An introduction to shape and topology optimization

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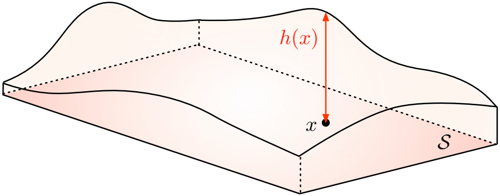
Foreword

- In this lecture, we focus on parametric optimization, or optimal control:
    - The shape is described by a set h of parameters, lying in a fixed vector space.
    - The state equations, accounting for the physical behavior of the shape, depend on h in a "simple" way.

- Many key concepts and methods of the course can be exposed in this framework, with a minimum amount of technicality.



An elastic plate can be described by its height $h : \mathcal{S} \to \mathbb{R}$ with respect to a fixed cross-section $\mathcal{S}$.

Part II

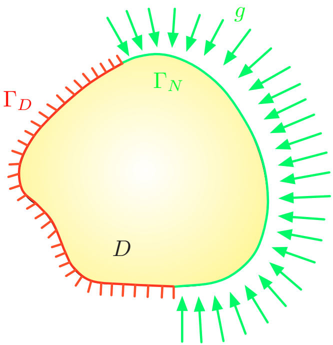
Optimal control and parametric optimization problems

A model problem involving the conductivity equation (I)

- We return 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 "state", conductivity equation:

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

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



The considered cavity

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

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

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

A model problem involving the conductivity equation (II)

- We consider a problem of the form:

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

  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. featuring 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 $h \in \mathcal{U}_{\mathrm{ad}}$;
  - The design variable h acts as a parameter in the coefficients of the state equation.

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

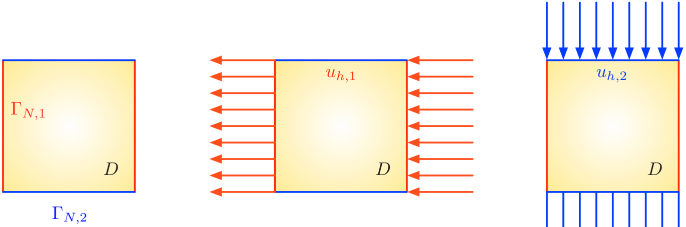
Part II

Optimal control and parametric optimization problems

Non existence of optimal design (I)

- This counter-example is discussed in details in [All] §5.2.
- The defining domain 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 in this example is:

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

where the considered objective function is:

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

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

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

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 $\min_{h \in \mathcal{U}_{\rm ad}} J(h)$ *does not have a global solution.*

Hint of the proof: The proof comprises three stages:

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

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

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

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

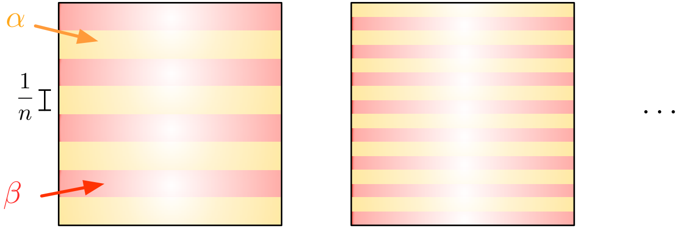
Step 3: One constructs a minimizing sequence of designs $h^n \in \mathcal{U}_{\rm ad}$:

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

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

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 a minimizing sequence h^n of conductivities.

Homogenization effect: *To get more optimized, 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 global solutions, for deep physical reasons.

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

- To ensure existence of an optimal shape, two techniques are usually employed:
  - Relaxation: the set $\mathcal{U}_{\text{ad}}$ 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 $\mathcal{U}_{\text{ad}}$ is restricted to, e.g. more regular designs.

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

Part II

Optimal control and parametric optimization problems

Derivative of the objective function (I)

Let us return to our (further simplified) problem:

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

where

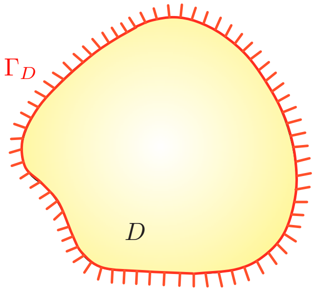
$$J(h) = \int_D j(u_h)\,\mathrm{d}x,$$

the set of admissible designs is:

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

and the temperature u_h is the solution in $H^1_0(D)$ to:

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



Remark Again, for simplicity, we omit constraints on h or u_h.

Derivative of the objective function (II)

For a fixed design $h \in \mathcal{U}_{\mathrm{ad}}$,

- One variational formulation characterizing u_h is:

$$\text{Search for } u_h \in H^1_0(D) \text{ s.t. } \forall v \in H^1_0(D), \quad \int_D h \nabla u_h \cdot \nabla v \, \mathrm{d}x = \int_D f v \, \mathrm{d}x.$$

- This problem has a unique solution $u_h \in H^1_0(D)$, which satisfies:

$$||u_h||_{H^1_0(D)} \leq C ||f||_{L^2(D)},$$

for some constant $C > 0$, owing to the Lax-Milgram theorem.

Derivative of the objective function (III)

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

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. Identify a descent direction $\widehat{h}^n$ for $J(h)$ from h^n, i.e. a direction such that $J'(h^n)(\widehat{h}) < 0$;
3. Select an appropriate time step $\tau^n > 0$;
4. Update the design as: $h^{n+1} = h^n + \tau^n \widehat{h}^n$.

- The cornerstone any such method is the calculation of the derivative of $J(h)$.
- This task is uneasy since $J(h)$ depends on h in a complicated way – via the solution u_h to a PDE whose coefficients depend on h.

Derivative of the objective function (IV)

Theorem 2.

The objective function

$$J(h) = \int_D j(u_h)\,\mathrm{d}x$$

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

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

where the adjoint state $p_h \in H^1_0(D)$ *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 (V)

Proof: The proof is divided into three steps:

1. Using the implicit function theorem, we prove that the state mapping
$$\mathcal{U}_{\mathrm{ad}} \ni h \longmapsto u_h \in H^1_0(D)$$
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. We calculate the derivative of $J(h)$ by using the chain rule.

3. We give a more convenient structure to this derivative, introducing an adjoint state p_h to eliminate the occurrence of $u_h'(\widehat{h})$.

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

For any $h \in \mathcal{U}_{\mathrm{ad}}$, u_h is the unique solution in $H^1_0(D)$ to the variational problem:
$$\forall v \in H^1_0(D), \;\; \int_D h \nabla u_h \cdot \nabla v \,\mathrm{d}x = \int_D fv \,\mathrm{d}x.$$

Derivative of the objective function (VI)

Let

$$\mathcal{F} : \mathcal{U}_{\rm ad} \times H^1_0(D) \to H^{-1}(D)$$

be the mapping defined by:

$$\mathcal{F}(h,u) : v \mapsto \int_D h \nabla u \cdot \nabla v \,{\rm d}x - \int_D fv \,{\rm d}x.$$

One verifies that

- $\mathcal{F}$ is a mapping of class $\mathcal{C}^1$;
- For given $h \in \mathcal{U}_{\rm ad}$, u_h is the unique solution u to the equation

$$\mathcal{F}(h,u) = 0.$$

- The differential of the partial mapping $u \mapsto \mathcal{F}(h,u)$ reads:

$$H^1_0(D) \ni \widehat{u} \longmapsto \left[v \mapsto \int_D h \nabla \widehat{u} \cdot \nabla v \,{\rm d}x \right] \in H^{-1}(D).$$

It is an isomorphism, owing to the Lax-Milgram theorem:

For all $g \in H^{-1}(D)$, there exists a unique $u \in H^1_0(D)$ s.t.

$$\forall v \in H^1_0(D), \int_D h \nabla u \cdot \nabla v \,{\rm d}x = \langle g, v \rangle_{H^{-1}(D), H^1_0(D)}.$$

Derivative of the objective function (VII)

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:

$$\forall v \in H_0^1(D), \int_D h \nabla u_h \cdot \nabla v \, \mathrm{d}x = \int_D fv \, \mathrm{d}x.$$

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

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

and so, for all $\widehat{h} \in L^\infty(D)$, $u_h'(\widehat{h})$ is the unique solution in $H_0^1(D)$ to:

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

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:

$$\forall \widehat{h} \in L^\infty(D), \;\; J'(h)(\widehat{h}) = \int_D j'(u_h) u_h'(\widehat{h}) \, \mathrm{d}x.$$

- 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 $\widehat{h} \in L^\infty(D)$ 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 (IX)

Step 3: *Reformulation of $J'(h)$ using an adjoint state:*

The adjoint state p_h is the unique solution in $H^1_0(D)$ to the variational problem:

$$\forall v \in H^1_0(D), \;\; \int_D h \nabla p_h \cdot \nabla v \,\mathrm{d}x = -\int_D j'(u_h) v \,\mathrm{d}x,$$

to be compared with the variational formulation for $u_h'(\widehat{h}) \in H^1_0(D)$:

$$\forall v \in H^1_0(D), \;\; \int_D h \nabla u_h'(\widehat{h}) \cdot \nabla v \,\mathrm{d}x = -\int_D \widehat{h} \nabla u_h \cdot \nabla v \,\mathrm{d}x.$$

Then, we calculate:

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

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

About the adjoint state

- The adjoint state p_h satisfies

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

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.

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

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

which 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:

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

Part II

Optimal control and parametric optimization problems

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:

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

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

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

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

$$\forall \widehat{p} \in H_0^1(D), \; \int_D h \nabla u \cdot \nabla \widehat{p} \, \mathrm{d}x - \int_D f \widehat{p} \, \mathrm{d}x = 0;$$

this is the variational formulation for $u = u_h$.

- Imposing the partial derivative of $\mathcal{L}$ with respect to u to vanish amounts to

$$\forall \widehat{u} \in H_0^1(D), \; \int_D h \nabla p \cdot \nabla \widehat{u} \, \mathrm{d}x = - \int_D j'(u) \widehat{u} \, \mathrm{d}x;$$

since $u = u_h$, we recognize the variational formulation for $p = p_h$.

The formal method of Céa

- Recall that, for arbitrary $\widehat{p} \in H^1_0(D)$,

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

- Since we have assumed that $h \mapsto u_h$ is differentiable, the chain rule yields:

$$J'(h)(\widehat{h}) = \frac{\partial \mathcal{L}}{\partial h}(h, u_h, \widehat{p})(\widehat{h}) + \frac{\partial \mathcal{L}}{\partial u}(h, u_h, \widehat{p})(u_h'(\widehat{h})).$$

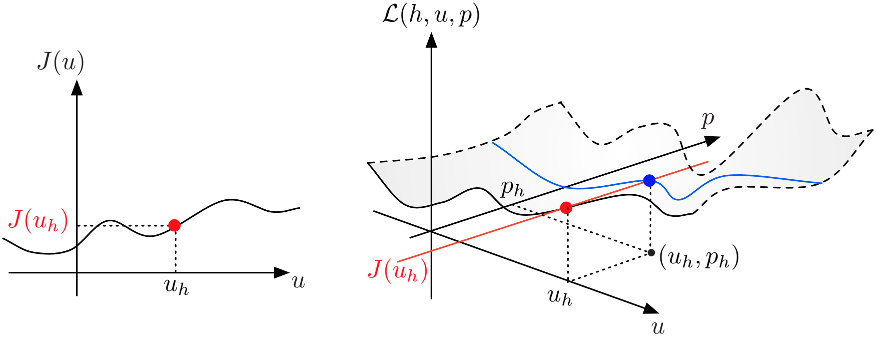
- Now taking $\widehat{p} = p_h$, the last term in the above right-hand side vanishes:

$$J'(h)(\widehat{h}) = \frac{\partial \mathcal{L}}{\partial h}(h, u_h, p_h)(\widehat{h}).$$

- The above derivative is the derivative of the mapping $h \mapsto \int_D h \nabla u \cdot \nabla p \, \mathrm{d}x$ evaluated at $u = u_h$ and $p = p_h$:

$$J'(h)(\widehat{h}) = \int_D \widehat{h} \nabla u_h \cdot \nabla p_h \, \mathrm{d}x.$$

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 (u_h, p_h), which is easy to differentiate with respect to h.

Part II

Optimal control and parametric optimization problems

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 coercive bilinear form on V given by: $a(u,v) = \int_D \nabla u \cdot \nabla v \, \mathrm{d}x$;
  - $\ell(\cdot)$ is the linear form on V defined by: $\ell(v) = \int_D f v \, \mathrm{d}x$.

- 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 consists in searching for an approximation u_h to h inside a finite-dimensional subspace $V_h \subset V$.

- The exact variational problem is replaced by:

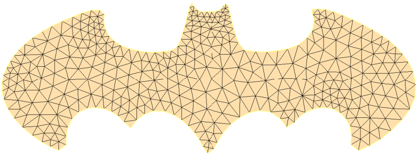
$$\boxed{\text{Search for } u_h \in V_h \text{ s.t. } \forall v_h \in V_h, \; a(u_h, v_h) = \ell(v_h),}$$

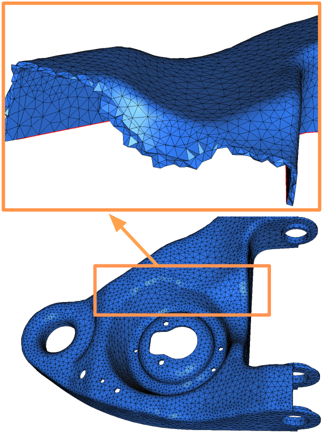
  which is also well-posed owing to the Lax-Milgram theorem.

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

Meshing the physical domain (I)

In practice, the domain D is discretized by means of a mesh $\mathcal{T}$, i.e. a covering by simplices (triangles in 2d, tetrahedra in 3d).





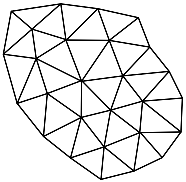
Meshing the physical domain (II)

A mesh $\mathcal{T}$ is defined by the datum of:

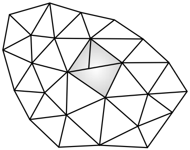
- A set of vertices $\{a_i\}_{i=1,\dots,N_V}$;
- A set of (open) simplices $\{T_j\}_{j=1,\dots,N_T}$, with vertices in $\{a_i\}$.

We also require that the mesh $\mathcal{T}$ be:

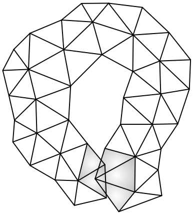
- Valid: For all simplices T_i, T_j with $i \neq j$, $T_i \cap T_j = \emptyset$.
- Conforming: For all simplices T_i, T_j, the intersection $\overline{T_i} \cap \overline{T_j}$ is either a vertex, or an edge, or a triangle (or a tetrahedron in 3d) of $\mathcal{T}$.



Valid, conforming mesh



Non conforming mesh



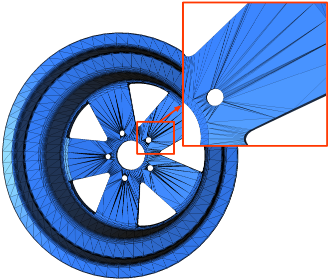
Invalid mesh

Meshing the physical domain (III)

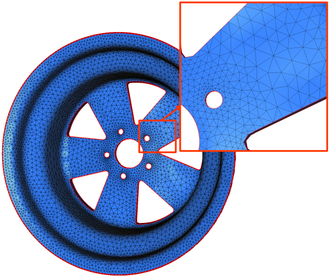
- It is often crucial in applications that $\mathcal{T}$ have good quality, i.e. that its elements be close to equilateral.
- The quality of a simplex T, with edges a_j can be evaluated e.g. by the function:

$$Q(T) = \alpha \frac{\mathrm{Vol}(T)}{\left(\sum_{j=1}^{d(d+1)/2} |a_j|^2 \right)^{\frac{d}{2}}},$$

where $\alpha \in \mathbb{R}$ is such that $Q(T) = 1$ if T is equilateral and $Q(T) = 0$ if T is flat.



Bad quality mesh, with nearly flat elements



Good quality mesh, with almost regular elements

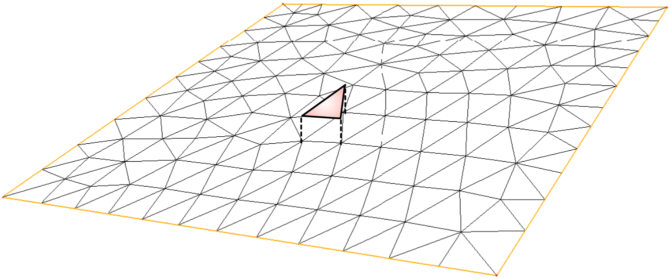
Construction of the finite element space V_h (I)

- In the finite element context, the mesh $\mathcal{T}_h$ is labelled by the size h of its elements.
- The finite element space V_h and its basis $\{\varphi_1, ..., \varphi_{N_h}\}$ are defined according to $\mathcal{T}_h$.

Example: the $\mathbb{P}_0$ Finite element method

- N_h is the number N_T of simplices $T_1, ..., T_{N_h}$ in the mesh;
- For $i = 1, ..., N_h$, φ_i is constant on each simplex $T \in \mathcal{T}_h$ and

$$\varphi_i(x) = 1 \text{ on } T_i \text{ and } \varphi_i(x) = 0 \text{ for } x \notin T_i.$$

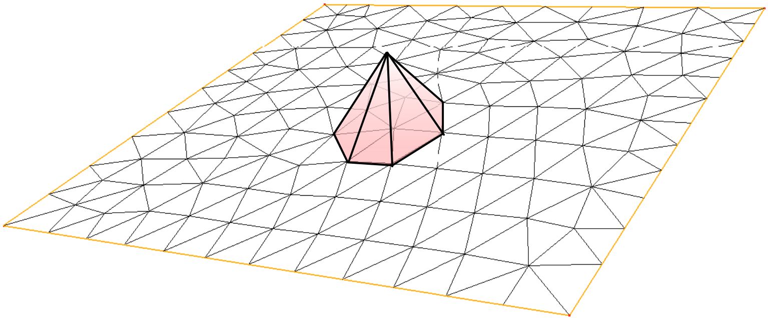


Construction of the finite element space V_h (II)

Example: the $\mathbb{P}_1$ Finite element method

- N_h is the number N_V 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:

$$u_h = \sum_{j=1}^{N_h} u_j \varphi_j,$$

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

$$KU = F,$$

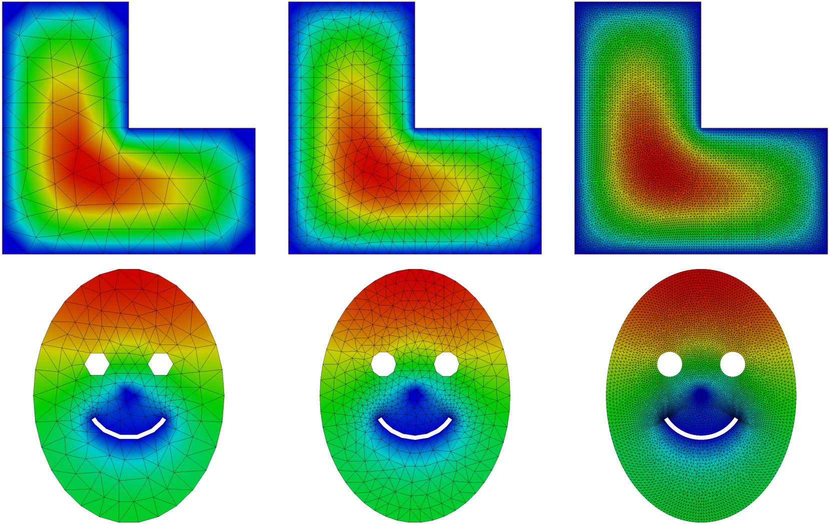
where

- $U = \begin{pmatrix} u_1 \\ \vdots \\ u_{N_h} \end{pmatrix}$ is the vector of unknowns,
- K is the stiffness matrix, defined by its entries:

$$K_{ij} \ = a(\varphi_j, \varphi_i), \quad i, j, = 1, \ldots, N_h;$$

- 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 $\mathcal{T}$.

Some practical aspects about the finite element method

- In practice, the discrete finite element system

$$KU = F$$

is a large $N_h \times N_h$ linear system, which is sparse.

- In realistic examples, its resolution can only be achieved thanks to iterative methods, such as the Conjugate Gradient algorithm, GMRES, etc.

- The numerical efficiency of such methods depends on the condition number of the matrix K, which is directly related to the quality of the computational mesh.

- The resolution of this system can also take advantage of recent Domain Decomposition methods.

- In shape optimization algorithms, such systems have to be solved multiple times: this is the main source of computational burden.

Final remarks about the finite element method

- The Finite Element 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 reference monographs [All] and [ErnGue].

Part II

Optimal control and parametric optimization problems

Refresher: differential and gradient (I)

Definition 1.

Let $(X, ||\cdot||_X)$ be a Banach space. A real-valued function $F : X \to \mathbb{R}$ is differentiable at $u \in X$ if there exists a linear, continuous mapping $F'(u) : X \to \mathbb{R}$ such that:

$$F(u+v) = F(u) + F'(u)(v) + \mathrm{o}(||v||), \text{ where } \frac{\mathrm{o}(||v||_X)}{||v||_X} \xrightarrow{v \to 0} 0.$$

The linear mapping $F'(u) \in X^*$ is the differential, or Fréchet derivative of F at u.

Definition 2.

If in addition X is a Hilbert space $(H, \langle \cdot, \cdot \rangle_H)$, the Riesz representation theorem allows to identify the derivative $F'(u)$ with an element $\nabla F(u) \in H$:

$$\forall v \in H, \; F'(u)(v) = \langle \nabla F(u), v \rangle_H;$$

$\nabla F(u)$ is called the gradient of F at u.

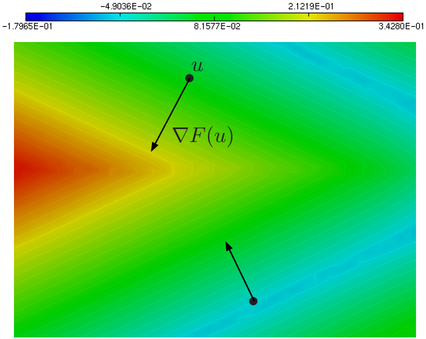
Refresher: differential and gradient (II)

Physical interpretation: If F is differentiable at $u \in H$, it holds, for "small" $\tau > 0$:

$$\forall \widehat{u} \in H, \ ||\widehat{u}||_H \leq 1, \quad F(u + \tau \widehat{u}) \approx F(u) + \tau \langle \nabla F(u), \widehat{u} \rangle_H, \\ \leq F(u) + \tau ||\nabla F(u)||_H,$$

where equality holds if and only if $\widehat{u} = \frac{\nabla F(u)}{||\nabla F(u)||_H}$ (Cauchy-Schwarz inequality).

$\Rightarrow$ $\nabla F(u)$ (resp. $-\nabla F(u)$) is the best ascent (resp. descent) direction for F from u.



Some isolines of a function $F : \mathbb{R}^2 \to \mathbb{R}$ and the gradient $\nabla F(u) \in \mathbb{R}^2$ at some point $u \in \mathbb{R}^2$.

The gradient algorithm (I)

In a Hilbert space H, we consider the unconstrained minimization problem:

$$\min_{h \in H} J(h),$$

where $J(h)$ is a differentiable function.

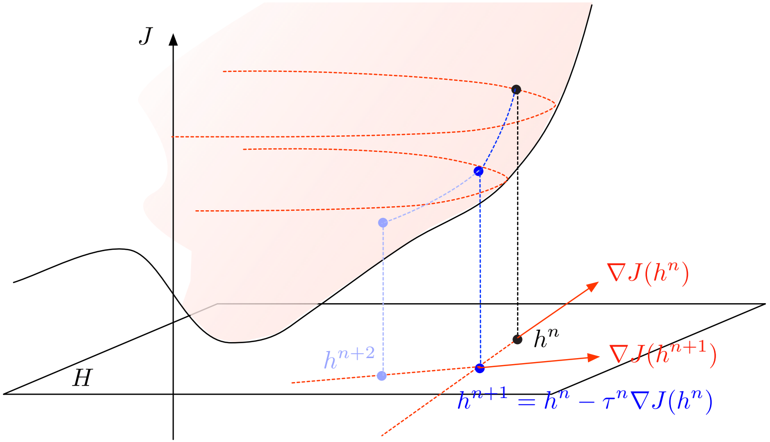
Initialization: Start from an initial design h^0.

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

1. Calculate the derivative $J'(h^n)$ of J at h^n and the gradient $\nabla J(h^n) \in H$; infer a descent direction $\widehat{h^n} = -\nabla J(h^n)$.
2. Take a suitably small time step $\tau^n > 0$ such that:
$$J(h^n + \tau^n \widehat{h^n}) < J(h^n).$$
3. The new iterate is $h^{n+1} = h^n + \tau^n \widehat{h^n}$.

Return: h^n.

The gradient algorithm (II)



The gradient algorithm proceeds by successive steps in the negative direction of the gradient of $J(h)$.

The augmented Lagrangian algorithm (I) [NoWri]

- Let us now consider the equality-constrained problem

$$\min_{h \in H} J(h) \text{ s.t. } C(h) = 0,$$

where $J : H \to \mathbb{R}$ and $C : H \to \mathbb{R}$ are differentiable.

- One possibility is to replace this problem with the unconstrained one:

$$\min_{h \in H} J(h) + \ell C(h),$$

where $J(h)$ is penalized by the constraint $C(h)$, using a fixed weight $\ell > 0$.

- In practice, the "suitable" value ℓ^* for ℓ, i.e. that driving the optimization process to the desired level of constraint $C(h) = 0$, is estimated after a few trial and errors.

- This value ℓ^* can be interpreted as the Lagrange multiplier associated to the constraint $C(h) = 0$ at the obtained local minimum.

The augmented Lagrangian algorithm (II)

The augmented Lagrangian algorithm reduces the resolution of a constrained optimization problem to a series of unconstrained ones, with updated parameters.

Initialization: Start from an initial design h^0, initial parameters ℓ^0, b^0.

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

1. Solve the unconstrained optimization problem:

$$\min_{h \in H} \; J(h) + \ell^n C(h) + \frac{b^n}{2} C(h)^2,$$

   starting from h^n to obtain h^{n+1}.

2. Update the optimization parameters via:

$$\ell^{n+1} = \ell^n + b^n C(h^n), \text{ and } b^{n+1} = \begin{cases} \alpha b^n & \text{if } b < b_{\max}, \\ b^n & \text{otherwise.} \end{cases}$$

- ℓ^n and b^n are updated so that the constraint $C(h) = 0$ holds at convergence;
- ℓ^n converges to the optimal Lagrange multiplier for the constraint $C(h) = 0$;
- b^n is a weight for the quadratic penalization of the constraint function $C(h)$.

The augmented Lagrangian algorithm (III)

The following "pragmatic" version involves fewer (costly) evaluations of $J(h)$, $C(h)$, and the derivatives $J'(h)$, $C'(h)$.

Initialization: Start from an initial design h^0, initial parameters ℓ^0, b^0.

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

1. Calculate a descent direction $\widehat{h^n}$ for the functional:
$$h \mapsto \mathcal{L}(h, \ell^n, b^n) := J(h) + \ell^n C(h) + \frac{b^n}{2} C(h)^2.$$
2. Select a suitably small time step so that:
$$\mathcal{L}(h^n + \tau^n \widehat{h^n}, \ell^n, b^n) < \mathcal{L}(h^n, \ell^n, b^n).$$
3. Update the design via:
$$h^{n+1} = h^n + \tau^n \widehat{h^n}.$$
4. Update the optimization parameters via:
$$\ell^{n+1} = \ell^n + b^n C(h^{n+1}), \text{ and } b^{n+1} = \begin{cases} \alpha b^n & \text{if } b < b_{\max}, \\ b^n & \text{otherwise.} \end{cases}$$

Part II

Optimal control and parametric optimization problems

Numerical algorithms (I)

We solve the optimization problem:

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

in there:

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

A basic projected gradient algorithm then reads:

Initialization: Start from an initial design h^0,

For $n = 0, \dots$ **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 optimized 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:

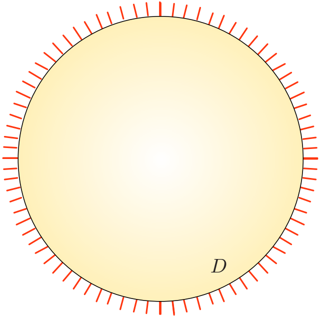
$$\min_{h \in \mathcal{U}_{\text{ad}}} J(h), \text{ where } J(h) = \int_D u_h \,\mathrm{d}x + \ell \int_D h \,\mathrm{d}x,$$

the temperature $u_h \in H^1_0(D)$ is the solution to:

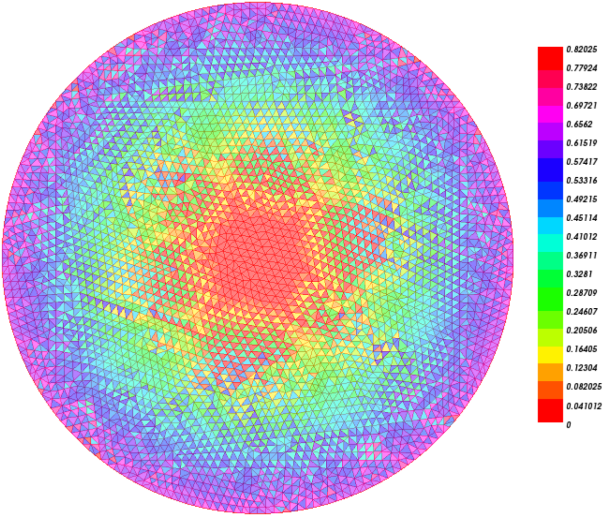
$$\begin{cases} -\mathrm{div}(h \nabla u_h) = 1 & \text{in } D, \\ u_h = 0 & \text{on } \partial D. \end{cases}$$

In other terms,

- 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:
$$J(h + \tau\widehat{h}) = J(h) + \tau J'(h)(\widehat{h}) + \mathrm{o}(\tau),$$
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
$$J'(h)(\widehat{h}) = \int_D \widehat{h} \nabla u_h \cdot \nabla p_h \, \mathrm{d}x$$
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.

- This choice is actually awkward: ∇u_h and ∇p_h are not very regular, and nor is $\widehat{h}$. In the theoretical framework, $\widehat{h}$ does not even belong to $L^\infty(D)$!

- 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 H be a Hilbert space with inner product $\langle \cdot, \cdot \rangle_H$.

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

$$\forall w \in H, \;\; \langle V, w \rangle_H = J'(h)(w) = \int_D w \nabla u_h \cdot \nabla p_h \, \mathrm{d}x.$$

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

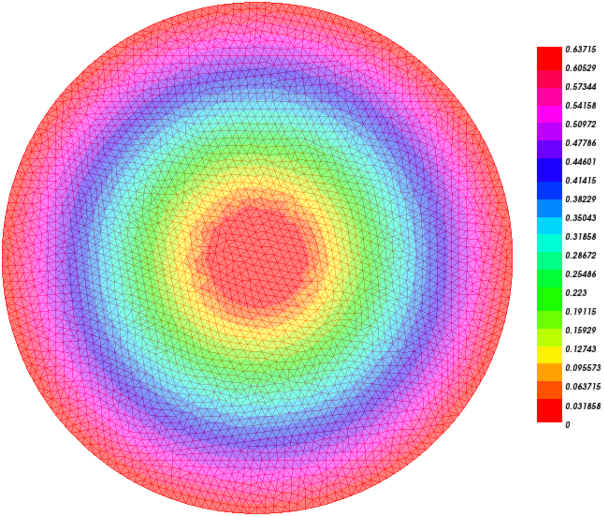
$$\begin{array}{rcl} J(h - \tau V) & = & J(h) - \tau J'(h)(V) + \mathrm{o}(\tau) \\ & = & J(h) - \tau \langle V, V \rangle_H + \mathrm{o}(\tau) \\ & < & J(h). \end{array}$$

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

$$H = H^1(D), \text{ and } \langle u, v \rangle_H = \int_D (\alpha^2 \nabla u \cdot \nabla v + uv) \, \mathrm{d}x,$$

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.

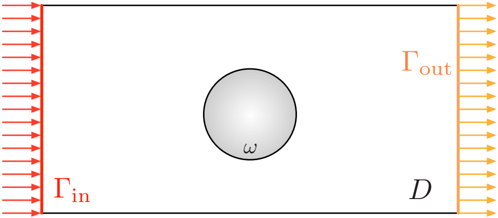
Another example: design of a "heat lens" (I)

As proposed in [Che], the problem

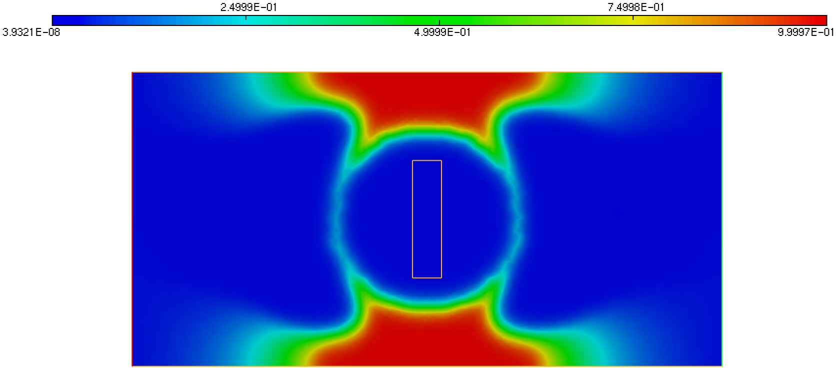
$$\min J(h) \text{ where } J(h) = \int_\omega \left| \alpha \frac{\partial u_h}{\partial x_1} \right|^2 \mathrm{d}x + \ell \int_D h \, \mathrm{d}x$$

is considered:

- The horizontal heat flux through a non optimizable region ω is minimized;
- A penalization on 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.

Technical appendix

The Lax Milgram theorem

In a Hilbert space H, let $a : H \times H \to \mathbb{R}$ be a bilinear form and $\ell : H \to \mathbb{R}$ be a linear form such that:

- a is continuous, i.e. there exists $M > 0$ such that:

$$\forall u, v \in H, \ |a(u,v)| \leq M||u||_H||v||_H.$$

- a is coercive, i.e. there exists $\alpha > 0$ such that:

$$\forall u \in H, \ \alpha||u||_H^2 \leq a(u,u).$$

- ℓ is continuous (i.e. ℓ belongs to the dual space H^*):

$$||\ell||_{H^*} := \sup_{\substack{v \in H \\ v \neq \mathbf{0}}} \frac{|\ell(v)|}{||v||_H} < \infty.$$

Theorem 3.

Under the above hypotheses, the variational problem

$$\textit{Search for } u \in H \textit{ s.t. for all } v \in H, \ a(u,v) = \ell(v)$$

has a unique solution $u \in H$, which depends continuously on ℓ:

$$||u||_H \leq \frac{M}{\alpha}||\ell||_{H^*}.$$

Fréchet and Gateaux derivatives

Several notions of derivative are available for a function $F : U \to V$ between two normed vector spaces $(U, ||\cdot||_U)$ and $(V, ||\cdot||_V)$.

Definition 3 (Fréchet differentiability).

- *A function $F : U \to V$ is called Fréchet differentiable at some point $x \in U$ if there exists a linear, continuous mapping $L_x : U \to V$ such that:*

$$F(x+v) = F(x) + L_x(v) + \mathrm{o}(||v||_U), \text{ where } \frac{||\mathrm{o}(||v||_U)||_V}{||v||_U} \xrightarrow{v \to 0} 0.$$

- *The mapping $v \mapsto L_x(v)$ is denoted by $v \mapsto F'(x)(v)$, or $\mathrm{d}_x F(v)$ and is called the differential or the Fréchet derivative of F at x.*

- *The function $F : U \to V$ is called Gateaux differentiable at $x \in U$ if for any direction $v \in U$, the following limit exists:*

$$\lim_{\substack{t \to 0 \\ t > 0}} \frac{F(x+tv) - F(x)}{t}.$$

Remark: The notion of Fréchet differentiability is stronger than that of Gateaux differentiability, which is a generalization of directional differentiability.

Fréchet derivatives: the "chain rule"

The chain rule is a *fundamental result*, which supplies the Fréchet derivative of the composite $G \circ F$ of two functions

$$F : U \to V \text{ and } G : V \to W$$

between three normed vector spaces $(U, ||\cdot||_U)$, $(V, ||\cdot||_V)$ and $(W, ||\cdot||_W)$.

Theorem 4 (Chain rule).

Let $x \in U$ be a point such that:

- *F is Fréchet differentiable at x;*
- *G is Fréchet differentiable at $F(x) \in V$.*

Then, the composite function $G \circ F : U \to W$ is Fréchet differentiable at x, and its Fréchet derivative $v \mapsto (G \circ F)'(x)(v)$ is the linear mapping defined by:

$$\forall v \in U, \ (G \circ F)'(x)(v) = G'(F(x))(F'(x)(v)).$$

The implicit function theorem

The implicit function theorem is a key result, ensuring the existence and smoothness of a solution $u = u_\theta$ to a parametrized, non linear equation of the form:

$$\mathcal{F}(\theta, u) = 0,$$

where u is the unknown and θ is a "parameter"; see [La], Chap. I, Th. 5.9.

Theorem 5 (Implicit function theorem).

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

$$\text{The derivative } \frac{\partial \mathcal{F}}{\partial u}(\theta_0, u_0) : E \to F \text{ is a linear isomorphism.}$$

Then there exist open subsets $\mathcal{V}' \subset \mathcal{V}$ of θ_0 in Θ and $U' \subset U$ of u_0 in E, and a mapping $g : \mathcal{V}' \to U'$ of class $\mathcal{C}^p$ satisfying the properties:

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

First-order necessary optimality conditions (I)

Let H be a Hilbert space, and let $J : H \to \mathbb{R}$ be a differentiable function; we consider the unconstrained minimization problem:

$$\min_{u \in H} J(u). \qquad \text{(UC)}$$

Definition 4.

A point $u \in H$ is a local minimizer for (UC) if there exists an open neighborhood $V \subset H$ containing u such that:

$$\forall v \in V, \; J(u) \leq J(v).$$

Theorem 6.

Let u be a local minimize for (UC); then:

$$\nabla J(u) = 0.$$

First-order necessary optimality conditions (II)

Proof: Let $h \in H$ be given; by the definition of u, it holds for $t > 0$ small enough:

$$J(u + th) \geq J(u), \text{ and so } \frac{J(u + th) - J(u)}{t} \geq 0.$$

Letting $t \to 0$, the differentiability of J yields:

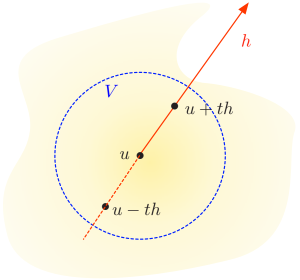
$$J'(u)(h) = \langle \nabla J(u), h \rangle \geq 0.$$

Replacing h by $-h$ in the previous argument yields the converse inequality

$$\langle \nabla J(u), h \rangle \leq 0,$$

which completes the proof. □

Remark The above proof uses in a crucial way that the point u in (UC) minimizes $J(v)$ (locally) in any direction $h \in H$.



First-order necessary optimality conditions (III)

Let H be a Hilbert space, and let $J : H \to \mathbb{R}$ and $C : H \to \mathbb{R}^p$ be differentiable functions; we consider the equality-constrained minimization problem:

$$\min_{h \in H} J(h) \text{ s.t. } C(h) = 0. \qquad \text{(EC)}$$

Definition 5.

A point $u \in H$ is a local minimizer for (EC) if there exists an open neighborhood $V \subset H$ containing u such that:

$$\forall v \in V \text{ s.t. } C(v) = 0, \; J(u) \leq J(v).$$

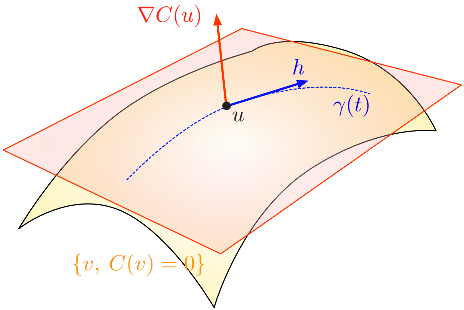
Theorem 7 (First-order necessary optimality conditions).

Let u be a local minimizer for (EC), and assume that the gradients $\nabla C_1(u), \ldots, \nabla C_p(u)$ are linearly independent. Then there exist Lagrange multipliers $\lambda_1, \ldots, \lambda_p \in \mathbb{R}$ such that:

$$\nabla J(u) + \sum_{i=1}^{p} \lambda_i \nabla C_i(u) = 0.$$

Hint of proof:

- The local optimality of u no longer implies that, for *arbitrary* $h \in H$ and t small enough,
$$J(u+th) \geq J(u).$$
- Such an inequality can only be written with directions h in the admissible space:
$$K(u) := \{h \in H, \text{ there exists } \varepsilon > 0 \text{ and a curve } \gamma : [-\varepsilon, \varepsilon] \to H \text{ s.t. } \gamma(0) = u,\ \gamma'(0) = h \text{ and } C(\gamma(t)) = 0 \text{ for } t > 0\}.$$
- $K(u)$ is a vector space, which rewrites, using the implicit function theorem:
$$K(u) = \bigcap_{i=1}^{p} \{\nabla C_i(u)\}^{\perp}.$$



First-order necessary optimality conditions (II)

- For any $h \in K(u)$, introducing a curve $\gamma(t)$ with the above properties:

$$J(\gamma(t)) \geq J(u), \text{ and so } \frac{J(\gamma(t)) - J(u)}{t} \geq 0.$$

  Taking limits, it follows,

$$\langle \nabla J(u), h \rangle \geq 0.$$

  Since $K(u)$ is a vector space, the same argument applies to $-h$, and so:

$$\langle \nabla J(u), h \rangle = 0.$$

- Hence, we have proved that

$$\forall h \in K(u) \;\; \langle \nabla J(u), h \rangle = 0, \text{ that is } \nabla J(u) \in \left(\bigcap_{i=1}^{p} \{\nabla C_i(u)\}^{\perp} \right)^{\perp}.$$

- Finally, using the general fact that, for arbitrary subsets $A_1, \ldots, A_p \subset H$,

$$(\mathrm{span}\,\{A_i, \;\; i = 1, \ldots, p\})^{\perp} = \bigcap_{i=1}^{p} A_i^{\perp},$$

  the desired result follows.

First-order necessary optimality conditions (III)

Interpretation (when $p = 1$): The above optimality condition implies that:

- Either $\nabla J(u) = 0$, which is the necessary first-order optimality condition for u to be an unconstrained minimizer of $J(v)$.
- Or $\lambda \neq 0$, and so,

$$\nabla C(u) = -\frac{1}{\lambda}\nabla J(u).$$

- "At first order", a direction $h \in H$ such that $J(u+th) < J(u)$ for small $t > 0$, has a non zero coordinate along $\nabla J(u)$:

$$h = \alpha \nabla J(u) + v, \text{ where } v \perp \nabla J(u), \alpha < 0.$$

- Alternatively, h rewrites:.

$$h = \beta \nabla C(u) + w, \text{ where } w \perp \nabla C(u), \beta \neq 0.$$

- Hence, $C(u+th) \neq 0$, so that $u + th$ is not an admissible point in (EC).

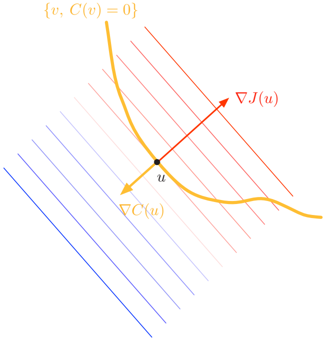


Illustration when $H = \mathbb{R}^2$, $p = 1$ and J is an affine function, whose isolines are depicted. At a local optimum u of (EC), $\nabla J(u)$ and $\nabla C(u)$ are aligned.

Bibliography

References I

[All] G. Allaire, *Conception optimale de structures*, Mathématiques & Applications, **58**, Springer Verlag, Heidelberg (2006).

[All2] G. Allaire, *Shape optimization by the homogenization method*, Springer Verlag, (2012).

[All] G. Allaire, *Analyse Numérique et Optimisation*, Éditions de l'École Polytechnique, (2012).

[Bre] H. Brezis, *Functional analysis, Sobolev spaces and partial differential equations*, Springer Science & Business Media, (2010).

[Che] A. Cherkaev, *Variational methods for structural optimization*, vol. 140, Springer Science & Business Media, 2012.

[ErnGue] A. Ern and J.-L. Guermond, *Theory and Practice of Finite Elements*, Springer, (2004).

[FreyGeo] P.J. Frey and P.L. George, *Mesh Generation : Application to Finite Elements*, Wiley, 2nd Edition, (2008).

References II

[HenPi] A. Henrot and M. Pierre, *Variation et optimisation de formes, une analyse géométrique*, Mathématiques et Applications 48, Springer, Heidelberg (2005).

[La] S. Lang, *Fundamentals of differential geometry*, Springer, (1991).

[NoWri] J. Nocedal and S.J. Wright, *Numerical Optimization*, Springer Science, (1999).

[Mu] F. Murat, *Contre-exemples pour divers problèmes où le contrôle intervient dans les coefficients*, Annali di Matematica Pura ed Applicata, 112, 1, (1977), pp. 49–68.