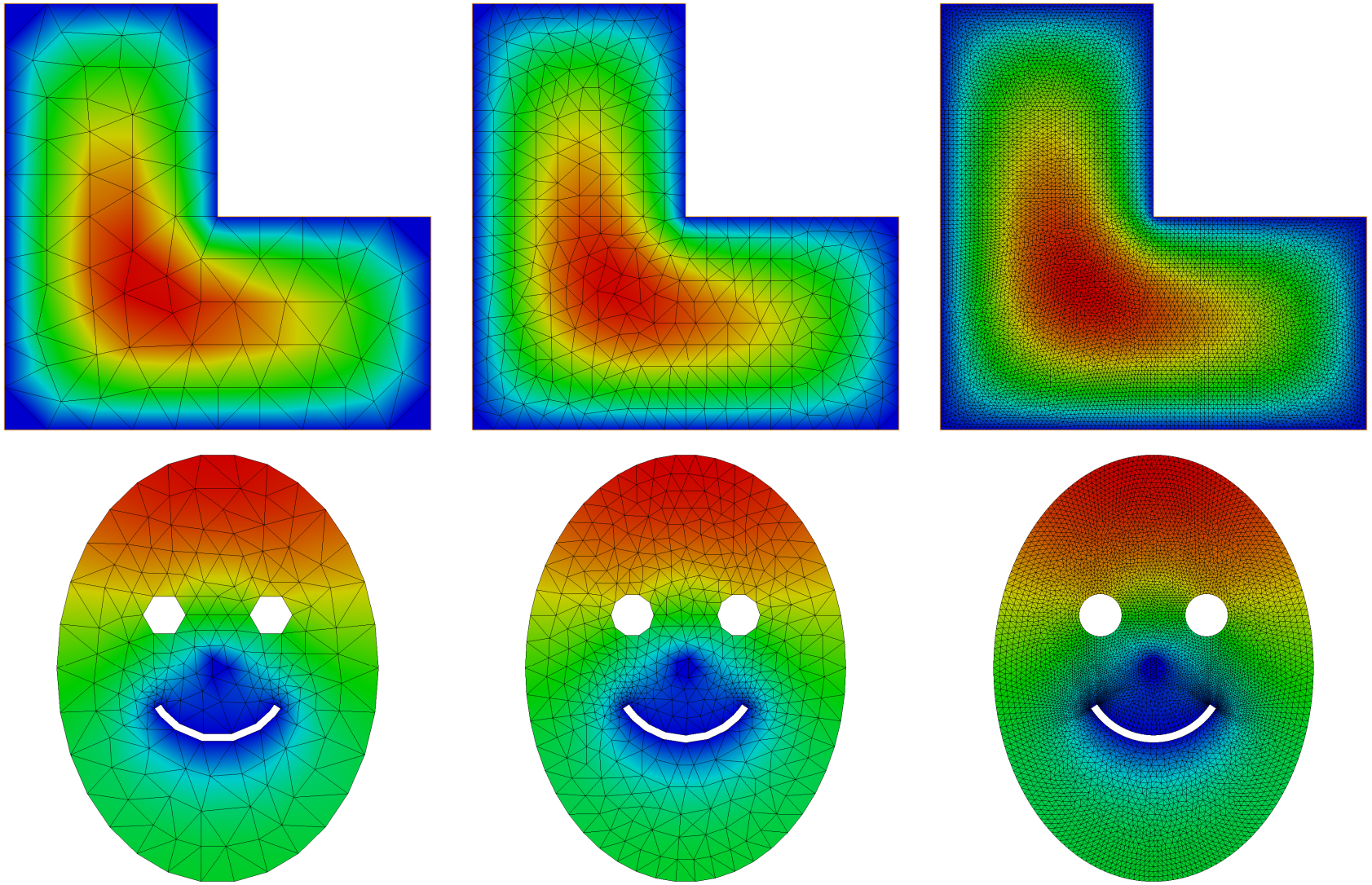
the variational problem becomes a $N_h \times N_h$ linear system:

$$KU = F,$$

where

- $U = \begin{pmatrix} u_1 \\ \vdots \\ u_{N_h} \end{pmatrix}$ is the unknown vector,
- K is the stiffness matrix, defined by its entries $K_{ij} = a(\varphi_j, \varphi_i)$,
- F is the right-hand side vector: $F_i = \ell(\varphi_i)$.

The finite element method in a nutshell (II)



Resolution of the Laplace equation with the finite element method on several domains D, using various meshes $\mathcal{T}$.

The finite element method in a nutshell (III)

- This paradigm extends (with some work!) to various frameworks:
  - Mixed variational formulations, like in the case of the Stokes equations;
  - Eigenvalue problems;
  - non linear PDE, such as the Navier-Stokes equations, or the non linear elasticity system.
- To go further, see the introductory and references monographs [All] and [ErnGue].

Part III

Parametric optimization problems

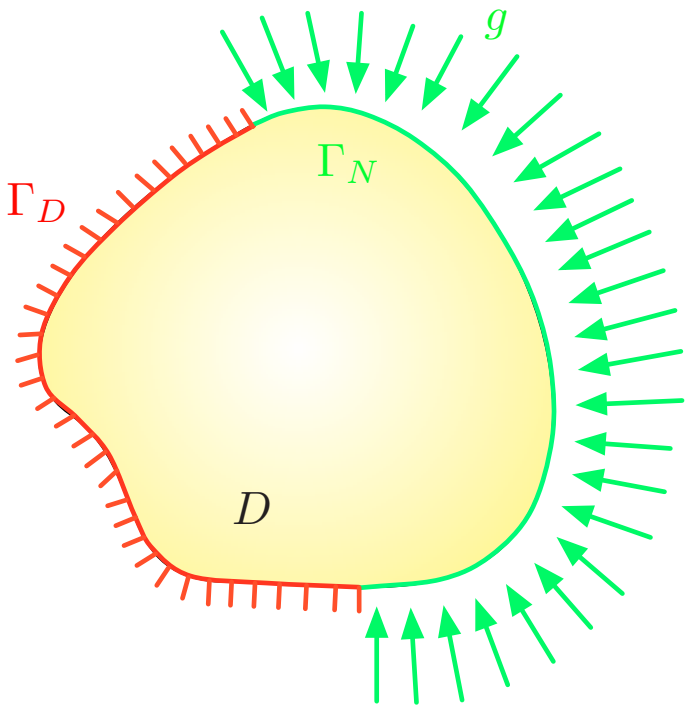
- Presentation of the model problem
- Non existence of optimal design
- Calculation of the derivative of the objective function
- The formal method of Céa
- Numerical algorithms

A model problem involving the conductivity equation (I)

- We turn back to the problem of optimizing the thermal conductivity $h : D \to \mathbb{R}$.
- The temperature u_h is the solution in $H^1(D)$ to the equation:

$$\begin{cases} -\mathrm{div}(h\nabla u_h) & = & f & \text{in } D, \\ u_h & = & 0 & \text{on } \Gamma_D, \\ h\frac{\partial u_h}{\partial n} & = & g & \text{on } \Gamma_N, \end{cases}$$

where $f \in L^2(D)$ and $g \in L^2(\Gamma_N)$.



The considered cavity

- The set $\mathcal{U}_{\mathrm{ad}}$ of design variables is:

$$\mathcal{U}_{\mathrm{ad}} = \{h \in L^\infty(D),\ \alpha \leq h(x) \leq \beta \text{ a.e. } x \in D\} \subset L^\infty(D),$$

where $0 < \alpha < \beta$ are fixed bounds.

A model problem involving the conductivity equation (II)

- Our purpose is to consider a problem of the form:

$$\min_{h \in \mathcal{U}_{\mathrm{ad}}} J(h), \text{ where } J(h) = \int_D j(u_h)\, dx,$$

and $j : \mathbb{R} \to \mathbb{R}$ is a smooth function satisfying growth conditions:

$$\forall s \in \mathbb{R}, \ |j(s)| \leq C(1 + |s|^2), \text{ and } j'(s) \leq C(1 + |s|).$$

- Many variants are possible, e.g. including constraints on h or u_h.

- In this simple setting, the state u_h is evaluated on the same domain D, regardless of the actual value of the design variable $h \in \mathcal{U}_{\mathrm{ad}}$.

- Even in this simple case, the optimization problem has no (global) solution in general...

Part III

Parametric optimization problems

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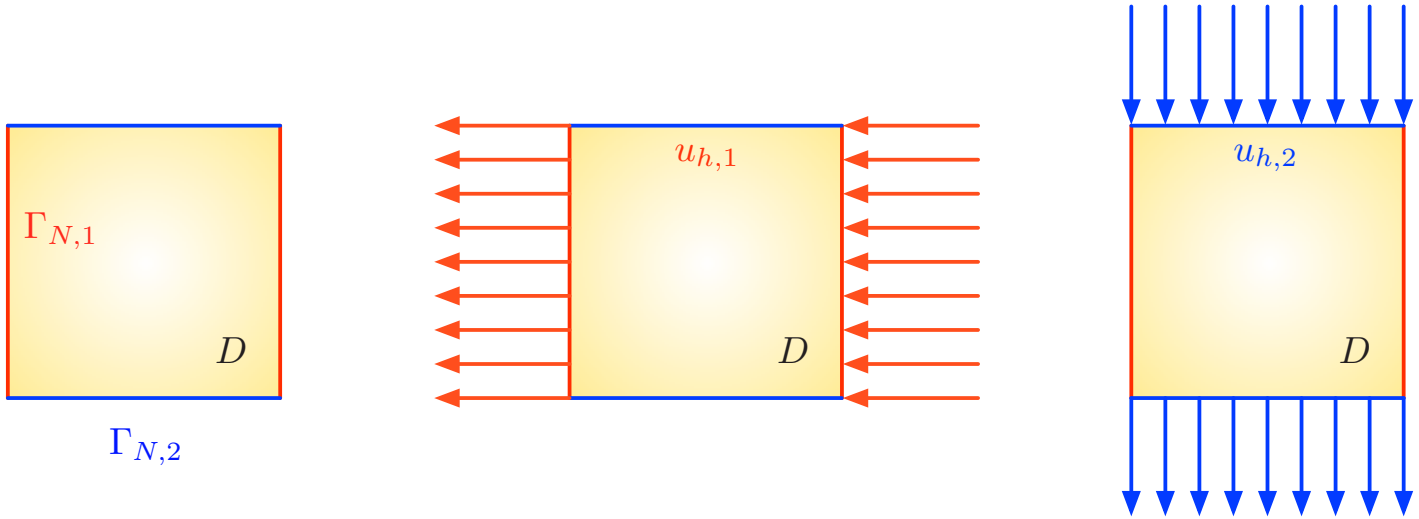
Non existence of optimal design (I)

- This counter-example is discussed in details in [All] §5.2.
- The considered cavity is the unit square $D = (0,1)^2$.
- We consider two physical situations:

$$\begin{cases} -\mathrm{div}(h\nabla u_{h,1}) = 0 & \text{in D}, \\ h\frac{\partial u_{h,1}}{\partial n} = e_1 \cdot n & \text{in } \Gamma_{N,1}, \\ h\frac{\partial u_{h,1}}{\partial n} = 0 & \text{in } \Gamma_{N,2}, \end{cases} \quad \text{and} \quad \begin{cases} -\mathrm{div}(h\nabla u_{h,2}) = 0 & \text{in D}, \\ h\frac{\partial u_{h,2}}{\partial n} = 0 & \text{in } \Gamma_{N,1}, \\ h\frac{\partial u_{h,2}}{\partial n} = e_2 \cdot n & \text{in } \Gamma_{N,2}. \end{cases}$$



(Left) Boundary conditions, (middle) boundary data for $u_{h,1}$; (right) boundary data for $u_{h,2}$.

Non existence of optimal design (II)

The optimization problem of interest is:

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

where the considered objective function is:

$$J(h) = \int_{\Gamma_{N,1}} e_1 \cdot n \, u_{h,1} \, ds - \int_{\Gamma_{N,2}} e_2 \cdot n \, u_{h,2} \, ds,$$

and the set $\mathcal{U}_{\mathrm{ad}}$ of admissible designs is augmented with a volume constraint:

$$\mathcal{U}_{\mathrm{ad}} = \left\{ h \in L^\infty(D), \quad \begin{array}{c} \alpha < h(x) < \beta \text{ a.e. } x \in D, \\ \int_D h \, dx = V_T \end{array} \right\}.$$

In other terms, one aims to

- Minimize the temperature difference between the left and right sides in Case 1.
- Maximize the temperature difference between the top and bottom sides in Case 2.

Non existence of optimal design (III)

Theorem 1.

The parametric optimization problem $\min_{h \in \mathcal{U}_{\mathrm{ad}}} J(h)$ *does not have a global solution.*

Hint of the proof: The proof unfolds in three stages:

Step 1: One calculates a lower bound m on the values of $J(h)$, $h \in \mathcal{U}_{\mathrm{ad}}$:

$$\forall h \in \mathcal{U}_{\mathrm{ad}}, \;\; J(h) \geq m.$$

Step 2: One proves that this lower bound is not attained by an element in $\mathcal{U}_{\mathrm{ad}}$:

$$\forall h \in \mathcal{U}_{\mathrm{ad}}, \;\; J(h) > m.$$

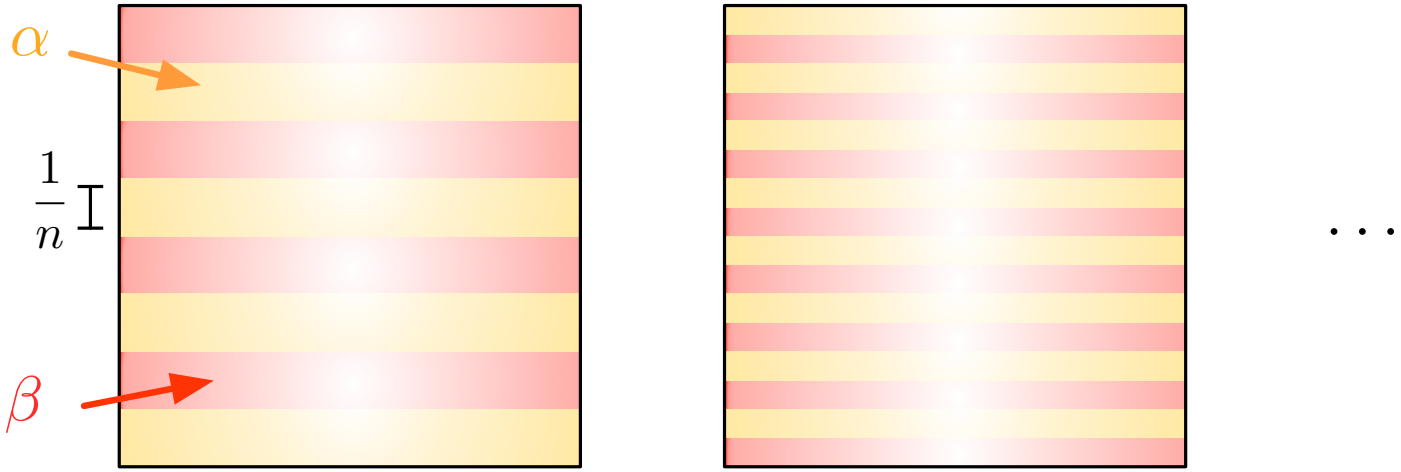
Step 3: One constructs a minimizing sequence of designs $h^n \in \mathcal{U}_{\mathrm{ad}}$:

$$J(h^n) \xrightarrow{n \to \infty} m.$$

Hence, m is the infimum of $J(h)$ over $\mathcal{U}_{\mathrm{ad}}$ but it is not attained by any $h \in \mathcal{U}_{\mathrm{ad}}$.

Non existence of optimal design (IV)

The minimizing sequence is constructed as a laminate, i.e. a succession of layers with maximum and minimum conductivities.



Two elements in the minimizing sequence h^n of conductivities.

Homogenization effect: *To get more optimal, designs tend to create very thin structures, at the microscopic level.*

Non existence of optimal design (V)

- In general, shape optimization problems, even under their simplest forms, do not have optimal solutions, for deep physical reasons.

- See [Mu] for many such examples of non existence of optimal design in optimal control problems.

- To retrieve existence of an optimal shape, two solutions are generally considered:

  - Relaxation: the set $\mathcal{U}_{\mathrm{ad}}$ of admissible designs is enlarged so that it contains 'microscopic designs': this is the essence of the Homogenization method for optimal design [All2].
  - Restriction: the set $\mathcal{U}_{\mathrm{ad}}$ is restricted to, e.g. more regular designs.

- In practice, we shall be interested in the search of local minimizers of such problems, which is e.g. 'close' to an initial design inspired by intuition.

Part III

Parametric optimization problems

- Presentation of the model problem
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Derivative of the objective function (I)

Let us return to our (still simplified) problem:

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

where

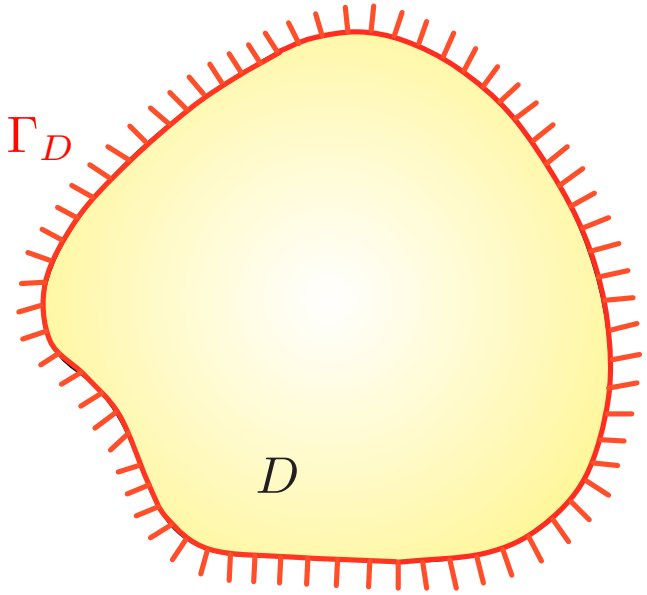
$$J(h) = \int_D j(u_h)\, dx,$$

the set of admissible designs is:

$$\mathcal{U}_{\mathrm{ad}} = \{h \in L^\infty(D),\ \alpha \leq h(x) \leq \beta \text{ a.e. } x \in D\},$$

and the temperature u_h is the solution in $H_0^1(D)$ to:

$$\begin{cases} -\mathrm{div}(h \nabla u_h) & = & f & \text{in } D, \\ u_h & = & 0 & \text{on } \partial D. \end{cases}$$



Remark For simplicity, we omit constraints on h or u_h.

Derivative of the objective function (II)

To solve this program numerically, we intend to apply a gradient-based algorithm, of the form:

Initialization: Start from an initial design h^0,

For $n = 0, \ldots$ **convergence:**

1. Calculate the derivative $J'(h^n)$ of the mapping $h \mapsto J(h)$ at $h = h^n$;
2. Select an appropriate time step $\tau^n > 0$;
3. Update the design as: $h^{n+1} = h^n - \tau^n J'(h^n)$.

The cornerstone in the practice of any such method is the calculation of the derivative of $J(h)$.

Derivative of the objective function (III)

Theorem 2.

The objective function

$$J(h) = \int_D j(u_h)\, dx$$

is Fréchet differentiable at any $h \in \mathcal{U}_{\mathrm{ad}}$*, and its derivative reads*

$$\forall \widehat{h} \in L^\infty(D),\ \ J'(h)(\widehat{h}) = \int_D (\nabla u_h \cdot \nabla p_h)\widehat{h}\, dx,$$

where the adjoint state $p_h \in H_0^1(D)$ *is the unique solution to the system:*

$$\begin{cases} -\mathrm{div}(h\nabla p_h) = -j'(u_h) & \text{in } D, \\ p_h = 0 & \text{on } \partial D. \end{cases}$$

Derivative of the objective function (IV)

Proof: The proof decomposes into two steps:

1. At first, we prove that the mapping
$$\mathcal{U}_{\mathrm{ad}} \ni h \longmapsto u_h \in H_0^1(D)$$
is Fréchet differentiable, with derivative $\widehat{h} \mapsto u_h'(\widehat{h})$.
(Here the fact that all the u_h belong to a fixed functional space is handy)

2. Then, we calculate the derivative of $J(h)$ using the chain rule, and we introduce the adjoint state p_h to eliminate $u_h'(\widehat{h})$.

Step 1: *Differentiability of $h \mapsto u_h$:*

For any $h \in \mathcal{U}_{\mathrm{ad}}$, u_h is the unique solution in $H_0^1(D)$ to the variational problem:
$$\forall v \in H_0^1(D), \quad \int_D h \nabla u_h \cdot \nabla v \, dx = \int_D f v \, dx.$$

Derivative of the objective function (V)

Let

$$\mathcal{F} : \mathcal{U}_{\mathrm{ad}} \times H_0^1(D) \to H^{-1}(D)$$

be the mapping defined by:

$$\mathcal{F}(h, u) : v \mapsto \int_D h \nabla u \cdot \nabla v \, dx - \int_D f v \, dx.$$

One verifies that

- $\mathcal{F}$ is a function of class $\mathcal{C}^1$;
- For given $h \in \mathcal{U}_{\mathrm{ad}}$, u_h is the unique solution to the equation
$$\mathcal{F}(h, u) = 0.$$
- The differential of the partial mapping $u \mapsto \mathcal{F}(h, u)$ reads:
$$H_0^1(D) \ni \widehat{u} \longmapsto \left[v \mapsto \int_D h \nabla \widehat{u} \cdot \nabla v \, dx \right] \in H^{-1}(D);$$
it is an isomorphism, owing to the Lax-Milgram theorem.

Derivative of the objective function (VI)

The implicit function theorem guarantees that the mapping $h \mapsto u_h$ is of class $\mathcal{C}^1$.

To calculate the derivative $\widehat{h} \mapsto u_h'(\widehat{h})$, we return to the variational formulation for u_h: for $v \in H_0^1(D)$,

$$\int_D h \nabla u_h \cdot \nabla v \, dx = \int_D f v \, dx.$$

Differentiating with respect to h in a direction $\widehat{h} \in H_0^1(D)$ yields:

$$\int_D \widehat{h} \nabla u_h \cdot \nabla v \, dx + \int_D h \nabla u_h'(\widehat{h}) \cdot \nabla v \, dx = 0,$$

and so

$$\boxed{\forall v \in H_0^1(D), \quad \int_D h \nabla u_h'(\widehat{h}) \cdot \nabla v \, dx = - \int_D \widehat{h} \nabla u_h \cdot \nabla v \, dx.}$$

Derivative of the objective function (VII)

Step 2: *Calculation of the derivative of $J(h)$:*

Since $h \mapsto u_h$ is of class $\mathcal{C}^1$, the chain rule yields immediately:

$$\forall \widehat{h} \in H_0^1(D), \;\; J'(h)(\widehat{h}) = \int_D j'(u_h) u_h'(\widehat{h}) \, dx.$$

- This expression is awkward: the dependence $\widehat{h} \mapsto J'(h)(\widehat{h})$ is not explicit and it is difficult to find a descent direction, i.e. a vector $\widehat{h} \in H_0^1(D)$ such that:

$$J'(h)(\widehat{h}) < 0.$$

- Fortunately, the expression of $J'(h)$ can be simplified thanks to the introduction of the adjoint state p_h.

Derivative of the objective function (VIII)

The adjoint state p_h is the unique solution in $H_0^1(D)$ to the variational problem:

$$\forall v \in H_0^1(D), \quad \int_D h\nabla p_h \cdot \nabla v \, dx = -\int_D j'(u_h) v \, dx.$$

Then, we calculate:

$$\begin{aligned} J'(h)(\widehat{h}) &= \int_D j'(u_h) u_h'(\widehat{h}) \, dx, \\ &= -\int_D h\nabla p_h \cdot \nabla u_h'(\widehat{h}) \, dx, \\ &= -\int_D h\nabla u_h'(\widehat{h}) \cdot \nabla p_h \, dx, \\ &= \int_D \widehat{h}\nabla u_h \cdot \nabla p_h \, dx. \end{aligned}$$

where the last line uses the variational formulation of $u_h'(\widehat{h})$ with p_h as test function.

Remark: From the last expression, one obviously obtains a descent direction:

$$\widehat{h} = -\nabla u_h \cdot \nabla p_h \;\Rightarrow\; J'(h)(\widehat{h}) < 0.$$

About the adjoint state

- The adjoint state p_h satisfies

$$\begin{cases} -\mathrm{div}(h\nabla p_h) = -j'(u_h) & \text{in } D, \\ p_h = 0 & \text{on } \partial D. \end{cases}$$

  It is therefore a 'virtual temperature' driven by a source (or sink) equal to the rate of change of the integrand of $J(h)$ at the state described by u_h.

- The descent direction:

$$\widehat{h} = -\nabla u_h \cdot \nabla p_h$$

  can be interpreted as the power induced by the 'virtual temperature' p_h.

- We shall see soon a second interpretation of p_h as the Lagrange multiplier associated to the PDE constraint if we formulate our optimization problem as:

$$\min_{(h,u)} \int_D j(u)\, dx, \text{ s.t. } \begin{cases} -\mathrm{div}(h\nabla u) = f & \text{in } D, \\ u = 0 & \text{on } \partial D. \end{cases}$$

Part III

Parametric optimization problems

- Presentation of the model problem
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The formal method of Céa

The method of Céa is a formal way to calculate the derivative of $J(h)$. It Assumes that the mapping $h \mapsto u_h$ is differentiable.

Let the Lagrangian

$$\mathcal{L} : \mathcal{U}_{\mathrm{ad}} \times H_0^1(D) \times H_0^1(D) \to \mathbb{R}$$

be defined by:

$$\mathcal{L}(h, u, p) = \underbrace{\int_D j(u)\, dx}_{\text{Objective function at stake}} + \underbrace{\int_D h \nabla u \cdot \nabla p \, dx - \int_D fp \, dx}_{\substack{\textbf{Enforcement of the PDE constraint } -\Delta u = f \\ \textbf{with a Lagrange multiplier } p}} .$$

In particular, for any $\widehat{p} \in H_0^1(D)$,

$$J(h) = \mathcal{L}(h, u_h, \widehat{p}).$$

For a given $h \in \mathcal{U}_{\mathrm{ad}}$, we search for the saddle points (u, p) of $\mathcal{L}(h, \cdot, \cdot)$.

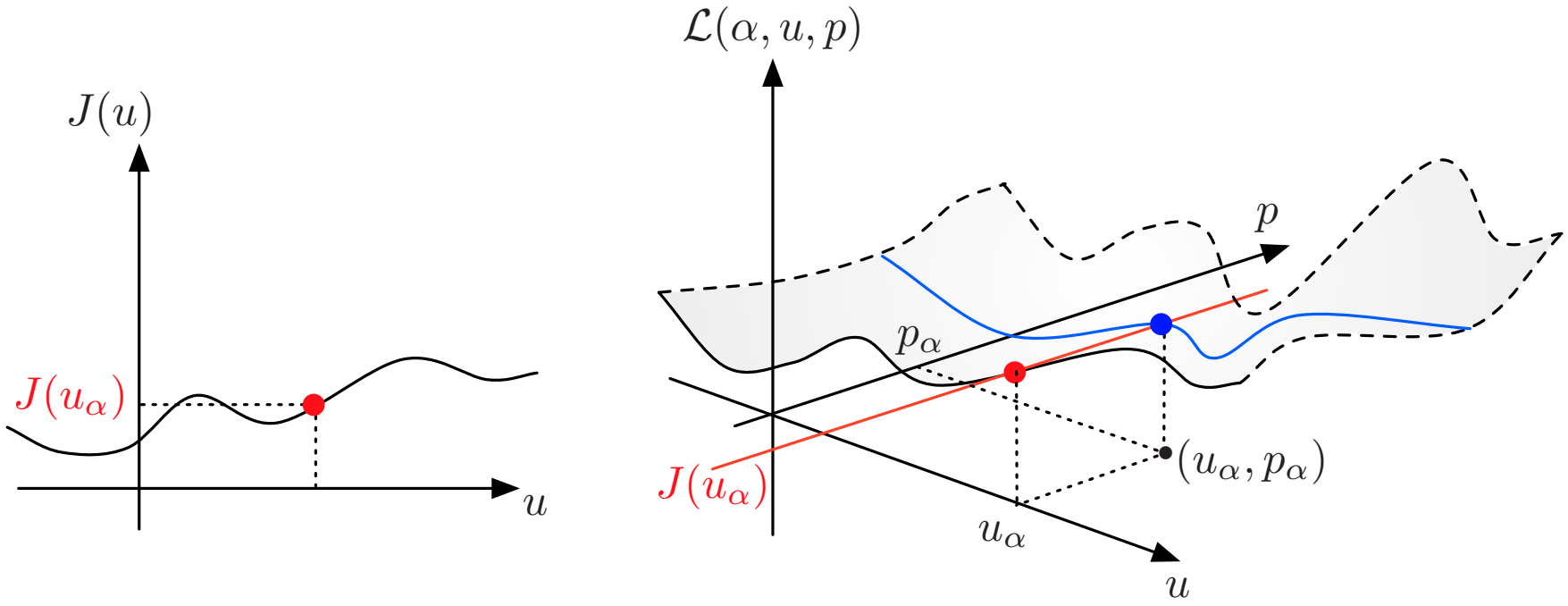
The formal method of Céa

- Imposing the partial derivative of $\mathcal{L}$ with respect to p to vanish amounts to
$$\forall \widehat{p} \in H_0^1(D), \quad \int_D h\nabla u \cdot \nabla \widehat{p}\, dx - \int_D f\widehat{p}\, dx = 0;$$
this is the variational formulation for $u = u_h$.
- Imposing the partial derivative of $\mathcal{L}$ with respect to u to vanish amounts to
$$\forall \widehat{u} \in H_0^1(D), \quad \int_D h\nabla p \cdot \nabla \widehat{u}\, dx = -\int_D j'(u)\widehat{u}\, dx;$$
since $u = u_h$, we recognize the variational formulation for $p = p_h$.

The formal method of Céa

- Recall that, for arbitrary $\widehat{p} \in H_0^1(D)$,
$$J(h) = \mathcal{L}(h, u_h, \widehat{p}).$$
- Since we have assumed that $h \mapsto u_h$ is differentiable, the chain rule yields:
$$J'(h)(\widehat{h}) = \frac{\partial \mathcal{L}}{\partial h}(h, u_h, \widehat{p})(\widehat{h}) + \frac{\partial \mathcal{L}}{\partial u}(h, u_h, \widehat{p})(u_h'(\widehat{h})).$$
- Now taking $\widehat{p} = p_h$, the last term in the above right-hand side vanishes:
$$J'(h)(\widehat{h}) = \frac{\partial \mathcal{L}}{\partial h}(h, u_h, p_h)(\widehat{h}).$$
- The above derivative is simply that of the mapping $h \mapsto \int_D h \nabla u \cdot \nabla p \, dx$ for given u, p. Hence:
$$J'(h)(\widehat{h}) = \int_D \widehat{h} \nabla u_h \cdot \nabla p_h \, dx.$$

The formal method of Céa: intuition



Physical intuition: The function $J(h)$ is 'twisted' into the value $\mathcal{L}(h, u_h, p_h)$ at the parametrized saddle point $\mathcal{L}(h, \cdot, \cdot)$, which is easy to differentiate with respect to the parameter.

Part III

Parametric optimization problems

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Numerical algorithms (I)

We solve the optimization problem:

$$\min_{h \in \mathcal{U}_{\rm ad}} J(h), \text{ where } J(h) = \int_D j(u_h)\, dx + \ell \int_D h\, dx;$$

in there:

- The set $\mathcal{U}_{\rm ad}$ reads: $\mathcal{U}_{\rm ad} = \{h \in L^\infty(D),\ \alpha < h(x) < \beta \text{ a.e. } x \in D\}$;
- A constraint on the high values of the h is added by a fixed penalization.

A basic projected gradient algorithm then reads:

Initialization: Start from an initial design h^0,

For $n = 0, \ldots$ **convergence:**

1. Calculate the state u_{h^n} and the adjoint p_{h^n} at $h = h^n$;
2. Calculate the descent direction $\widehat{h}^n = -\nabla u_{h^n} \cdot \nabla p_{h^n} - \ell$.
3. Select an appropriate time step $\tau^n > 0$;
4. Update the design as: $h^{n+1} = \min(\beta, \max(\alpha, h^n - \tau^n \widehat{h}^n))$.

Numerical algorithms (II)

In practice,

- The domain D is equipped with a fixed mesh $\mathcal{T}$, composed e.g. of triangles.
- The sought conductivity h is discretized on this mesh, e.g. as a $\mathbb{P}_0$ or $\mathbb{P}_1$ finite element function.
- For a given value of h, the solutions u_h and p_h to the state and adjoint equations are calculated by the finite element method on the mesh $\mathcal{T}$.

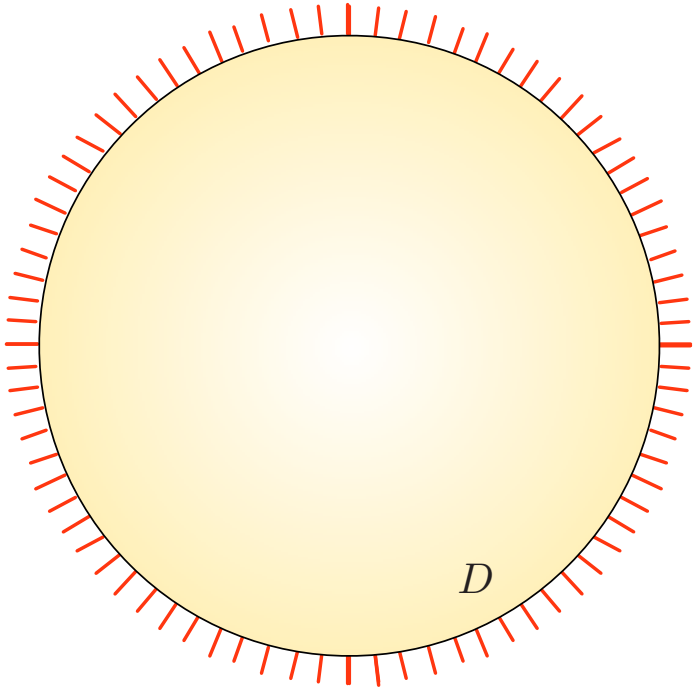
One first example: the optimal radiator (I)

We consider the problem:

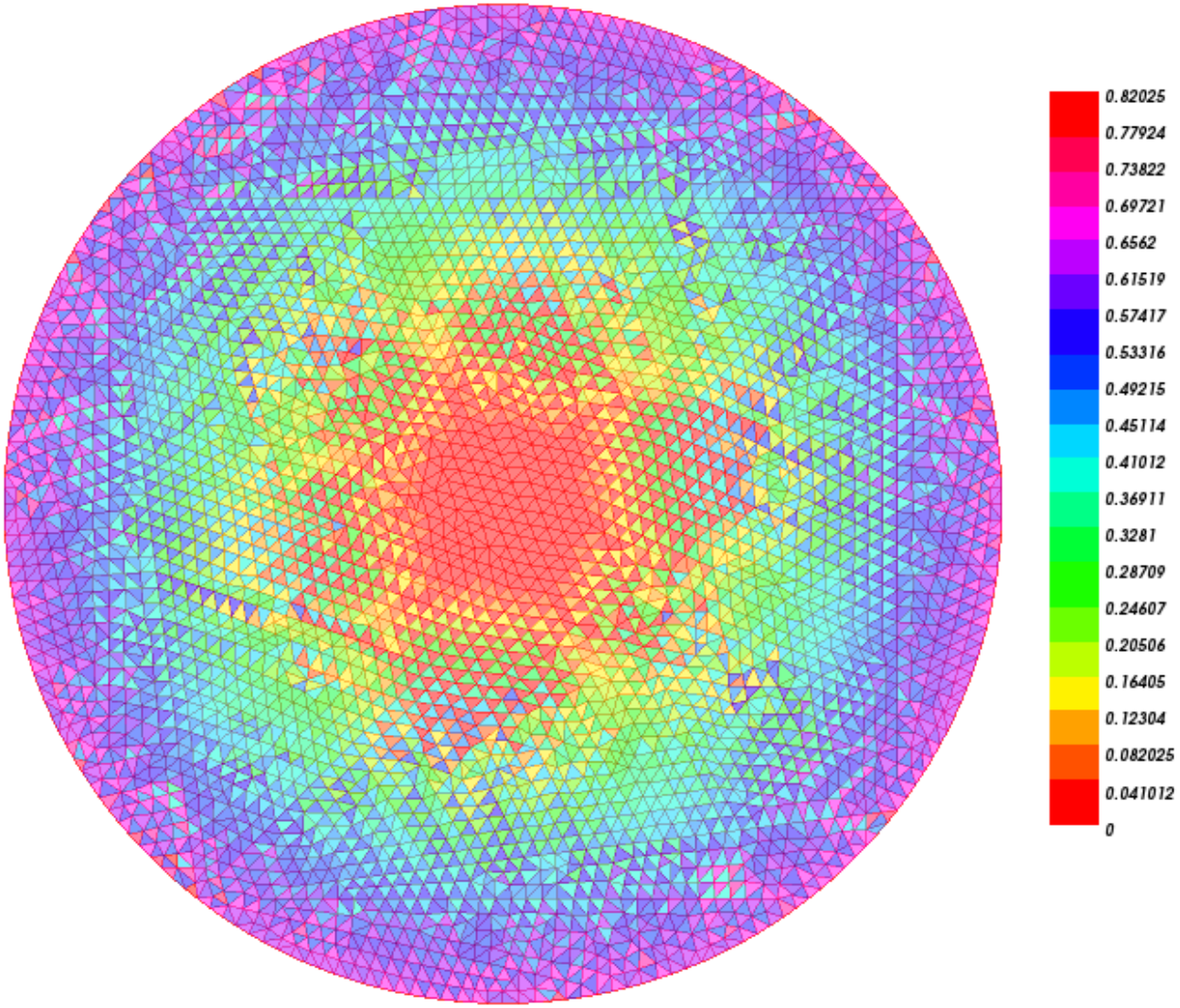
$$\min_{h \in \mathcal{U}_{\mathrm{ad}}} J(h), \text{ where } J(h) = \int_D u_h \, dx + \ell \int_D h \, dx;$$

that is,

- The mean temperature inside D is minimized;
- A constraint on the high values of the conductivity is added by a fixed penalization of the objective function.



One first example: the optimal radiator (II)



Optimized density in the thermal radiator problem.

One first example: the optimal radiator (III)

- This oscillatory behavior is actually not surprising: the algorithm tries to reproduce the 'homogenized' behavior of solutions.
- It is however highly undesirable in practice.
- One remedy consists in acting on the selected descent direction, by changing inner products, a general idea which fulfills many other purposes.
- Other solutions are presented later in the course.

Changing inner products (I)

By definition of the Fréchet derivative, the following expansion holds:

$$J(h+\tau\widehat{h}) = J(h) + \tau J'(h)(\widehat{h}) + o(\tau),$$

and a descent direction for J from h is any $\widehat{h} \in L^\infty(D)$ such that $J'(h)(\widehat{h}) < 0$.

The formula for the derivative

$$J'(h)(\widehat{h}) = \int_D \widehat{h}\nabla u_h \cdot \nabla p_h \, dx$$

makes it very natural to take as a descent direction the $L^2(D)$ gradient of $J'(h)$:

$$\widehat{h} = -\nabla u_h \cdot \nabla p_h,$$

i.e. the gradient associated to the differential $J'(h)$ via the $L^2(D)$ dual pairing.

Other, more adapted choices of a descent direction are possible, as gradients of $J'(h)$ obtained with other inner products than that of $L^2(D)$.

Changing inner products (II)

Let $\mathcal{H}$ be a Hilbert space with inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$.

Solve the following identification problem: Search for $V \in \mathcal{H}$ such that:

$$\forall w \in \mathcal{H}, \ \langle V, w \rangle_{\mathcal{H}} = J'(h)(w) = \int_D w \nabla u_h \cdot \nabla p_h \, dx.$$

Then $-V$ is also a descent direction for $J(h)$, since for $\tau > 0$ small enough:

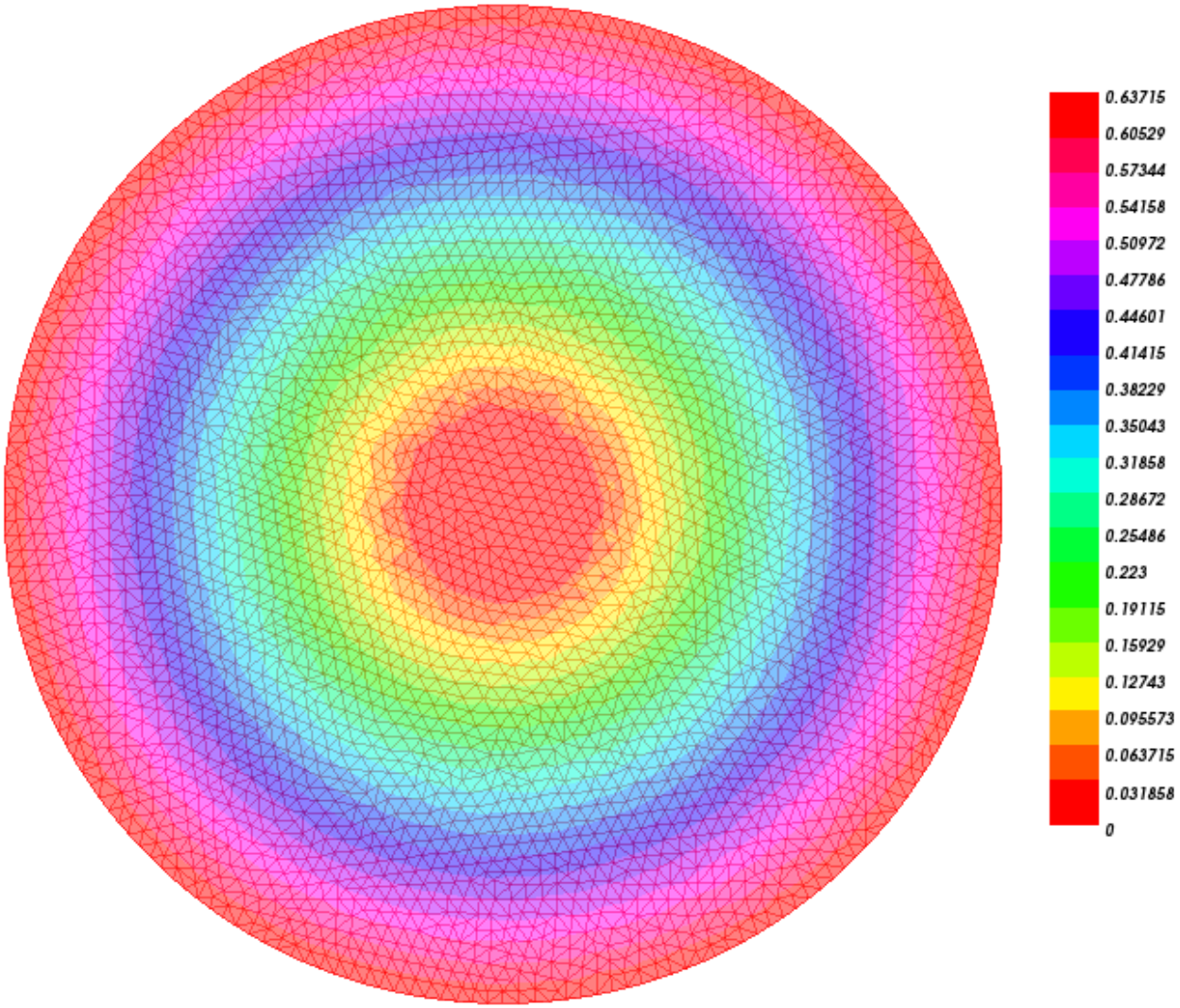
$$\begin{array}{rcl} J(h - \tau V) & = & J(h) - \tau J'(h)(V) + o(\tau) \\ & = & J(h) - \langle V, V \rangle_{\mathcal{H}} + o(\tau) \\ & < & J(h). \end{array}$$

Example: A descent direction which is more regular than that supplied by the $L^2(D)$ inner product is obtained with the choice:

$$\mathcal{H} = H^1(D), \text{ and } \langle u, v \rangle_{\mathcal{H}} = \int_D (\alpha^2 \nabla u \cdot \nabla v + uv) \, dx,$$

for α 'small' (of the order of the mesh size).

The optimal radiator again



Optimized density for the thermal radiator problem using the 'change of inner product' trick.

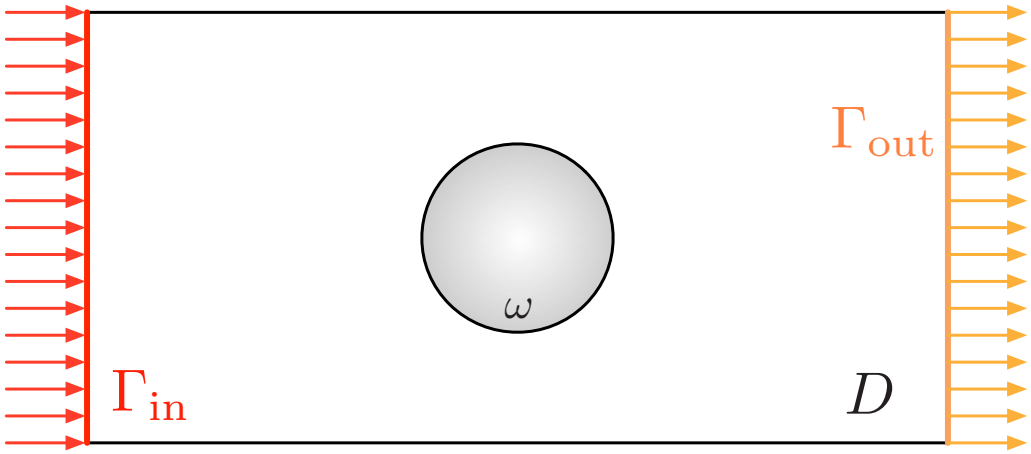
Another example: design of a 'heat lens' (I)

As proposed in [Che], the problem

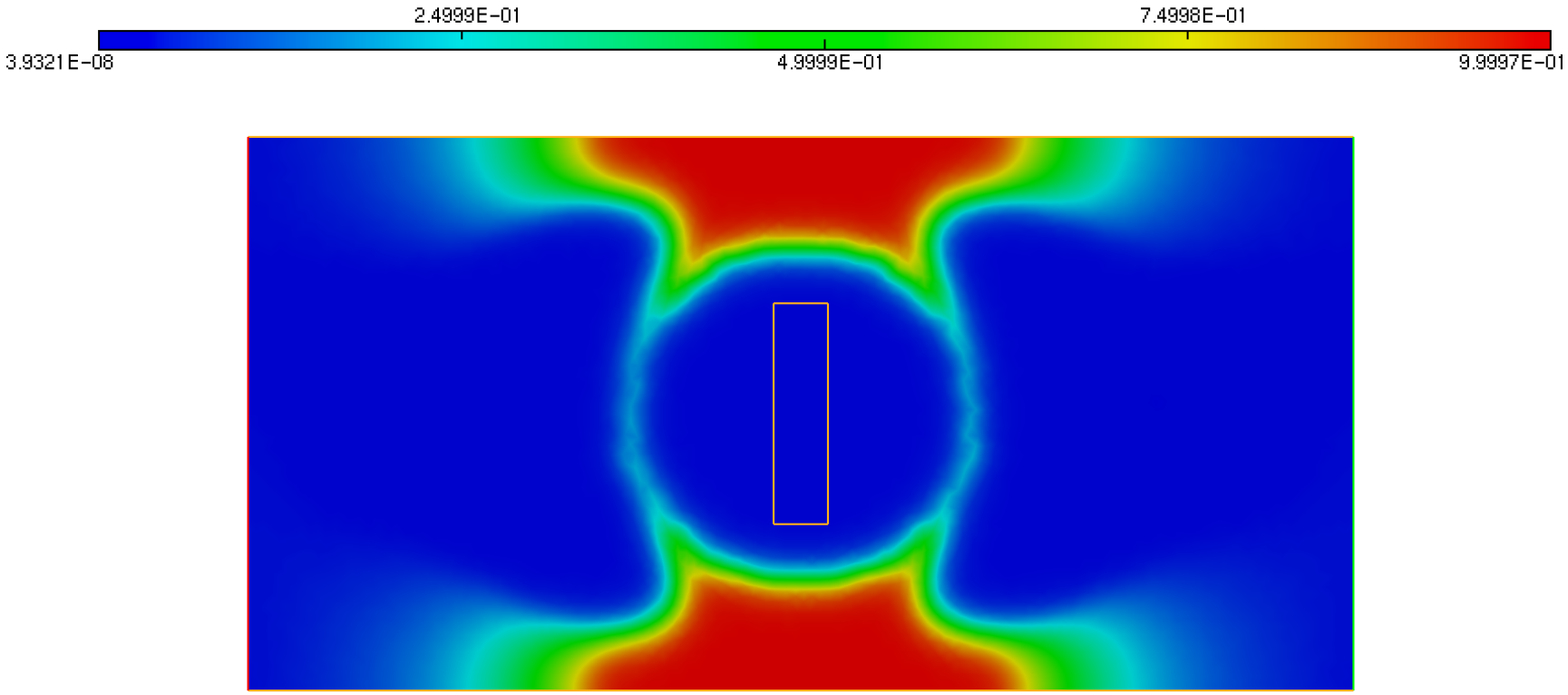
$$\min J(h) \text{ where } J(h) = \int_\omega \left| \alpha \frac{\partial u_h}{\partial x_1} \right|^2 dx + \ell \int_D h \, dx$$

is considered:

- The horizontal heat flux through a non optimizable region ω is minimized;
- A penalization on the high values of the conductivity h is added.



Another example: design of a 'heat lens' (II)



Optimized heat lens under a penalization of high values of the conductivity.

Remarks

- The above strategy to impose a constraint on the amount of high conductivity material is very crude. Other constrained optimization algorithms may be used, such as the Augmented Lagrangian algorithm.

- This parametric optimization framework lends itself to the use of:
  - Quasi-Newton methods, such as the Gauss-Newton or the BFGS algorithms;
  - 'True' second-order algorithms, based on the Hessian of the mapping $h \mapsto J(h)$.

- Density-based methods for topology optimization problems often rely on an adaptation of this parametric framework.

Part IV

Geometric optimization problems

- The method of Hadamard and shape derivatives
- Shape derivatives of PDE-constrained functionals
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- Céa's method for calculating shape derivatives
- Numerical aspects of geometric methods
- The level set method for shape optimization

Geometric shape optimization

We are now able to optimize shapes provided they are parametrized, be it:

- Via a set of parameters in a finite-dimensional space (thickness, etc.)
- By a function h in an adapted vector (Banach) space $h \mapsto J(h)$.

Asset: This is a very appealing setting, when available (methods from mathematical programming are readily available).

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 of shapes.
- Observe that we have only considered the (simpler) case where the state u_h lives in a fixed computational domain.

$\Rightarrow$ One needs to consider shape optimization problems in term of the geometry of shapes Ω:

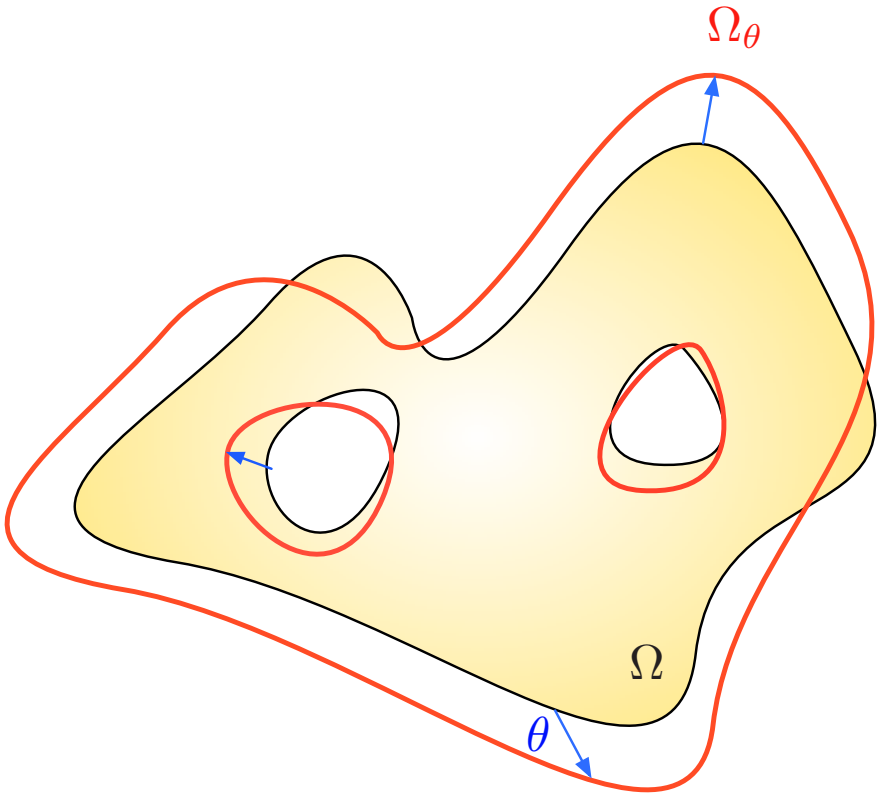
$$\min J(\Omega) \text{ s.t. } C(\Omega) \leq 0.$$

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

Hadamard's boundary variation method describes variations of a reference, 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 3.

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.

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

Definition 1.

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

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

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

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

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

First examples of shape derivatives (I)

Theorem 4.

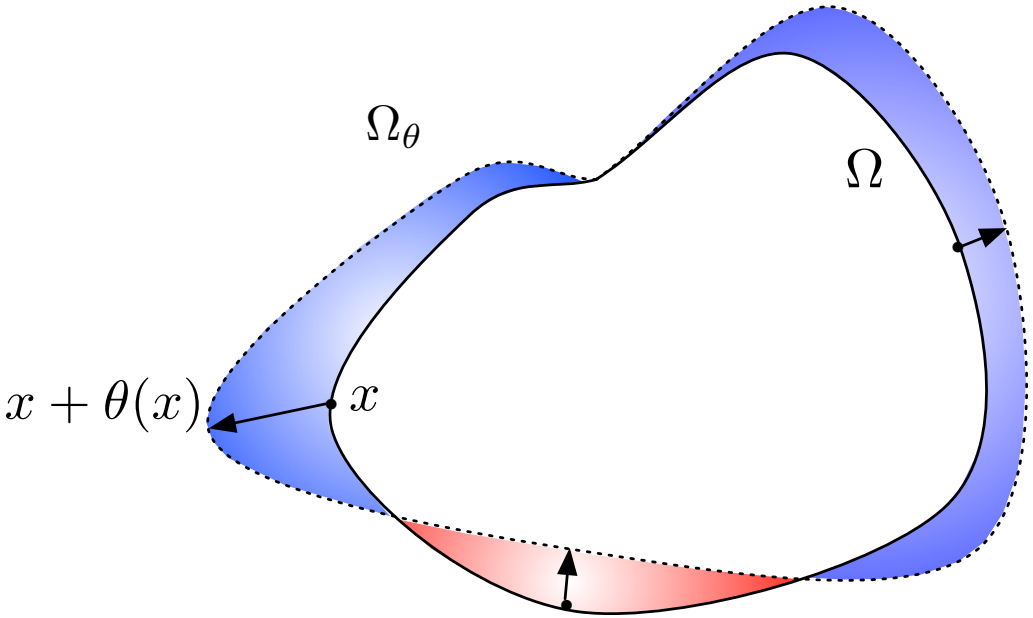
Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain, and let $f \in W^{1,1}(\mathbb{R}^d)$ be a fixed function. Consider the functional:

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

then J 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 (II)



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 (III)

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.

- It allows to calculate the shape derivative of the volume functional

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

Indeed, one has:

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

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; see Theorem 12:

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

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

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

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

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

- 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 map everything on the reference domain Ω,
2. Differentiating with respect to the deformation θ,

is the 'standard' way to calculate shape derivatives.

First examples of shape derivatives (V)

Theorem 5.

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:

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

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

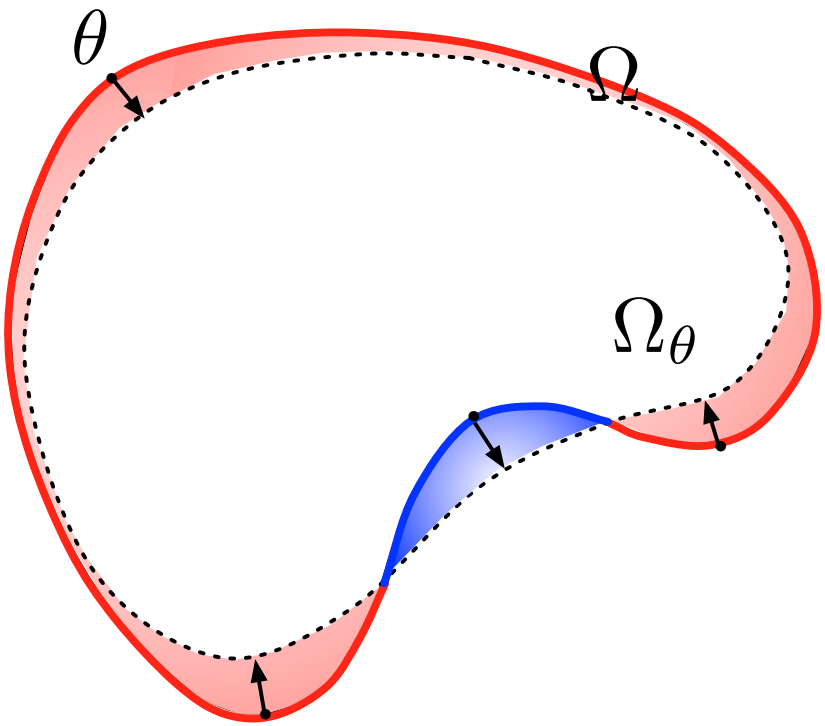
$$J'(\Omega)(\theta) = \int_{\partial\Omega} \left(\frac{\partial g}{\partial n} + \kappa g \right) (\theta \cdot n)\, ds,$$

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

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

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

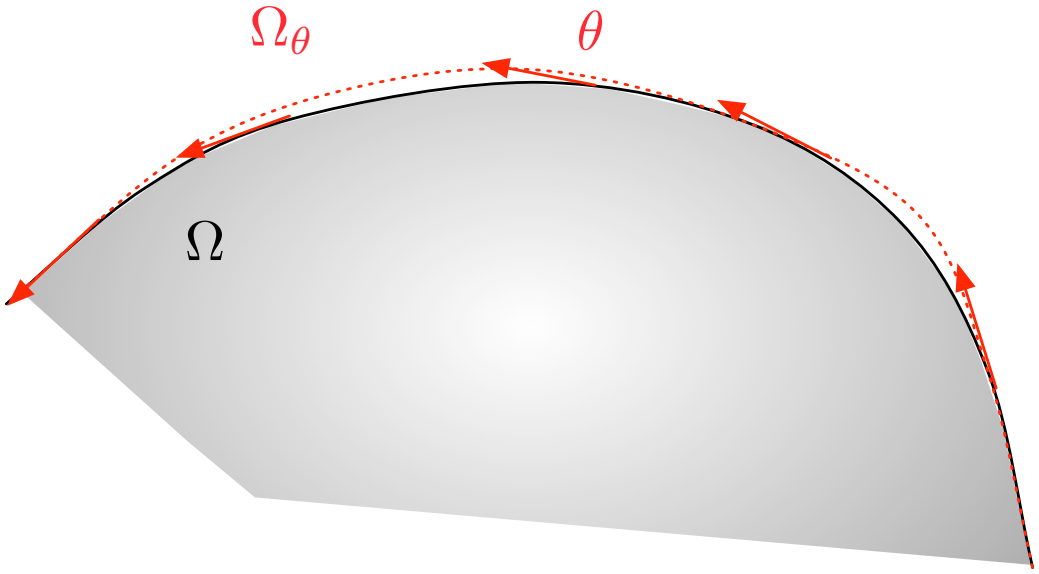
First examples of shape derivatives (VI)



Physical intuition: $\theta = -\kappa n$ *is a descent direction for the perimeter* $P(\Omega)$*: the perimeter 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 $J(\Omega)$ 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 $J'(\Omega)(\theta) = 0$.

Structure of shape derivatives (II)

Lemma 6.

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 7.

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 $t > 0$ in the definition of shape derivatives yields:

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

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Shape derivatives of PDE constrained functionals

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

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

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

- We now intend to consider functions of the form

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

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 borrows techniques from optimal control theory.

The considered framework

- Henceforth, we rely on the simplified 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:

$$\forall v \in H_0^1(\Omega)/H^1(\Omega), \quad \int_\Omega \nabla u \cdot \nabla v\, dx - \int_\Omega fv\, dx = 0.$$

- 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.

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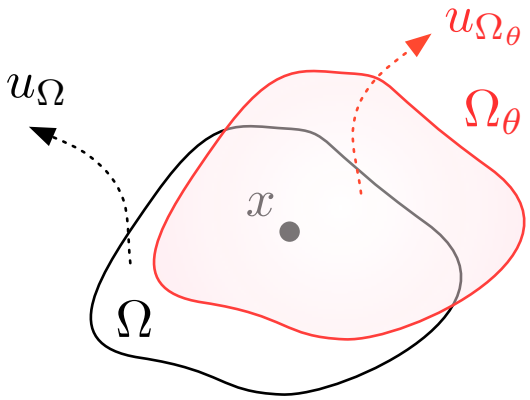
Eulerian and Lagrangian derivatives (I)

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

The Eulerian point of view:

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

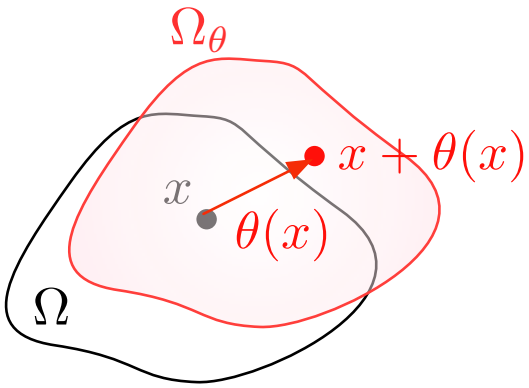
$$\theta \mapsto u_{\Omega_\theta}(x).$$



The Lagrangian point of view:

For a fixed $x \in \Omega$, $\mathring{u}_\Omega(\theta)(x)$ 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 satsified 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 Eulerian derivative $u'_\Omega(\theta)$ is defined from the Lagrangian derivative $\mathring{u}_\Omega(\theta)$,

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

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

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

Eulerian and Lagrangian derivatives (III)

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 $\mathring{u}_\Omega(\theta)$ at a given domain Ω provided the transported function

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

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

Eulerian and Lagrangian derivatives (IV)

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

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

Proposition 8.

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

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

is then shape differentiable at Ω, and:

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

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

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

Eulerian and Lagrangian derivatives (VI)

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

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

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

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

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

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

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

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

Then using the definition $u'_\Omega(\theta) = \mathring{u}_\Omega(\theta) - \nabla u_\Omega \cdot \theta$, with the Green formula:

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

$\square$

Eulerian and Lagrangian derivatives (VII)

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

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

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

Theorem 9.

Let $\Omega \subset \mathbb{R}^d$ be a smooth bounded domain. The mapping $\Omega \mapsto u_\Omega \in H_0^1(\Omega)$ has a Lagrangian derivative $\mathring{u}_\Omega(\theta)$, and for any $\theta \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$, $\mathring{u}_\Omega(\theta) \in H_0^1(\Omega)$ is the unique solution Y in $H_0^1(\Omega)$ to:

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

Eulerian and Lagrangian derivatives (VIII)

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

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

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

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

where

$$A(\theta) := |\det(\mathrm{I} + \nabla\theta)| (\mathrm{I} + \nabla\theta)^{-1} (\mathrm{I} + \nabla\theta)^{-T} \text{ and } \overline{f} = f \circ (\mathrm{Id} + \theta).$$

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

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:

  - $\mathcal{F} : W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d) \times H_0^1(\Omega) \to H^{-1}(\Omega)$,
  - $\mathcal{G} : W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d) \to H^{-1}(\Omega)$.

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

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

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

$\square$

Eulerian and Lagrangian derivatives (X)

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

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

Notice that, in particular:

$$\forall v \in H_0^1(\Omega), \quad \int_\Omega \nabla u'_\Omega(\theta) \cdot \nabla v \, dx = 0.$$

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 (XI): 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 $p_\Omega \in H_0^1(\Omega)$ be defined as the solution to the problem:

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

- Multiplying this equation by an arbitrary function $v \in H^1(\Omega)$, integrating over Ω and using Green's formula yields:

$$\int_\Omega \nabla p_\Omega \cdot \nabla v \, dx - \int_{\partial\Omega} \frac{\partial p_\Omega}{\partial n} v \, ds = -\int_\Omega j'(u_\Omega) \, v \, dx,$$

- ... to be compared with:

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

Thus,

$$\begin{aligned} J'(\Omega)(\theta) &= \int_{\partial\Omega} j(u_\Omega)\,\theta\cdot n\,ds + \int_\Omega j'(u_\Omega)u'_\Omega(\theta)\,dx \\ &= \int_{\partial\Omega} j(u_\Omega)\,\theta\cdot n\,ds - \int_\Omega \nabla p_\Omega\cdot\nabla u'_\Omega(\theta)\,dx + \int_{\partial\Omega}\frac{\partial p_\Omega}{\partial n}u'_\Omega(\theta)\,ds\,, \\ &= \int_{\partial\Omega} j(u_\Omega)\,\theta\cdot n\,ds - \int_{\partial\Omega}\frac{\partial p_\Omega}{\partial n}\frac{\partial u_\Omega}{\partial n}\theta\cdot n\,ds \end{aligned}$$

where we used the variational characteristics of u'_Ω:

$$\forall v\in H^1_0(\Omega),\ \int_\Omega \nabla u'_\Omega(\theta)\cdot\nabla v\,dx = 0,\ \text{and}\ u'_\Omega(\theta) = -\frac{\partial u_\Omega}{\partial n}\,\theta\cdot n\ \text{on}\ \partial\Omega.$$

Eventually, we obtain:

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

Eulerian and Lagrangian derivatives: summary

- Mathematically speaking, it is the rigorous way to assess the differentiability of shape functionals.
- 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 will allow for a formal, much simpler way to calculate shape derivatives.

Part IV

Geometric optimization problems

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

Céa's method

As we have seen, 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)

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:

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

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.

Céa's method: the Neumann case (II)

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

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

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

- $\forall q \in H^1(\mathbb{R}^d),\ \ \dfrac{\partial \mathcal{L}}{\partial q}(\Omega, u, p)(q) =$

$$\int_\Omega \nabla u \cdot \nabla q\, dx + \int_\Omega uq\, dx - \int_\Omega fq\, dx = 0.$$

- $\forall v \in H^1(\mathbb{R}^d),\ \ \dfrac{\partial \mathcal{L}}{\partial v}(\Omega, u, p)(v) =$

$$\int_\Omega j'(u) \cdot v\, dx + \int_\Omega \nabla v \cdot \nabla p\, dx + \int_\Omega vp\, dx = 0.$$

Céa's method: the Neumann case (III)

Step 1: *Identification of u:*

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

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

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

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

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

Conclusion: $u = u_\Omega$.

Céa's method: the Neumann case (IV)

Step 2: *Identification of p:*

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

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

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

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

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

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

Céa's method: the Neumann case (V)

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

- We go back to the fact that:

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

- 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 4, we end up with:

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

Céa's method: the Dirichlet case (I)

- We now consider the problem of derivating:

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

- **Warning:** When the state u_Ω satisfies essential boundary conditions, i.e. boundary conditions that are tied to the definition space of functions (here, $H_0^1(\Omega)$), 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 $v, q \in H_0^1(\Omega)$.

- 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 $v, q, \mu \in H^1(\mathbb{R}^d)$;

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

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:*

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

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

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

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

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

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:

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

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

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

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

Step 2 (continued):

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

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

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

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

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

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 4 (and after some calculation), we end up with:

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

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The generic numerical algorithm

Initialization: Start from an initial shape Ω^0.

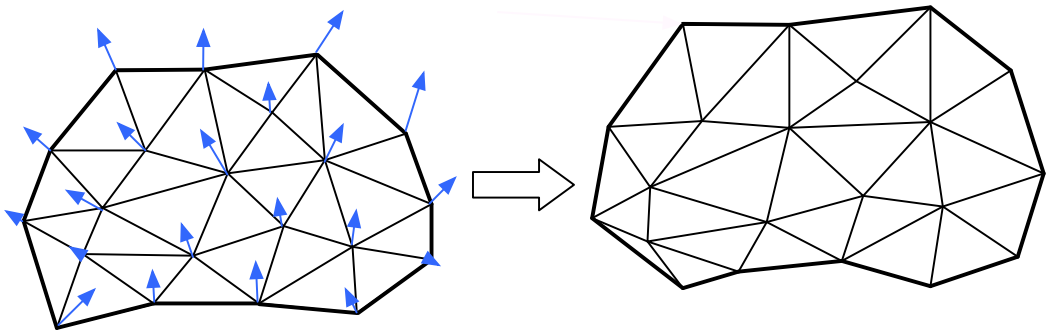
For $n = 0, \ldots$ **convergence,**

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 thence calculated by using the theoretical formula for the shape derivative $J'(\Omega)$.
- 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 $\mathcal{T}^{n+1}$.



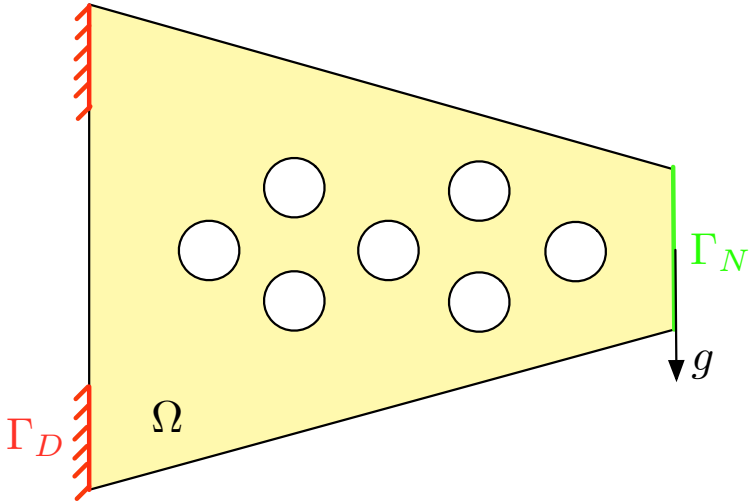
Deformation of a mesh by relocating its nodes to a prescribed final position.

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.

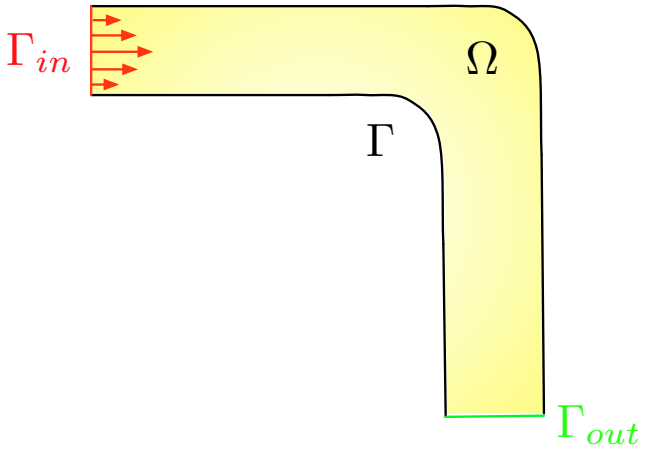


Numerical examples (II)

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

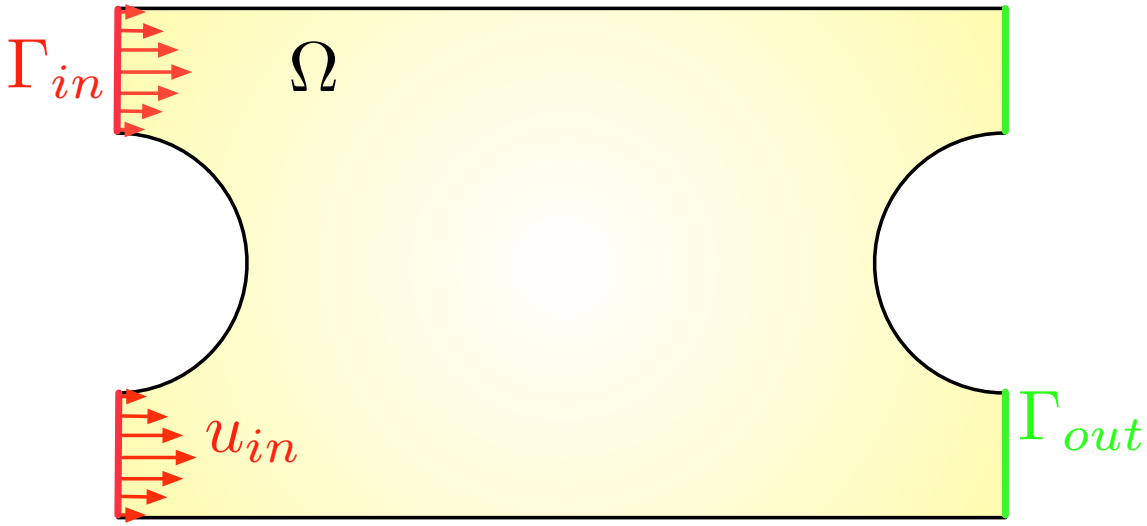
$$D(\Omega) = 2\nu \int_\Omega D(u_\Omega) : D(u_\Omega)\, dx.$$

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



Numerical examples (III)

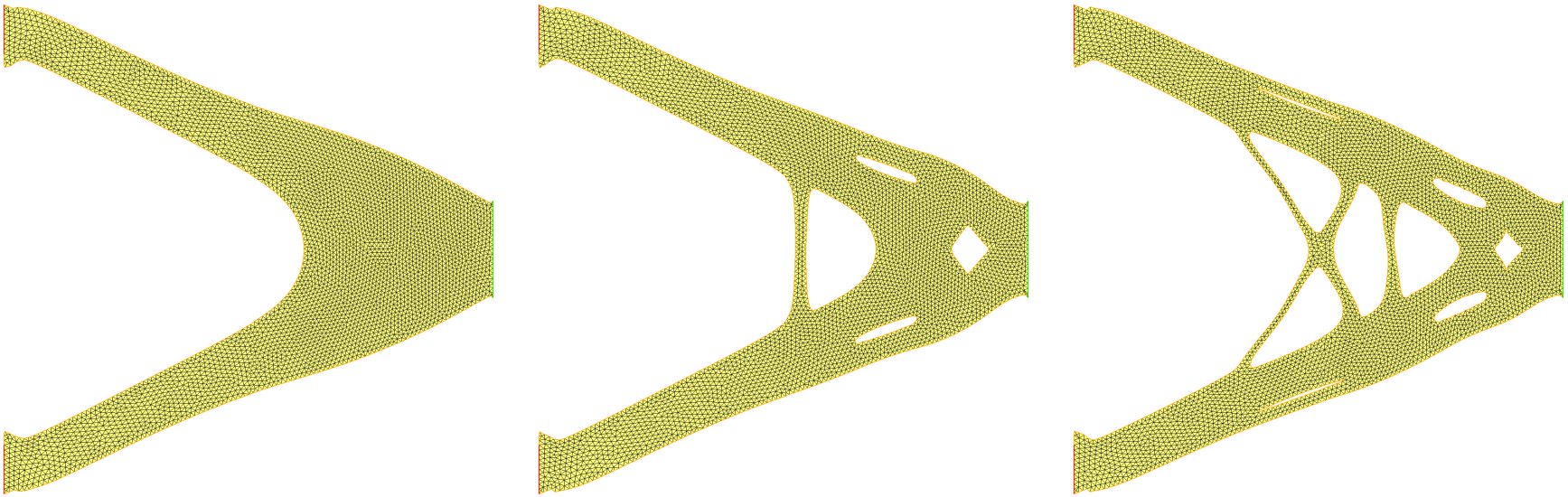
- Still in fluid mechanics, the viscous dissipation $D(\Omega)$ of a double pipe system is minimized.
- A volume constraint is imposed.



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.

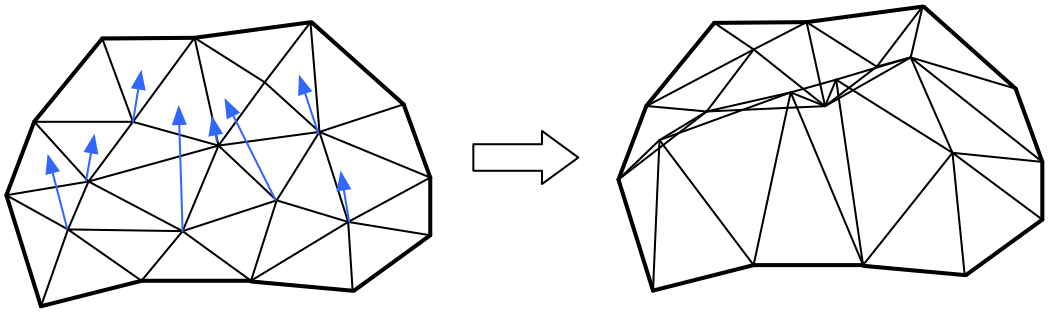


Several optimized cantilever beams associated to different initial designs.

Numerical issues and difficulties (II)

II - 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)

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.

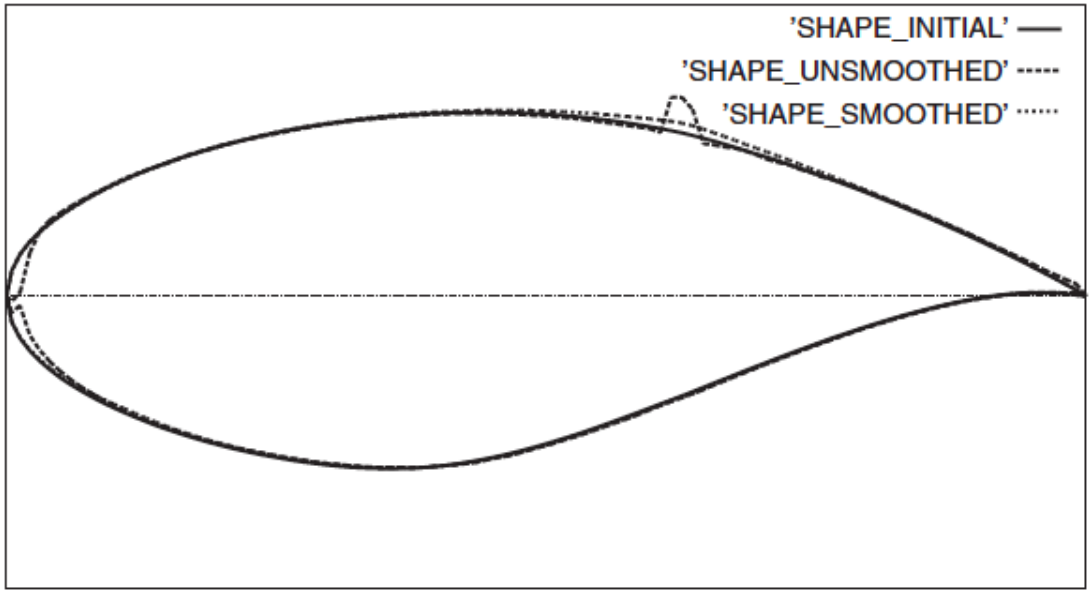
  (for instance, deforming a mesh of Ω using a 'nice' vector field θ defined on the whole Ω may considerably ease the process)

- 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 (III)

IV - 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).

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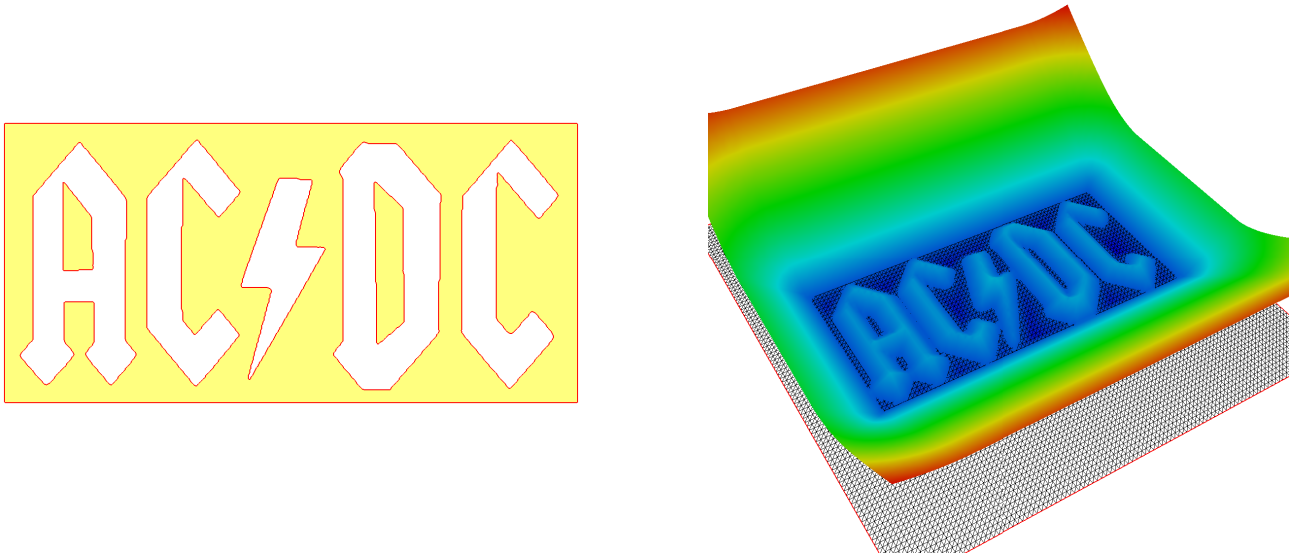
- The level set method for shape optimization

The level set method

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

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

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



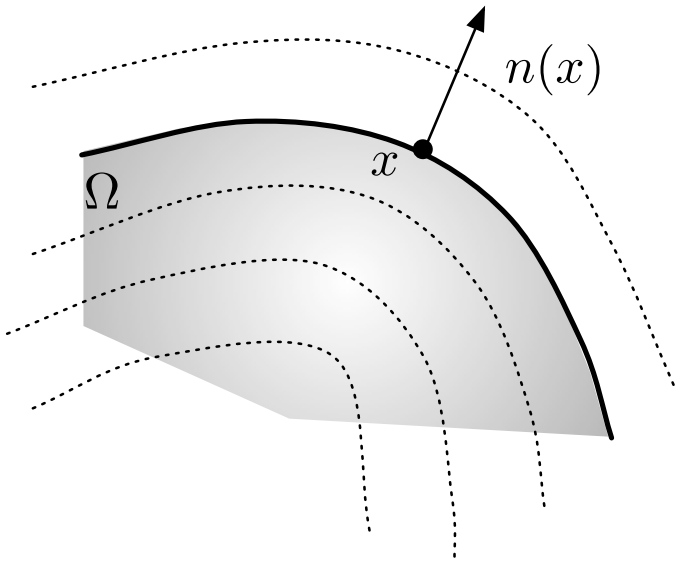
A domain $\Omega \subset \mathbb{R}^2$ (left), some level sets of an associated level set function (right).

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.

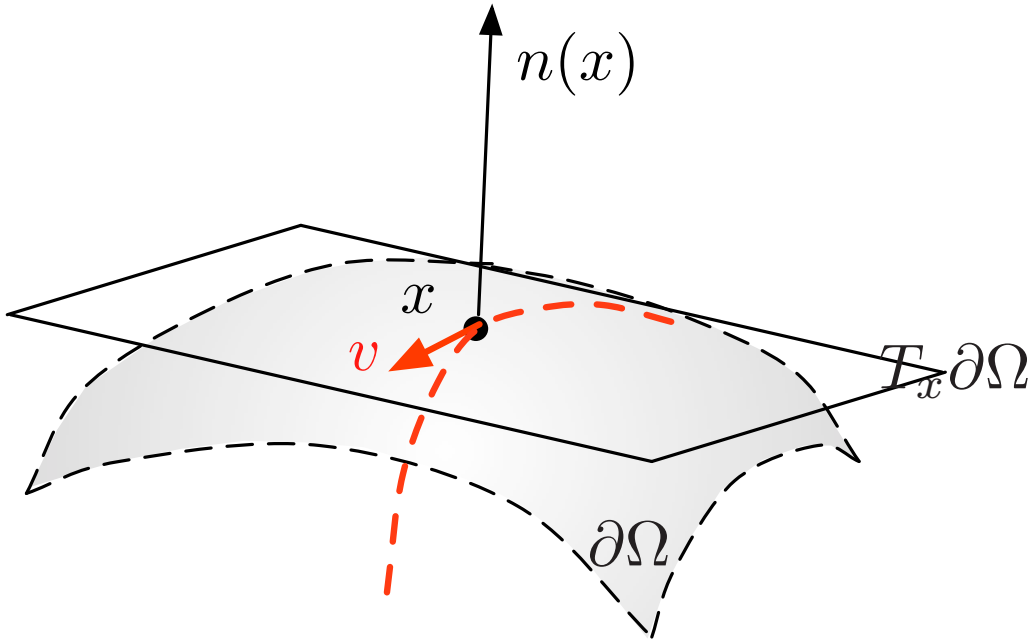
Level set functions and geometry (II)

- 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.

Evolution of domains with the level set method

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

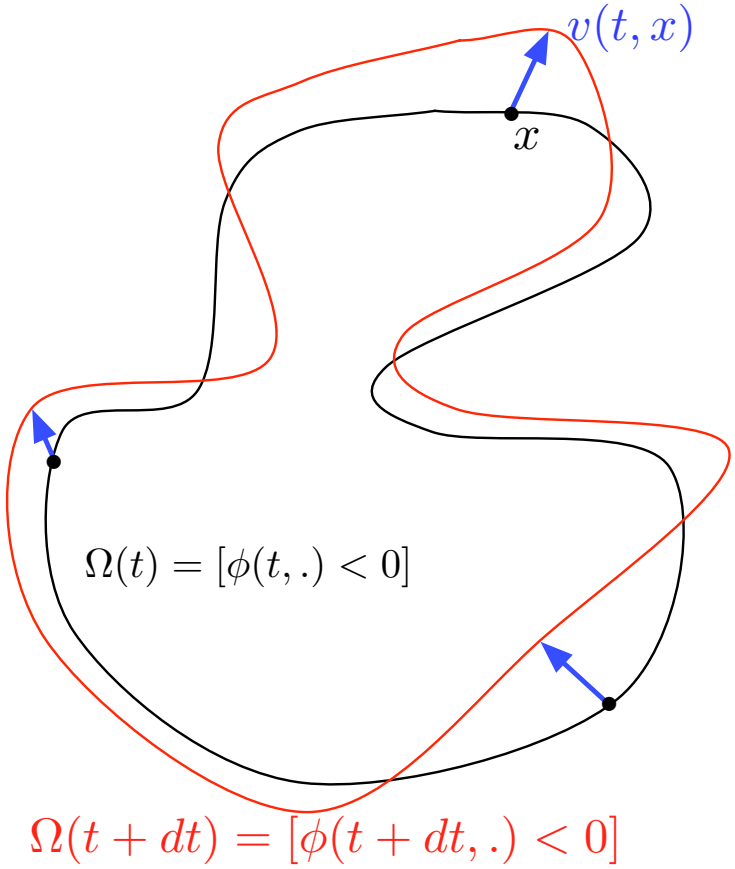
$$\boxed{\frac{\partial \phi}{\partial t}(t,x) + v(t,x).\nabla\phi(t,x) = 0}$$

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

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

this 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 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

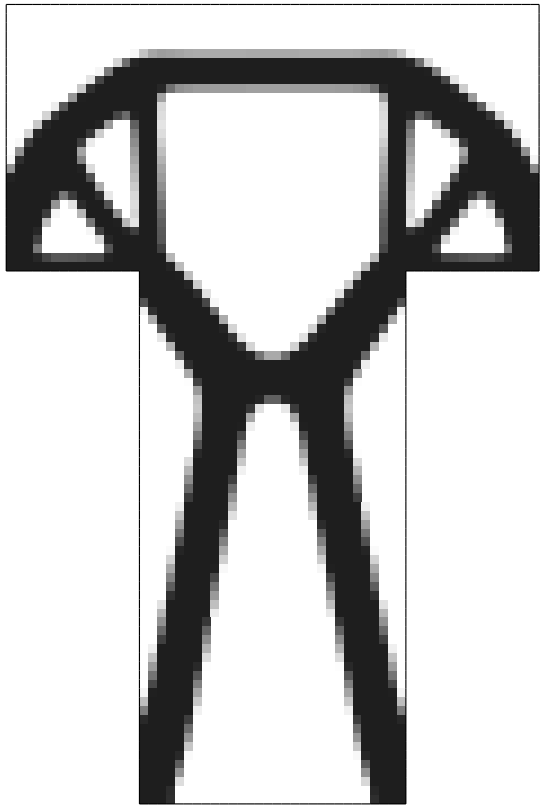
$$\Omega^n \mapsto \Omega^{n+1} = (\mathrm{Id} + \tau^n \theta^n)(\Omega^n)$$

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.

Example: the ersatz material approximation in linearized elasticity (I)

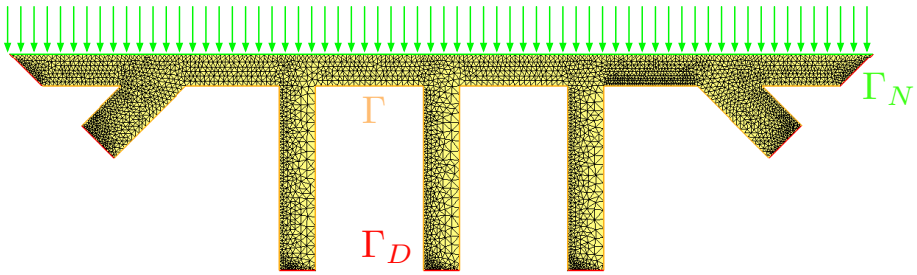
In the linear elasticity context, when the optimized part of the boundary Γ (i.e. that represented with the level set method) is traction-free, the ersatz material method approximates the elastic displacement $u_\Omega : \Omega \to \mathbb{R}^d$ by that $u_{\Omega,\varepsilon} : D \to \mathbb{R}^d$ of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

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

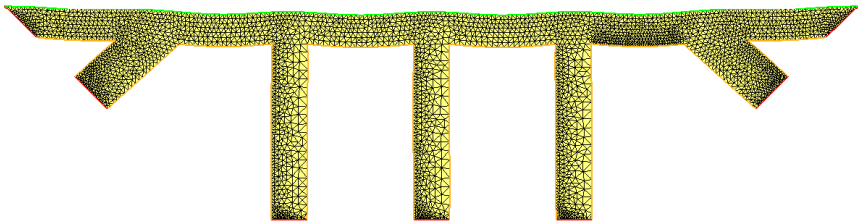
where the approximate Hooke's tensor A_ε reads:

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

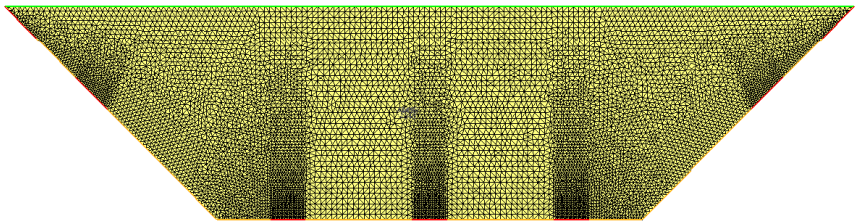
Example: the ersatz material approximation in linearized elasticity (II)

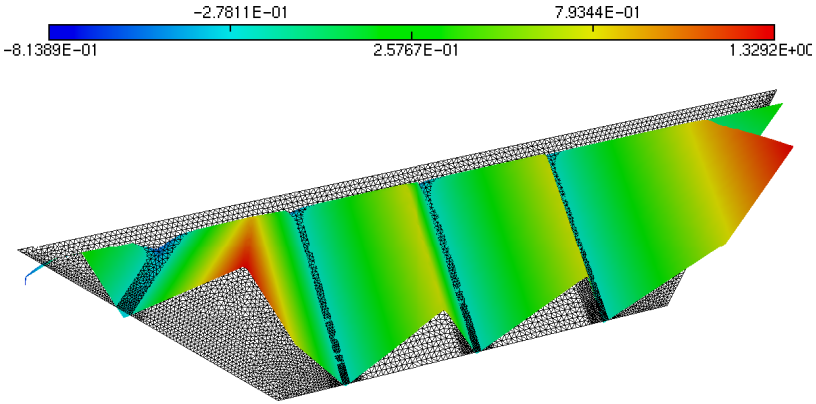


Physical situation of a bridge

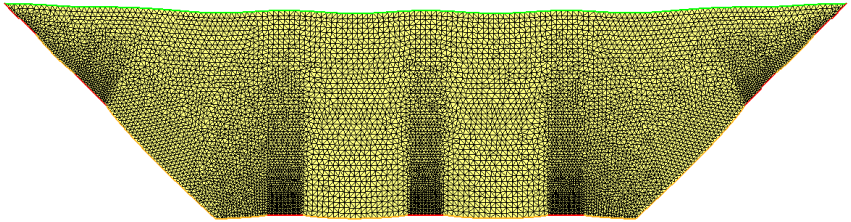


Deformed configuration of the bridge





Implicit definition of the bridge on a mesh of D



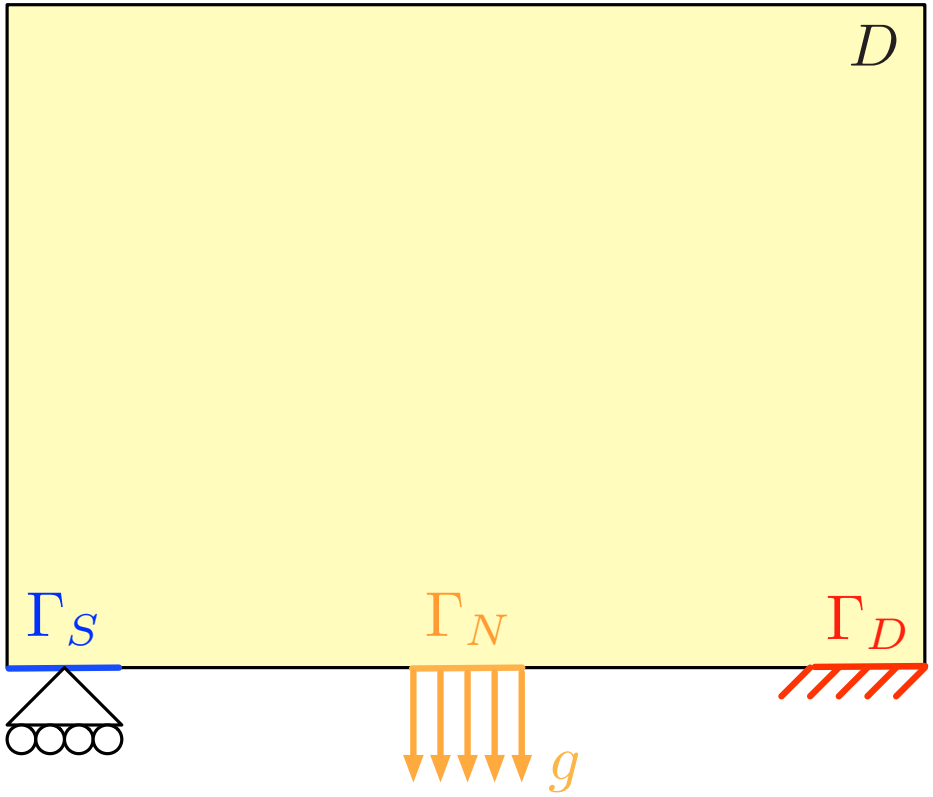
Deformed configuration of the domain D

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

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

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

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



Part V

Topology optimization

- Topological derivatives
- A glimpse of mathematical homogenization
- Density-based topology optimization problems

Topological derivatives (I)

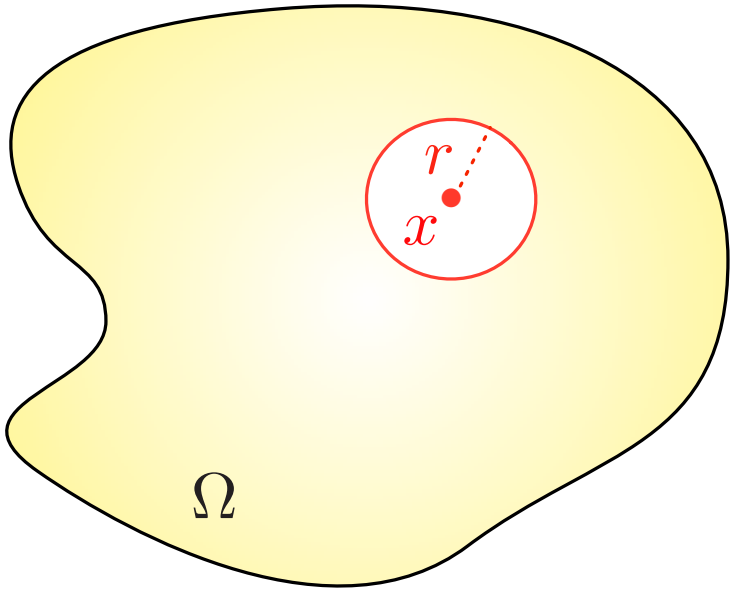
- The previous algorithms feature an update process of the shape by deformation of its boundary.
- In the mathematical framework, the shapes produced during the process are all diffeomorphic to one another; in particular, they have the same topology.
- With a little abuse of the mathematical theory (depending on the numerical representation), it is possible that holes merge during the process.
- However, holes cannot spring up.
- This may be enabled owing to the use of topological derivative, which measure the dependance of a function $J(\Omega)$ with respect to the nucleation of a small hole inside Ω.

Topological derivatives (II)

Topological derivatives appraise variations of a domain Ω of the form:

$$\Omega_{x,r} := \Omega \setminus \overline{B(x,r)},$$

where $B(x,r)$ is the open ball centered at $x \in \Omega$ with radius r.



Definition 4.

A functional $J(\Omega)$ of the domain has a topological derivative at a point $x \in \Omega$ if there exists $g_\Omega^T(x) \in \mathbb{R}$ such that the following asymptotic expansion holds around $r = 0$:

$$J(\Omega_{x,r}) = J(\Omega) + r^d g_\Omega^T(x) + o(r^d), \text{ where } \frac{|o(r^d)|}{r^d} \xrightarrow{r \to 0} 0.$$

Topological derivatives (III)

- *Intuition:* The value of $J(\Omega)$ decreases if a 'small' hole, centered at some point x where $g_\Omega^T(x) < 0$, is nucleated inside Ω.

- The mathematical calculation of topological derivatives is difficult. Fortunately, formulas for such derivatives have been achieved in a wide variety of situations; see for instance [Am, NoSo].

  Example: In the context of 2d linearly elastic shapes, the topological derivative of the compliance reads:

$$\forall x \in \Omega,\ \ g_\Omega^T(x) = \frac{\pi(\lambda+2\mu)}{2\mu(\lambda+\mu)}\,(4\mu Ae(u_\Omega) : e(u_\Omega) + (\lambda-\mu)\mathrm{tr}(Ae(u_\Omega))\mathrm{tr}(e(u_\Omega)))\,(x).$$

- This information is easily introduced into shape derivative-based algorithms: for instance, at every n_{top} iteration, a small hole is nucleated inside the shape Ω^n instead of modifying its boundary.

Topological derivatives (IV)

Initialization: Start from an initial shape Ω^0,

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

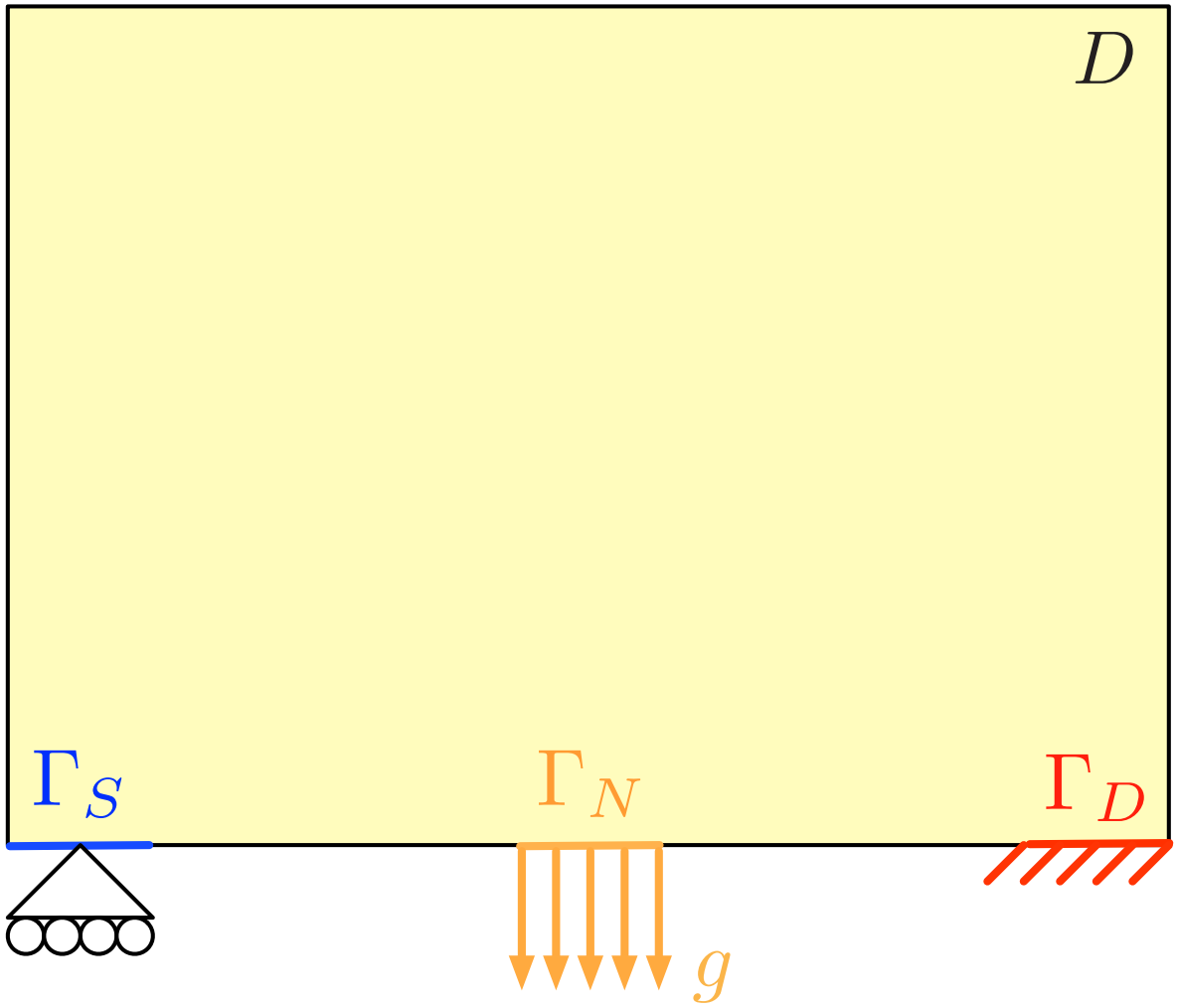
- Calculate the state u_{Ω^n} (and possibly the adjoint p_{Ω^n}) on Ω^n;
- **If** $n \bmod n_{\text{top}} = 0$**:**
  1. Calculate the topological derivative $g_\Omega^T(x)$ at every point $x \in \Omega$;
  2. The new shape Ω^{n+1} is obtained as:

$$\Omega^{n+1} = \Omega^n \setminus \overline{B(x_0, r)},$$

  where $g_\Omega^T(x_0)$ is minimum at x_0, and $r > 0$ is a 'small' parameter.
- **Else:**
  1. Calculate $J'(\Omega^n)$, and infer a descent direction θ^n for $J(\Omega)$.
  2. Advect the shape Ω^n along θ^n for a small pseudo-time step τ^n:

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

The bridge example using topological derivatives



Part V

Topology optimization

- Topological derivatives
- A glimpse of mathematical homogenization
- Density-based topology optimization problems

Mathematical homogenization (I)

Let us consider again the two-phase conductivity setting:

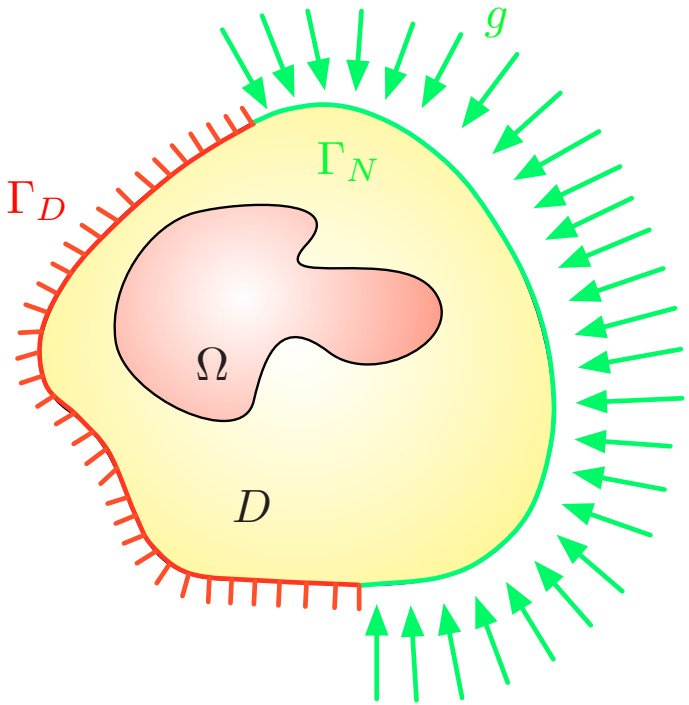
$$\min_{\Omega \in \mathcal{U}_{\mathrm{ad}}} J(\Omega), \text{ where } J(\Omega) = \int_D j(u_\Omega)\, dx,$$

and $u_\Omega : D \to \mathbb{R}$ is the solution to the conductivity equation:

$$\begin{cases} -\mathrm{div}(A_\Omega \nabla u_\Omega) = f & \text{in } D, \\ u_\Omega = 0 & \text{on } \Gamma_D, \\ (A_\Omega \nabla u_\Omega) n = g & \text{on } \Gamma_N, \end{cases}$$

where

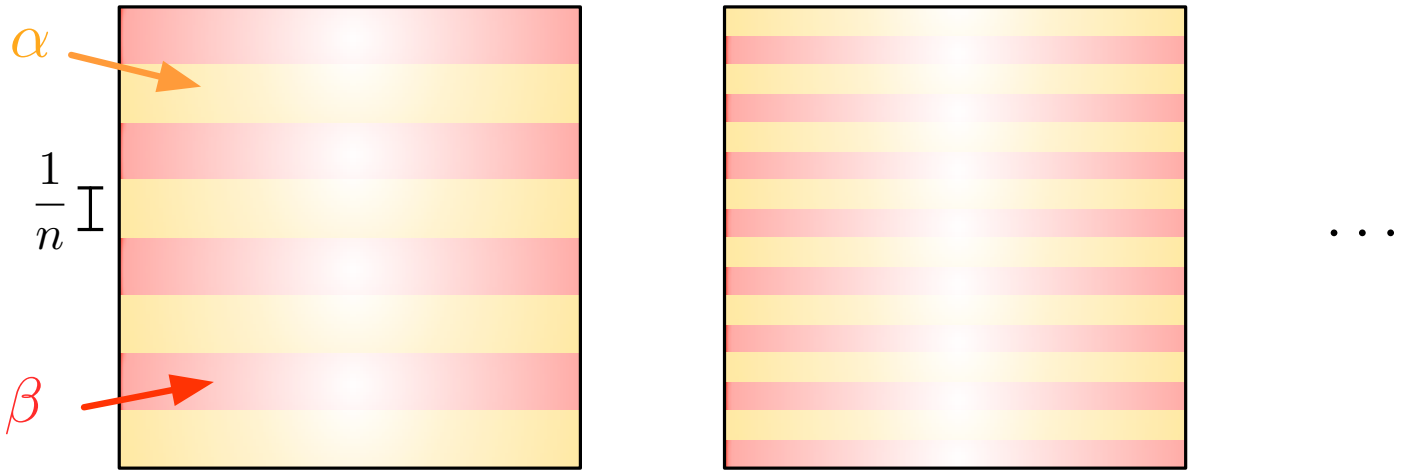
$$A_\Omega = \beta \chi_\Omega + (\alpha - \beta)\chi_\Omega.$$



As we have seen, 'most' such optimization problems do not have a solution.

Mathematical homogenization (II)

The main reason for this non existence of optimal solution is the homogenization effect: better and better values of $J(\Omega)$ are achieved by sequences of shapes showing smaller and smaller features.

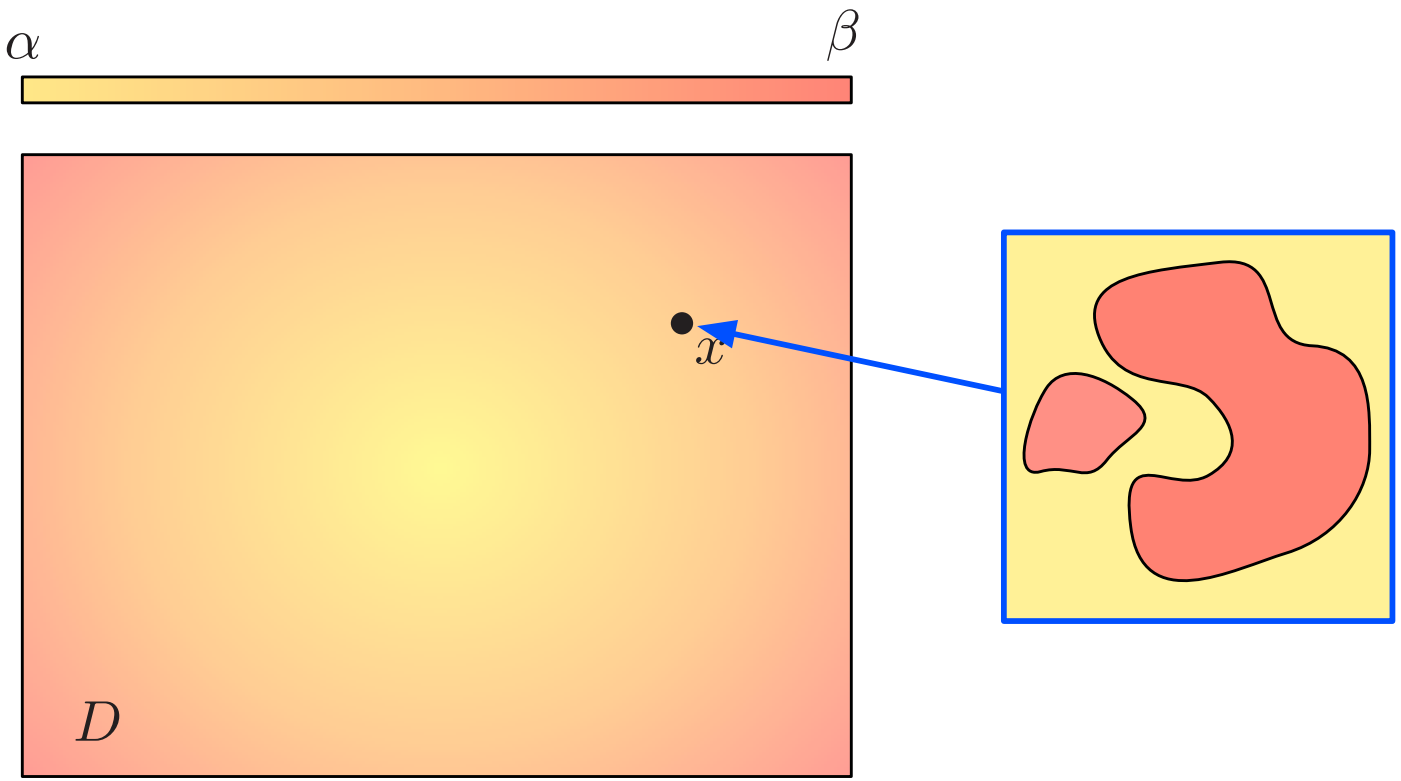


One sequence of shapes showing smaller and smaller features, making $J(\Omega)$ better and better.

Mathematical homogenization (III)

The homogenization method features shapes as couples $(h(x), A^*(x))$, where:

- For $x \in D$, $h(x)$ is the local fraction of materials α and β;
- For $x \in D$, $A^*(x)$ is the diffusion tensor describing the microscopic arrangement of α and β near x.



Around $x \in D$, the structure behaves as a microscopic arrangement of materials α and β in fraction $h(x)$; this amounts to an effective diffusion described by the tensor $A^*(x)$.

Mathematical homogenization (IV)

In the case of 'many' objective functions $J(\Omega)$, one proves that

$$\inf_{\Omega \in \mathcal{U}_{\mathrm{ad}}} J(\Omega) = \inf_{(h,A^*) \in \mathcal{D}_{\mathrm{ad}}} J^*(h, A^*),$$

where:

- $\mathcal{D}_{\mathrm{ad}}$ is the set of all couples (h, A^*) such that
  - $h \in L^\infty(\Omega, [0,1])$,
  - For all $x \in D$, $A^*(x)$ belongs to the set $\mathcal{G}_{h(x)}$ of diffusions tensors which can be obtained as a microscopic arrangement of α and β in proportion $h(x)$.
- The relaxed functional $J^*(h^*, A^*)$ reads:

$$J^*(h, A^*) = \int_D j(u_{h,A^*})\, dx,$$

where u_{h,A^*} is the solution to the equation:

$$\begin{cases} -\mathrm{div}(A^* \nabla u) = f & \text{in } D, \\ u = 0 & \text{on } \Gamma_D, \\ (A^* \nabla u_\Omega) n = g & \text{on } \Gamma_N. \end{cases}$$

Mathematical homogenization (V)

- The homogenized problem

$$\min_{(h,A^*)\in\mathcal{D}_{\mathrm{ad}}} J^*(h,A^*)$$

  is a relaxation of the original one: the set of admissible designs is enlarged.

- The homogenized version of the problem has a global solution!

- Unfortunately, this problem is very difficult to solve, since in general, the set $\mathcal{G}_h$ cannot be characterized easily.

- This problem has some very convenient simplifications in some cases however.

- It also inspires very popular, formal variants for topology optimization, including the SIMP method.

Part V

Topology optimization

- Topological derivatives
- A glimpse of mathematical homogenization
- Density-based topology optimization problems

Density-based topology optimization (I)

We take up again the two-phase conductivity setting:

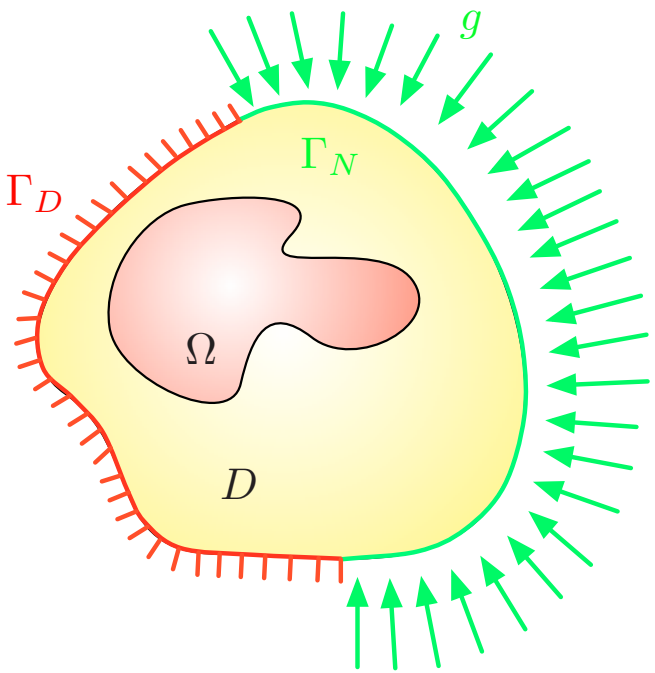
$$\min_{\Omega \subset D} J(\Omega), \text{ where } J(\Omega) = \int_D j(u_\Omega)\, dx.$$

In here, the temperature u_Ω is the solution to:

$$\begin{cases} -\mathrm{div}(h_\Omega \nabla u_\Omega) & = & f & \text{in } D, \\ u_\Omega & = & 0 & \text{on } \Gamma_D, \\ h_\Omega \frac{\partial u_\Omega}{\partial n} & = & g & \text{on } \Gamma_N, \end{cases}$$

where the diffusion h_Ω reads:

$$h_\Omega = \alpha + \chi_\Omega(\beta - \alpha).$$



The ideas presented here extend readily to the contexts of linearized elasticity and (with some work) fluid mechanics.

Density-based topology optimization (II)

- The (sought) 'black-and-white' characteristic function $\chi_\Omega : D \to \{0,1\}$ of Ω, is replaced by a 'greyscale' density function $h : D \to [0,1]$.
- The properties (diffusion) of a region with intermediate density h are coined via an empiric interpolation law $\zeta(h)$ between the extreme values α and β:

$$\zeta(0) = \alpha, \text{ and } \zeta(1) = \beta.$$

- The problem rewrites:

$$\min_{h \in \mathcal{U}_{\mathrm{ad}}} J(h), \text{ where } \mathcal{U}_{\mathrm{ad}} = L^\infty(D,[0,1]), \;\; J(h) = \int_D j(u_h)\, dx,$$

and u_h is the solution to:

$$\begin{cases} -\mathrm{div}(\zeta(h)\nabla u_h) = f & \text{in } D, \\ u_h = 0 & \text{on } \Gamma_D, \\ (\zeta(h)\nabla u_h)n = g & \text{on } \Gamma_N. \end{cases}$$

- It is a simplified and empiric version of the homogenized problem, where the microstructure tensor A^* is omitted.

Density-based topology optimization (III)

The resulting density-based problem is within the remit of parametric optimization!

Theorem 10.

The objective function

$$J(h) = \int_D j(u_h)\, dx$$

is Fréchet differentiable at any $h \in \mathcal{U}_{\mathrm{ad}}$, and its derivative reads

$$\forall \widehat{h} \in L^\infty(D),\ \ J'(h)(\widehat{h}) = \int_D \zeta'(h)(\nabla u_h \cdot \nabla p_h)\widehat{h}\, dx,$$

where the adjoint state $p_h \in H^1(D)$ is the unique solution to the system:

$$\begin{cases} -\mathrm{div}(\zeta(h)\nabla p_h) = -j'(u_h) & \text{in } D, \\ p_h = 0 & \text{on } \partial D, \\ \zeta(h)\frac{\partial p_h}{\partial n} = 0 & \text{on } \Gamma_N. \end{cases}$$

The same numerical methods as for parametric optimization may be used.

The interpolation profile

- The interpolation profile $\zeta(h)$ endows regions with (fictitious) intermediate densities with material properties (diffusion, etc.).

- In the practice of the Solid Isotropic Method with Penalization (SIMP), a power law of the form
$$\zeta(h) = \alpha + h^p(\beta - \alpha)$$
is used (often, $p = 3$).

- This has the effect to penalize the presence of 'greyscale' intermediate regions, and to urge the optimized density towards a 'black-and white' function.

- This interpolation law is empiric: there is not even a guarantee that a material with such properties does exist!

- In the article [Am2], other choices for $\zeta(h)$ are discussed, which are more consistent from the physical viewpoint.

Density filters (I)

- Often, desired properties (regularity, etc.) are imposed on h by filtering: h appears in the state (and adjoint) equations under the form Lh, where

$$L : L^\infty(D, [0,1]) \to L^\infty(D, [0,1])$$

is the filter operator.

- The problem rewrites:

$$\min_{h \in \mathcal{U}_{\mathrm{ad}}} J(h), \text{ where } J(h) = \int_D j(u_h)\, dx,$$

and u_h is the solution to:

$$\begin{cases} -\mathrm{div}(\zeta(Lh)\nabla u_h) = f & \text{in } D, \\ u_h = 0 & \text{on } \Gamma_D, \\ (\zeta(Lh)\nabla u_h)n = g & \text{on } \Gamma_N. \end{cases}$$

- The calculation of the derivative of $J(h)$ now yields:

$$\begin{aligned} J'(h)(\widehat{h}) &= \int_D \zeta'(h)(\nabla u_h \cdot \nabla p_h)(L\widehat{h})\, dx, \\ &= \int_D L^T \left(\zeta'(h)(\nabla u_h \cdot \nabla p_h)\right) \widehat{h}\, dx. \end{aligned}$$

Density filters (II)

Here are two examples of regularizing filters:

- *Convolution-based filter:* For ε 'small' ($\varepsilon \approx$ mesh size), one defines:

$$L_\varepsilon h = h * \eta_\varepsilon,$$

where η_ε is a mollifying kernel; i.e. $\eta_\varepsilon(x) = \frac{1}{\varepsilon^d}\eta(\frac{x}{\varepsilon})$,

$$\eta \in \mathcal{C}_c^\infty(\mathbb{R}^d), \ \operatorname{supp}(\eta) \subset B(0,1), \ \text{and} \ \int_{\mathbb{R}^d} \eta \, dx = 1.$$

- *PDE-based filter:* For ε small,

$$L_\varepsilon h = q,$$

where q is the unique solution in $H^1(D)$ to the problem:

$$\begin{cases} -\varepsilon^2 \Delta q + q = h & \text{in } D, \\ \frac{\partial q}{\partial n} = 0 & \text{on } \partial D. \end{cases}$$

See for instance [WanSig] for many other examples of filters.

Sensitivity filters

- As in the parametric optimization context, the derivative:

$$\forall \widehat{h} \in L^\infty(D),\ \ J'(h)(\widehat{h}) = \int_D \zeta'(h)(\nabla u_h \cdot \nabla p_h)\widehat{h}\, dx$$

  lends itself to a straightforward choice of a descent direction:

$$\widehat{h} = -\zeta'(h)(\nabla u_h \cdot \nabla p_h),$$

  that is, $\widehat{h}$ is the $L^2(D)$ gradient of $J'(h)$.

- Other choices are possible (and often more adequate) by changing inner products:

$$\widehat{h} = -V,$$

  where V solves:

$$\forall w \in \mathcal{H},\ \ \langle V, w\rangle_{\mathcal{H}} = J'(h)(w),$$

  for an adapted choice of Hilbert space and inner product $\mathcal{H}$ and $\langle \cdot, \cdot \rangle_{\mathcal{H}}$.

- This stage is often called sensitivity filtering in density-based methods.

Density-based relaxation

- As the result of a density-based topology optimization process, a density function h is obtained, which may present greyscale values.

- However, in general, a real 'black-and-white' design is expected.

- Hence there is the need to threshold the density h, i.e. to find the adequate value $\rho \in (0, 1)$ such that:
  - Regions where $0 \leq h(x) \leq \rho$ are considered to be 'void';
  - Regions where $\rho < h(x) \leq 1$ are considered to be 'full of material'.

- So as to stir the optimized density towards values 0 and 1 during the optimization, one may use a Heaviside filter:

$$\widetilde{H_{\beta,\eta}} h = \frac{\tanh(\beta\eta) + \tanh(\beta(h - \eta))}{\tanh(\beta\eta) + \tanh(\beta(1 - \eta))},$$

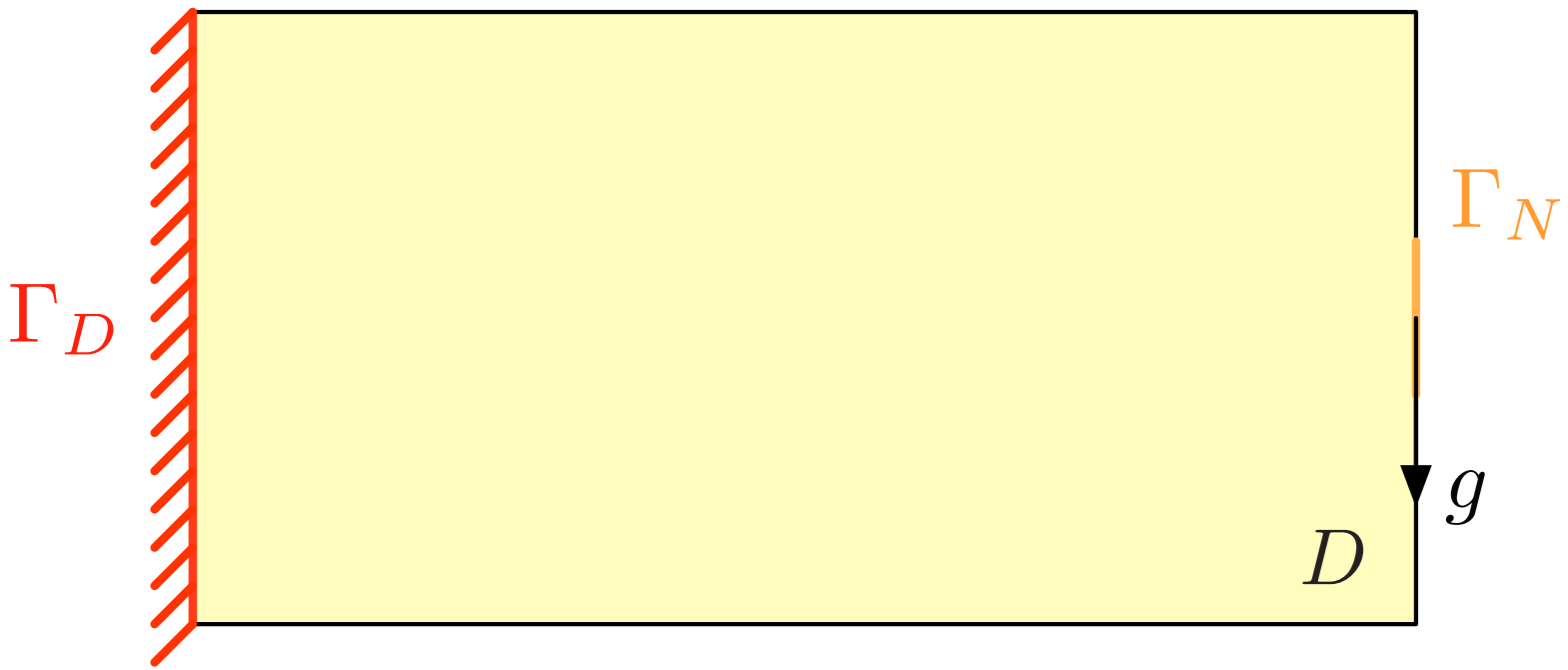
  where β and η are user-defined parameters which may be updated in the course of the process.

Example: the cantilever benchmark

- In the context of linearized elasticity, the compliance of a cantilever beam is minimized:

$$C(h) = \int_D \zeta(h) A e(u_h) : e(u_h)\, dx.$$

- A constraint on the volume $\mathrm{Vol}(h) = \int_D h\, dx$ of material is added.

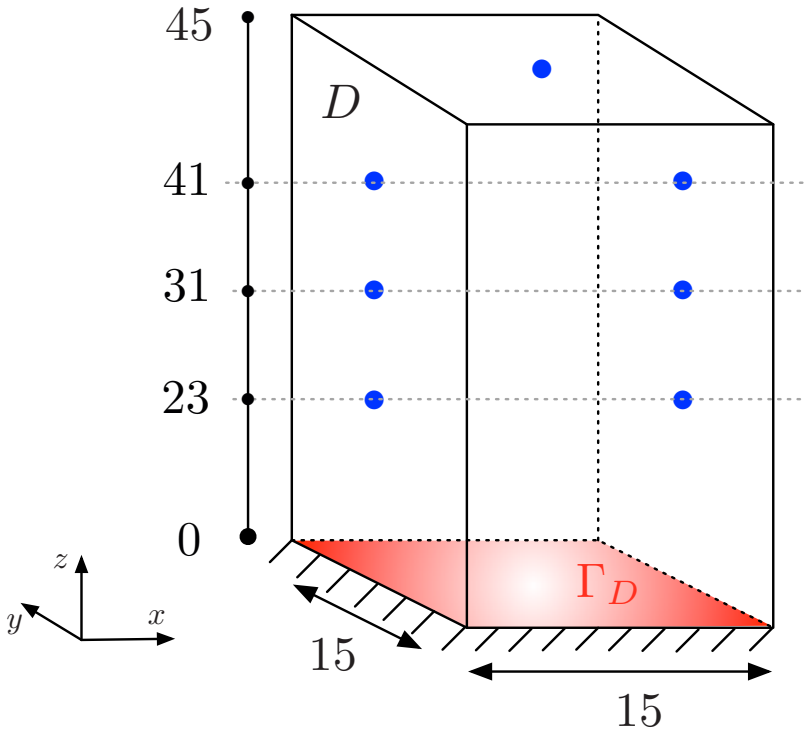


Part VI

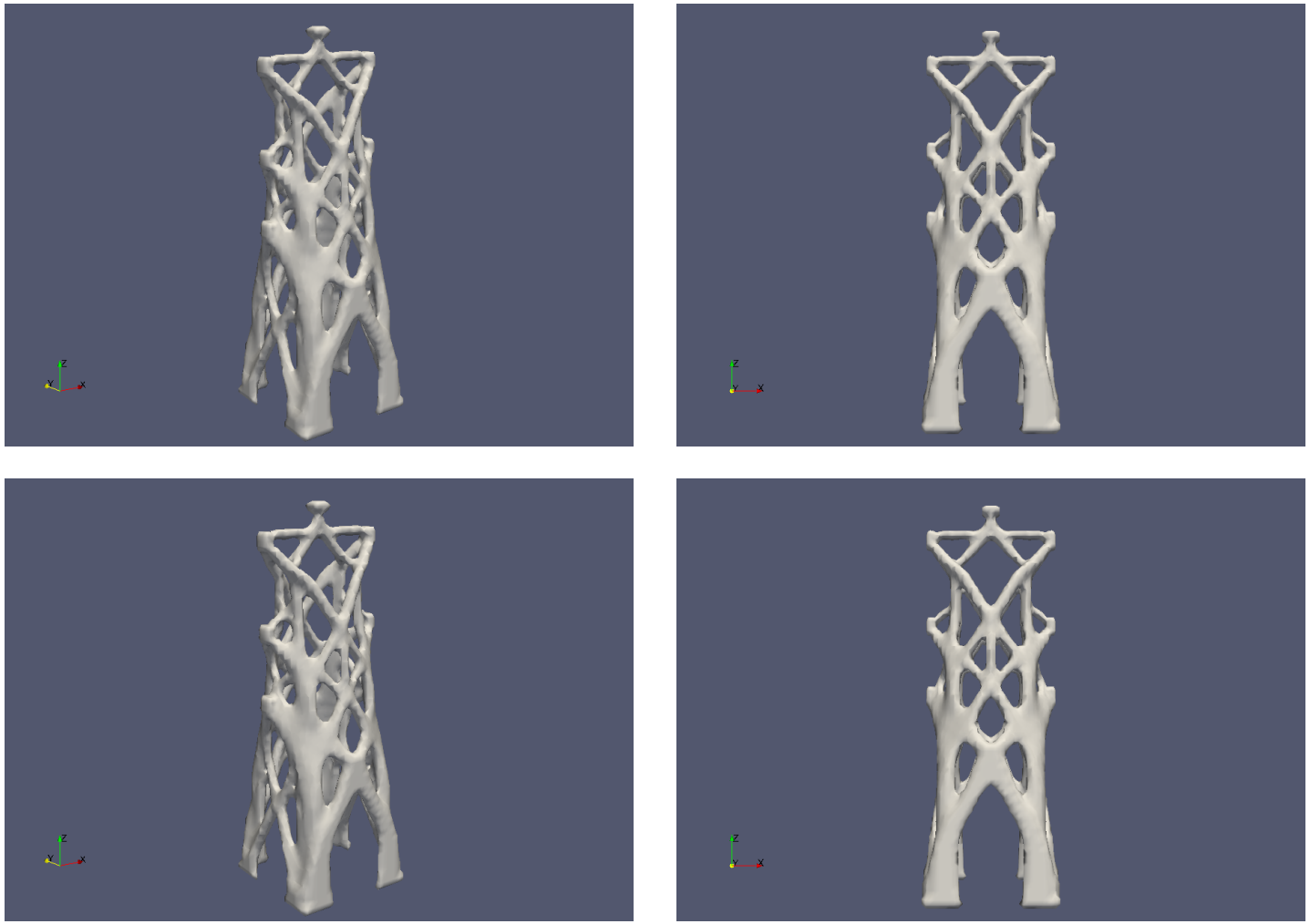
Further numerical results

Optimization of the shape of a pylon (I)

- A pylon Ω is fixed on a region Γ_D of its boundary;
- Several load scenarii may occur, depending on the conditions of the ambient medium (wind, etc.);
- The physical behavior of Ω is described by the linearized elasticity equations;
- The mean compliance of Ω under the various possible scenarii is minimized, under a volume constraint.



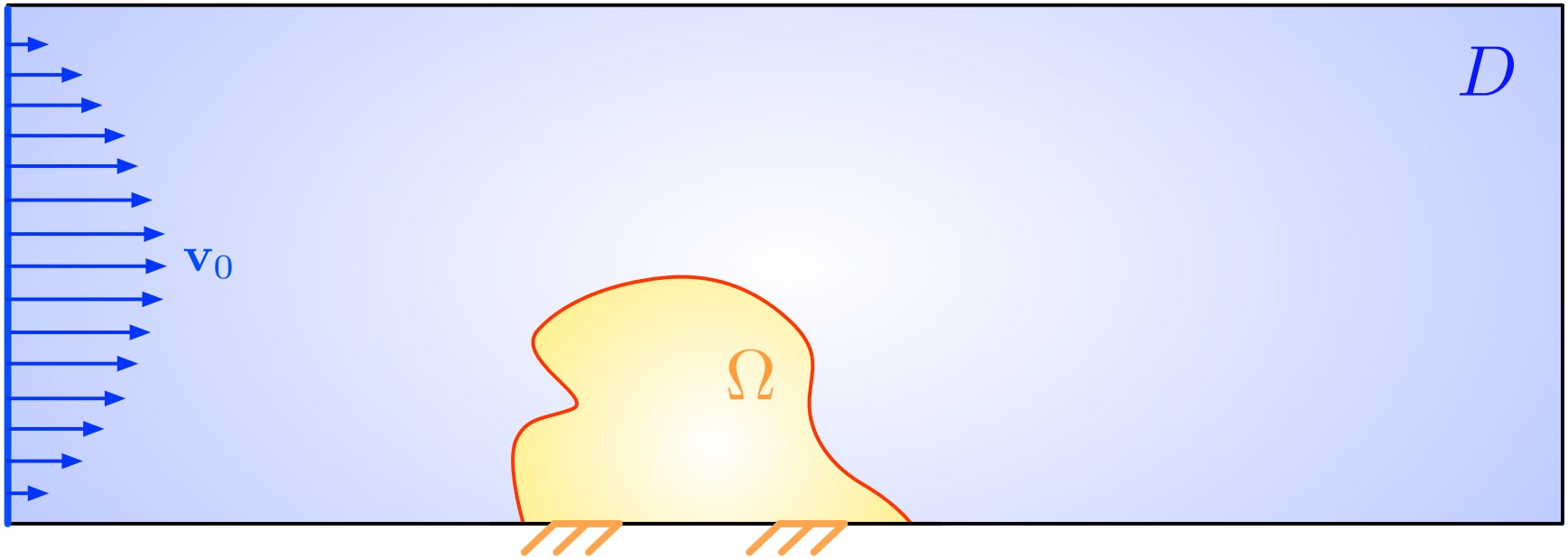
Optimization of the shape of a pylon (II)



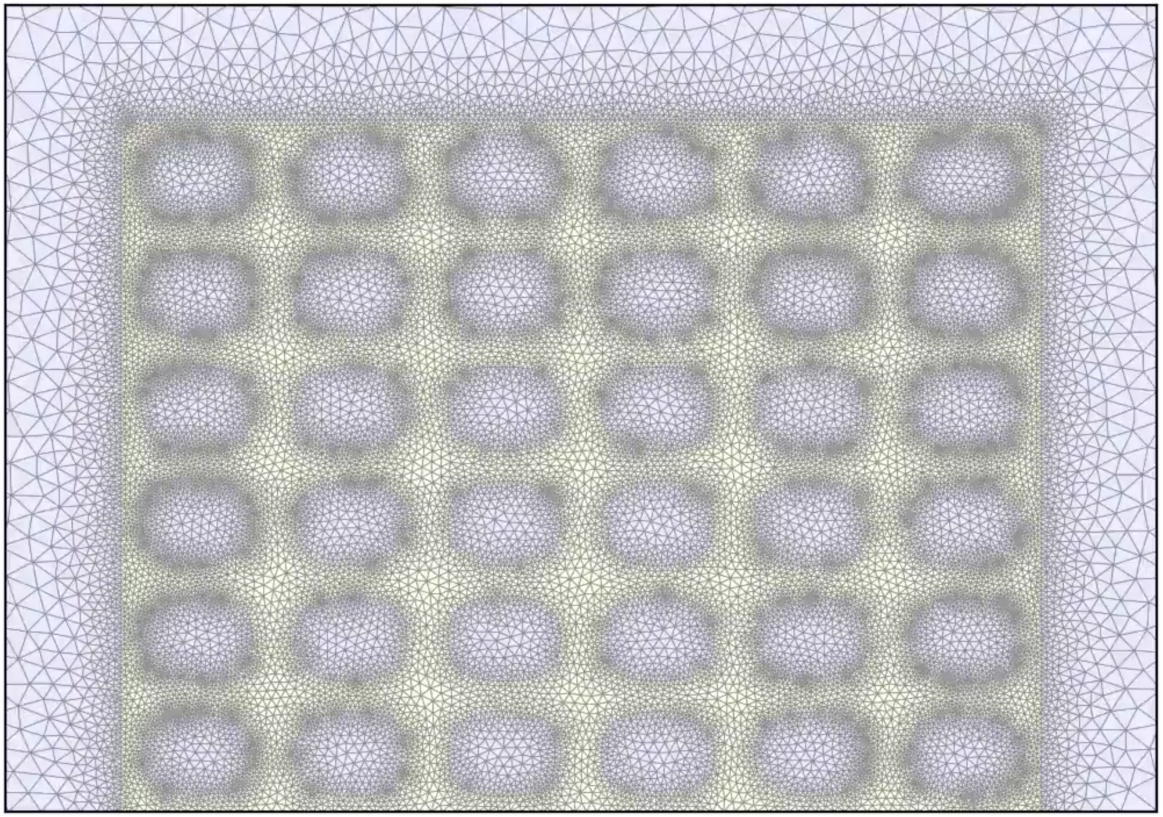
(Top / bottom) Two optimized pylons associated to various sets of constraints.

An example in fluid mechanics (I)

- A fluid is flowing through a pipe D with a given incoming velocity profile.
- An obstacle Ω occupies the pipe, which contains a non optimizable region.
- The fluid is governed by the Navier-Stokes equations, and the behavior of the obstacle is described by the linearized elasticity system.
- The work of the fluid on Ω is minimized under a volume constraint.



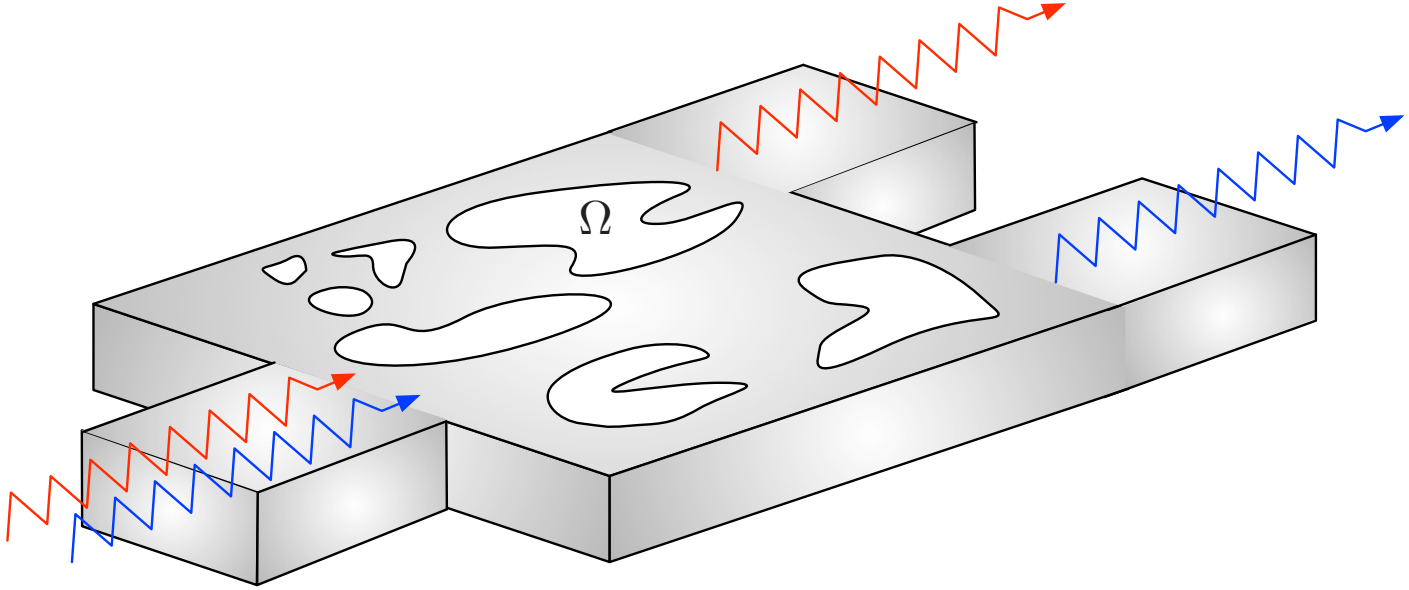
An example in fluid mechanics (II)



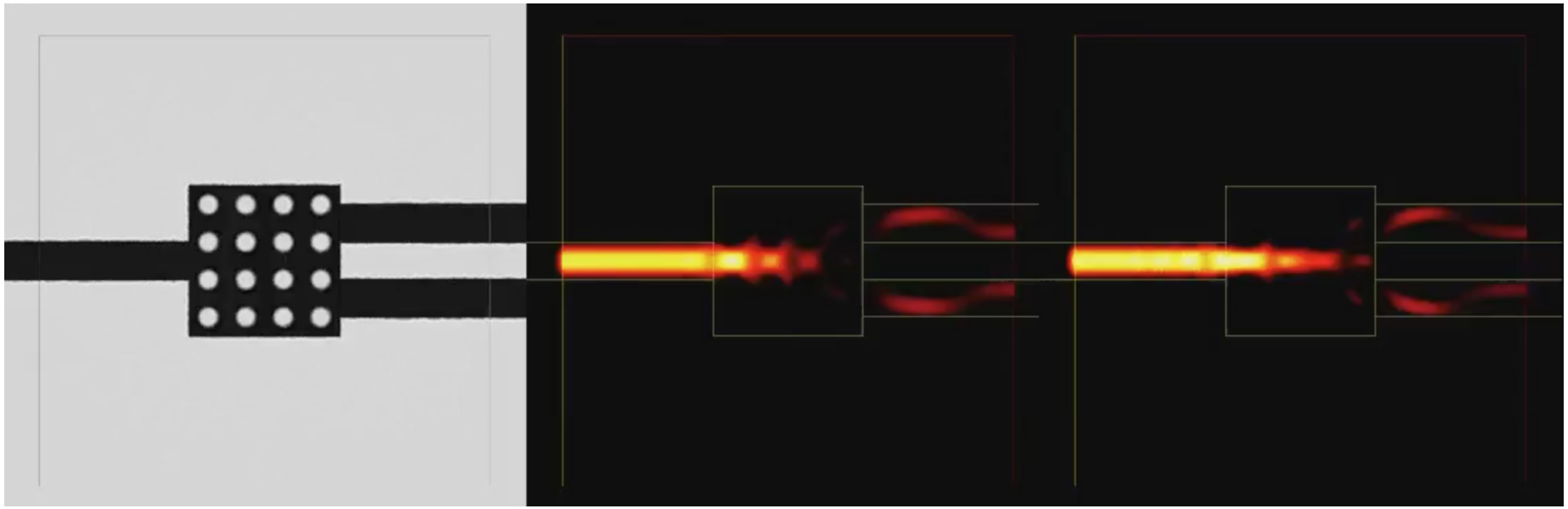
Optimized reinforcement of a pillar subjected to the pressure of a fluid ***(Thanks: Florian Feppon)***.

An example in electromagnetism (I)

- An electromagnetic wave is conveyed by a waveguide.
- Its eletric and magnetic fields fuflill the Maxwell equations.
- A demultiplexer is a device aimed to steer the incoming wave to different output ports depending on its wavelength.
- The aim is to optimize the distribution Ω of silica in the demultiplexer so as to impose this behavior?



An example in electromagnetism (II)



Optimized shape of a demultiplexer ***(Thanks: Nicolas Lebbe)***.

Part VII

Current challenges in shape and topology optimization

- Shape optimization and robustness
- Additive manufacturing shape and topology optimization

Shape optimization and robustness

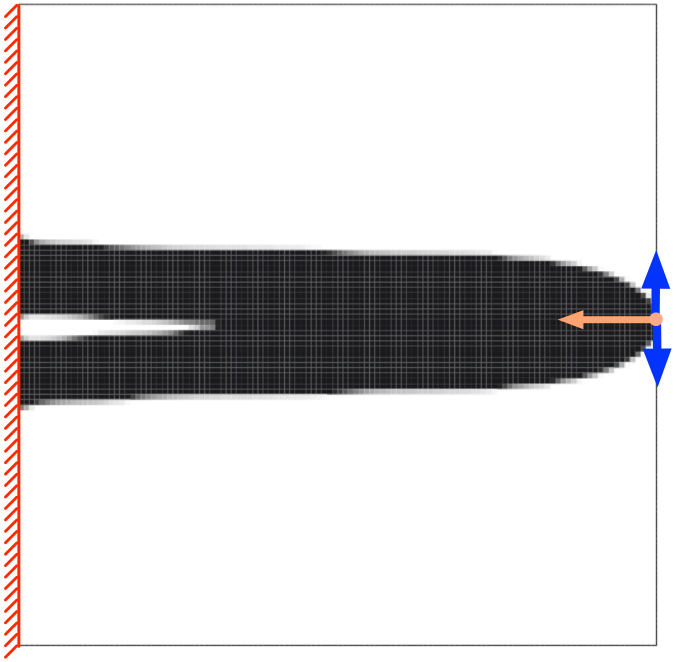
- The physical situations in which shape optimization problems arise are characterized by data :
  - The magnitude of the applied loads on an elastic structure;
  - The location where they are applied;
  - The wavelength of a wave conveyed by a guide;
  - The viscosity of a fluid passing through a channel.

- Often, these data are estimated, or measured, in a quite imprecise way.

- It is therefore natural to require that a shape be robust with respect to small perturbations on these data.

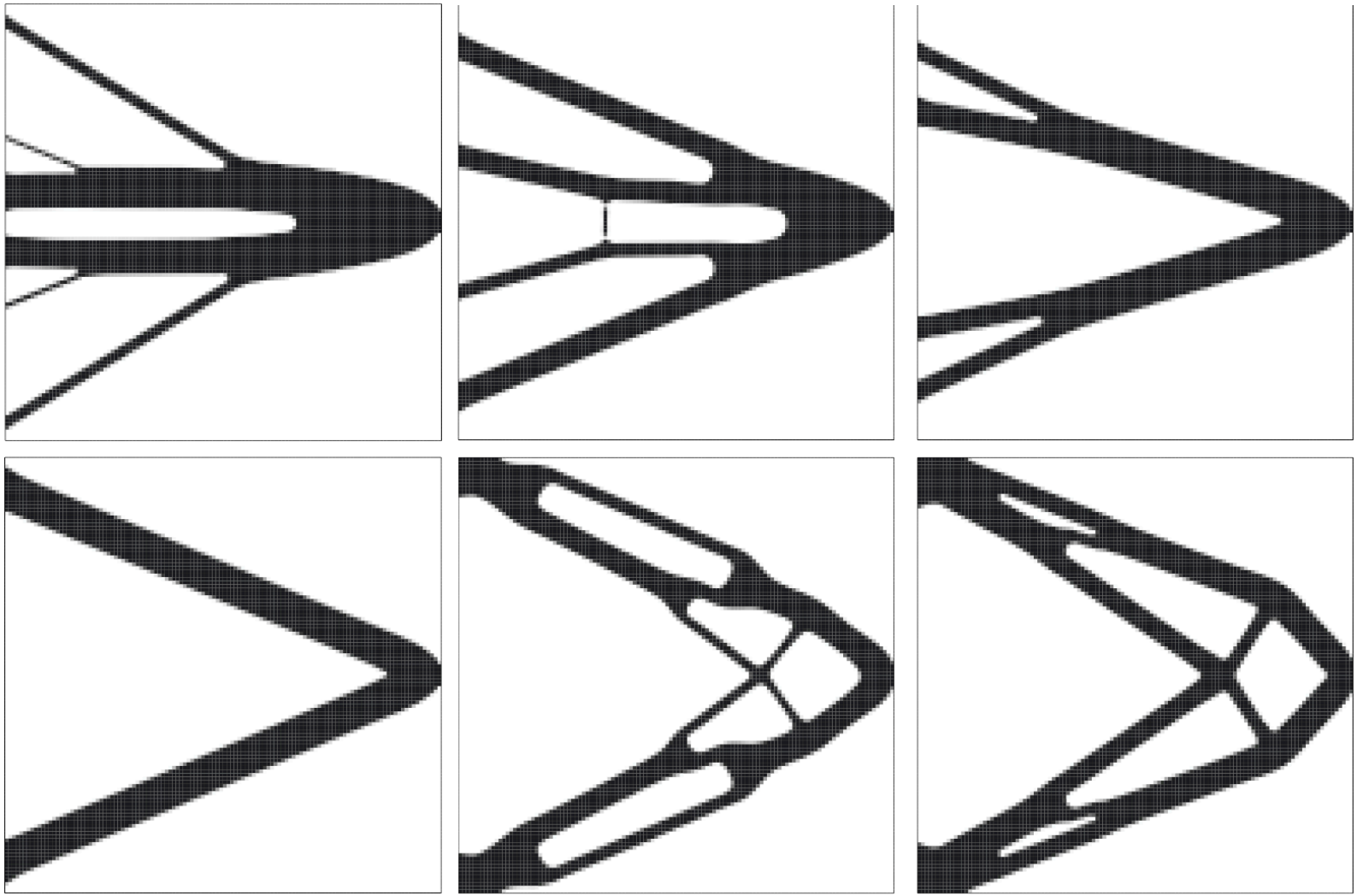
A revealing example [deGAlJou] (I)

- A cantilever beam is submitted to a horizontal load.
- 'Small' vertical perturbations are expected on this load.
- The shape of the beam is optimized under a volume constraint.
- In this particular situation, uncertainties can be taken into account in a rigorous way.



Optimized shape of the beam without taking into account uncertainties on the load.

A revealing example [deGAlJou] (II)



Optimized shape of the cantilever beam under larger and larger uncertainties on the vertical component of the load.

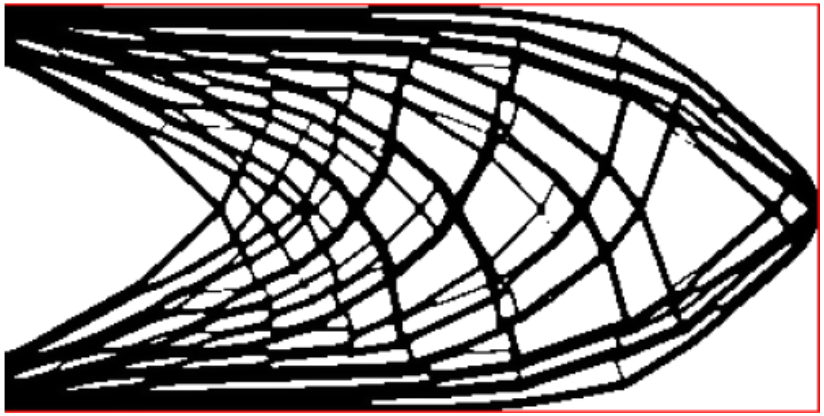
Part VII

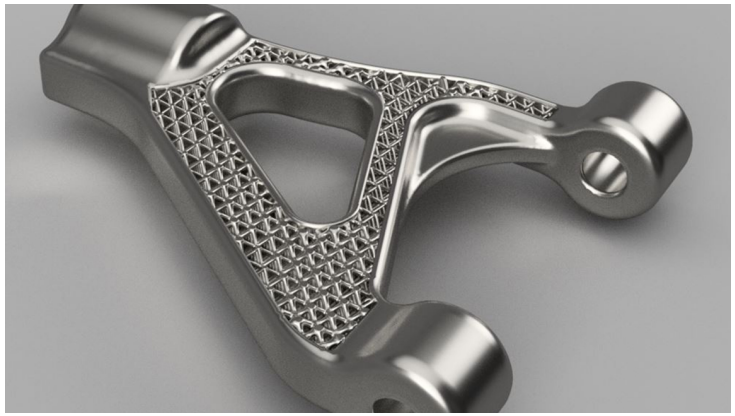
Current challenges in shape and topology optimization

- Shape optimization and robustness
- Additive manufacturing shape and topology optimization

Manufacturing the optimized shapes

- Optimized shapes are often too complex to be manufactured by traditional fabrication processes (milling, casting, etc.); for instance:
  - They show thin bars, which are likely to break in the course of the assembly;
  - They contain thick regions, where the cooling of the molten material is difficult.
- One burning challenge is to model the constraints imposed by the fabrication process on the optimized shape Ω
- The modern additive manufacturing (or 3d printing) techniques are expected to allow much more freedom in terms of the constructible designs.

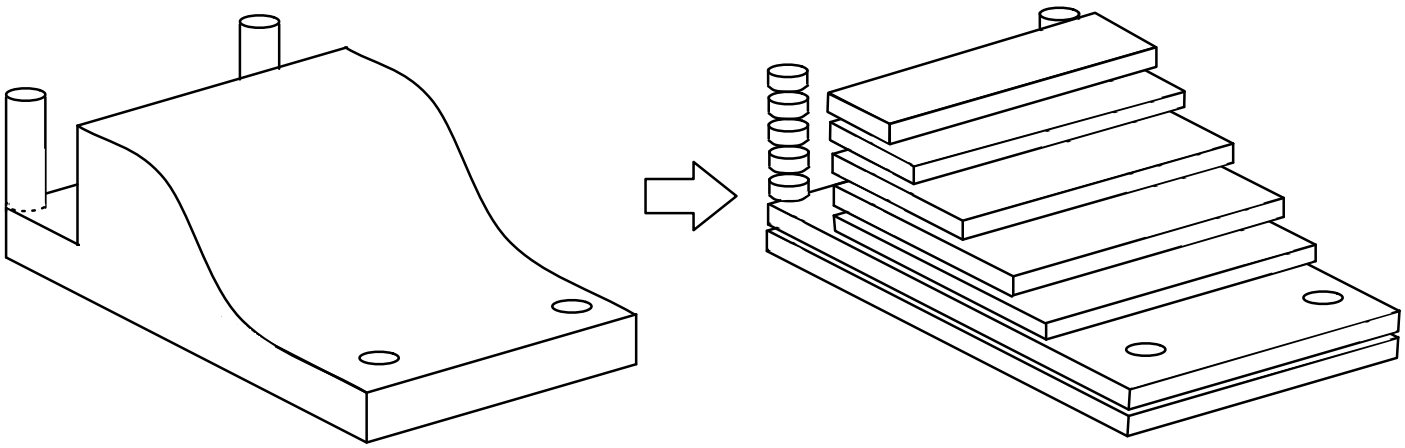




(Left) One 'optimized' shape; (right) one shape assembled by additive manufacturing.

Additive manufacturing in a nutshell (I)

- All additive manufacturing techniques begin with a slicing procedure: the shape is converted into a series of horizontal layers.
- These 2d layers are constructed one atop the other, according to the selected technology.



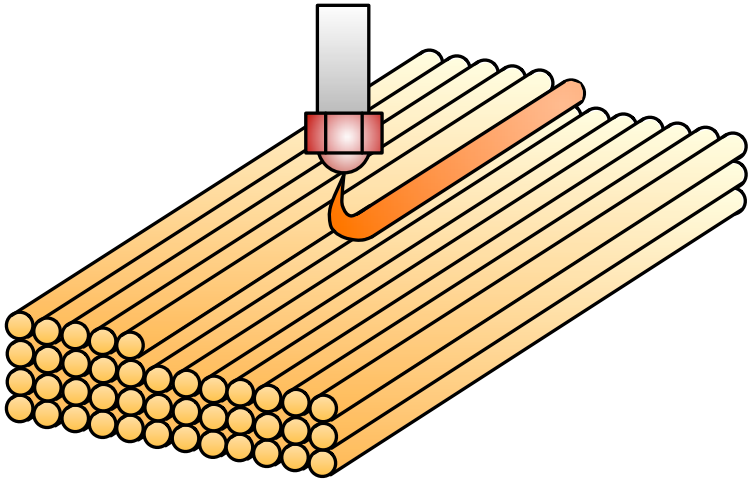
The slicing procedure, initiating any additive manufacturing process.

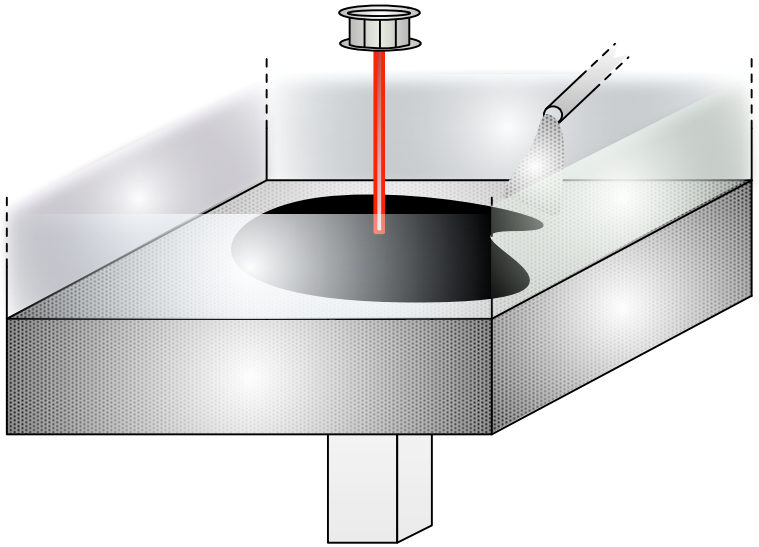
- In principle, these techniques allow to construct 'arbitrarily complex' shapes.

Additive manufacturing in a nutshell (II)

Two of the most popular additive manufacturing technologies are:

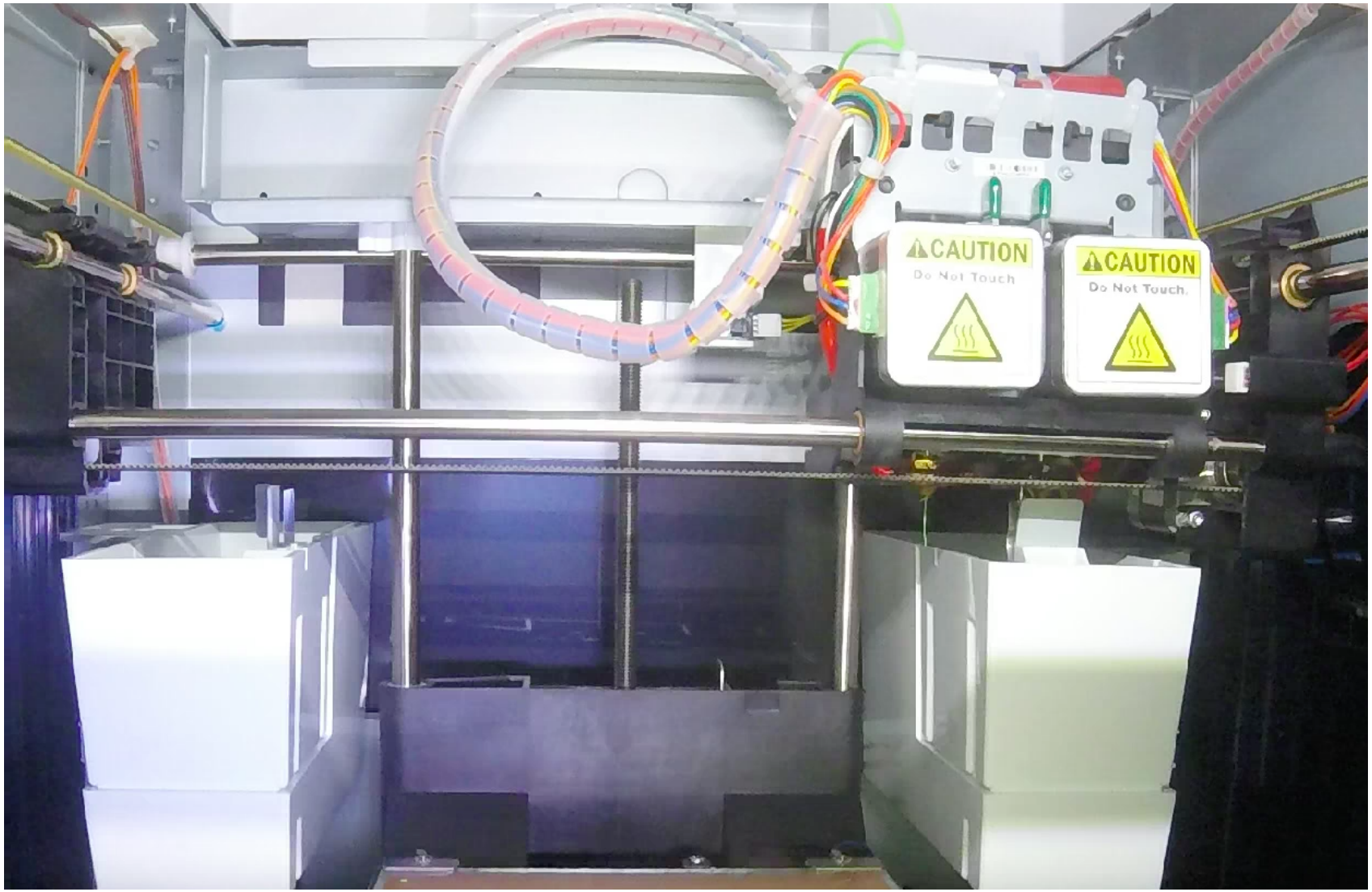
- Material extrusion methods (e.g. FDM): they proceed by depositing a molten filament of polymer (e.g. ABS) under the form of rasters.
- Powder bed fusion methods (e.g. EBM, SLS) are mainly used to process metal. The construction of each 2d layer starts by spreading metallic powder inside the build chamber, which is then selectively molten owing to a laser.





Sketch of the (left) FDM technology, and (right) EBM process.

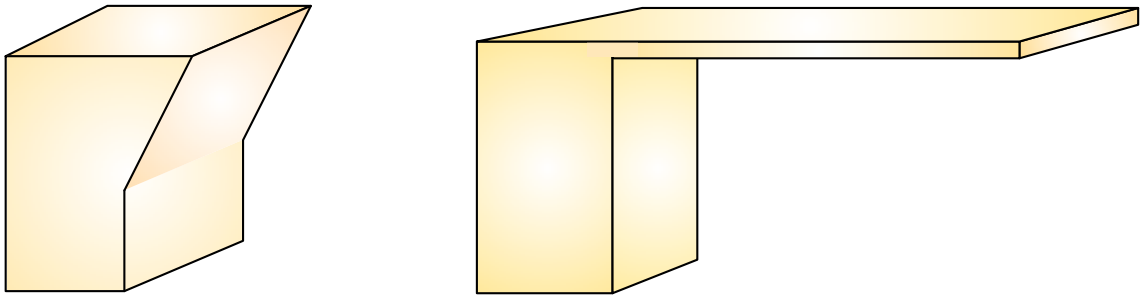
Additive manufacturing in a nutshell (III)



One machine tool for the FDM process in action.

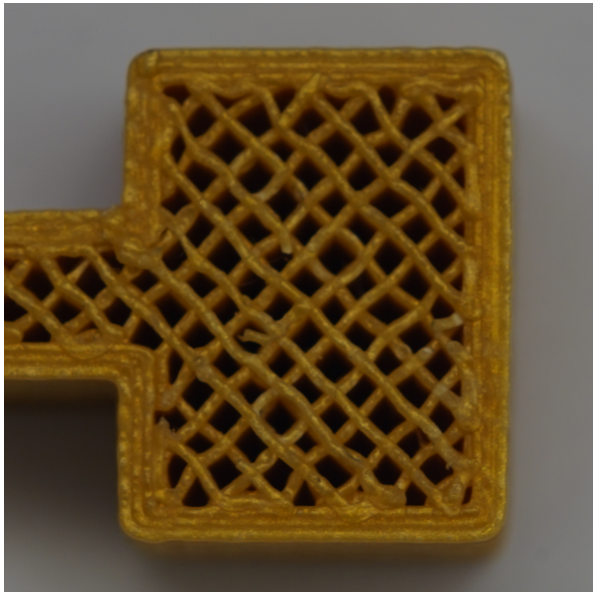
New challenges in connection with additive manufacturing!

- It is difficult to erect large overhanging regions with these techniques.



(Left) One 'small' and (right) one 'large' overhang.

- Materials assembled by additive manufacturing do not have the exact same physical properties as those predicted by theory.



One 2d layer of a structure produced by FDM.

Part VIII

Conclusions and take-home messages

Conclusions and take-home messages

- Shape and topology optimization methods arise in a wide range of physical contexts: heat conduction, structure mechanics, fluid mechanics, electromagnetism, etc. They are also used in imaging, or shape reconstruction.
- Several vantages are available: parametric, geometric or topology optimization, depending on the nature of the sought design, and on the available means (data, CPU, etc.).
- Accordingly, various notions of shape sensitivity exist: 'classical' Fréchet derivatives, shape derivatives, topological derivatives,...
- ... paving the way to multiple numerical frameworks: parametric optimization algorithms, algorithms featuring an evolving mesh, fixed mesh level set methods, etc.
- Recent, burning challenges have arisen in this thriving field of mathematics, physics and computer science!

Thank you for your attention!

Technical appendix

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 11 (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:

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

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

A Lipschitz function $f : \mathbb{R}^d \to \mathbb{R}$ 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 12 (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:

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

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.

The implicit function theorem

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

Theorem 13 (Implicit function theorem).

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

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

Then there exist an open subset $\mathcal{V}' \subset \mathcal{V}$ of θ_0 in Θ and a mapping $g : \mathcal{V}' \to U$ 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 $u \in E$, given by $u = g(\theta)$.*

Theorem 14 (Lax-Milgram theorem).

Let V be a Hilbert space, and let $(u, v) \mapsto a(u, v)$ and $v \mapsto \ell(v)$ be a bilinear and a linear form on V, respectively, such that:

- *a is continuous;*
- *a is elliptic (or coercive): there exists $\alpha > 0$ such that:*

$$\forall u \in V, a(u, u) \geq \alpha ||u||^2;$$

- *ℓ is continuous.*

Then the variational problem

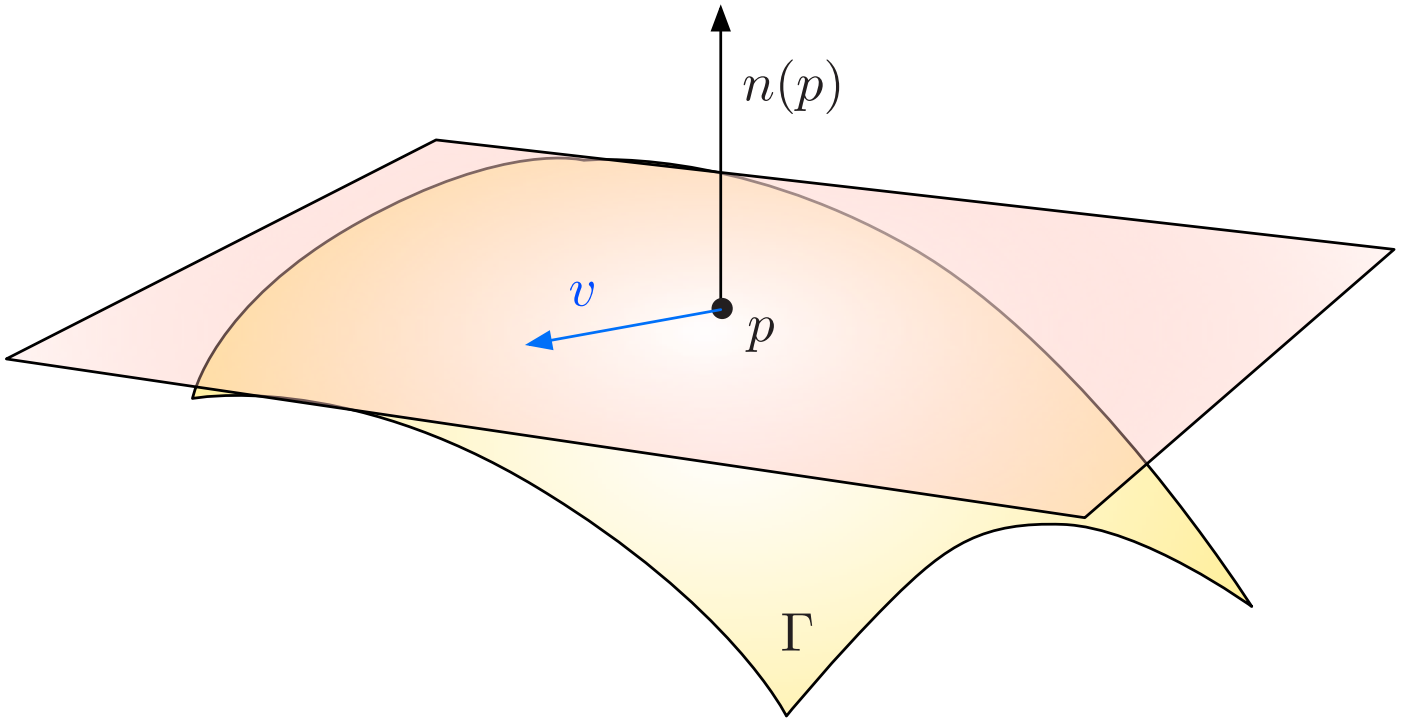
$$\text{Search for } u \in V \text{ s.t. } \forall v \in V, \ \ a(u, v) = \ell(v)$$

has a unique solution in V.

Surfaces and curvature (I)

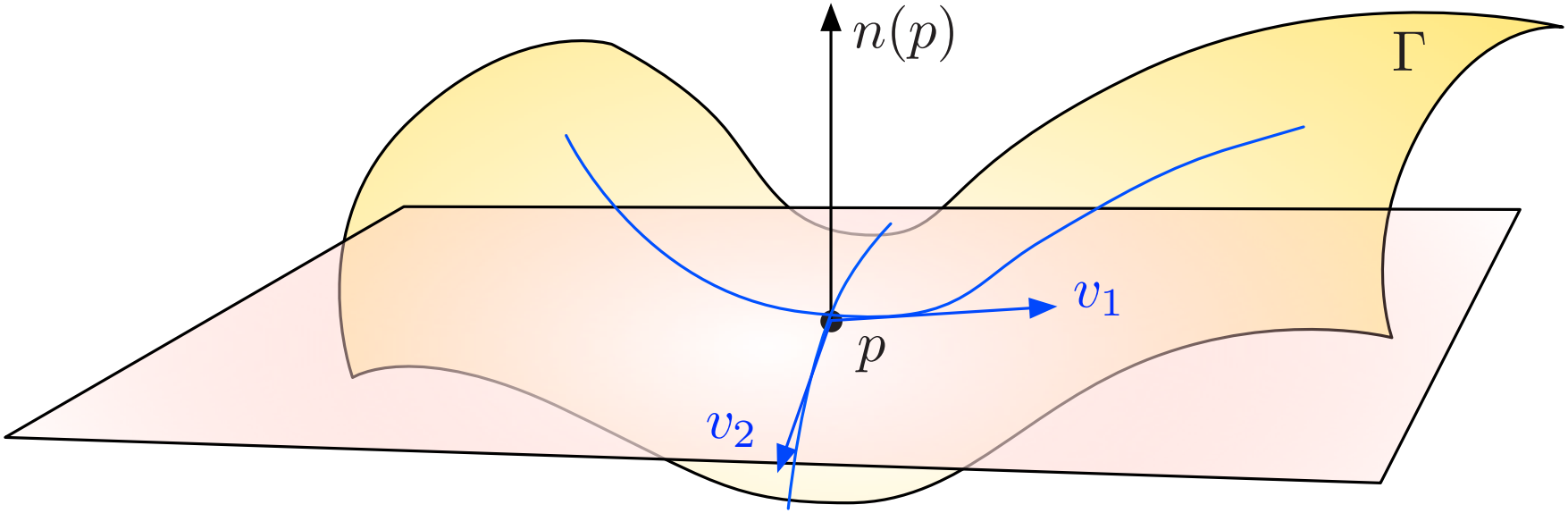
At first order, in the neighborhood of a point $p \in \Gamma$, a surface Γ behaves like a plane, the tangent plane,

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



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