OPTIMAL DESIGN OF STRUCTURES (MAP 562)

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CHAPTER VI

GEOMETRIC OPTIMIZATION

Geometric optimization of a membrane

A membrane is occupying a variable domain Ω in $\mathbb{R}^N$ with boundary

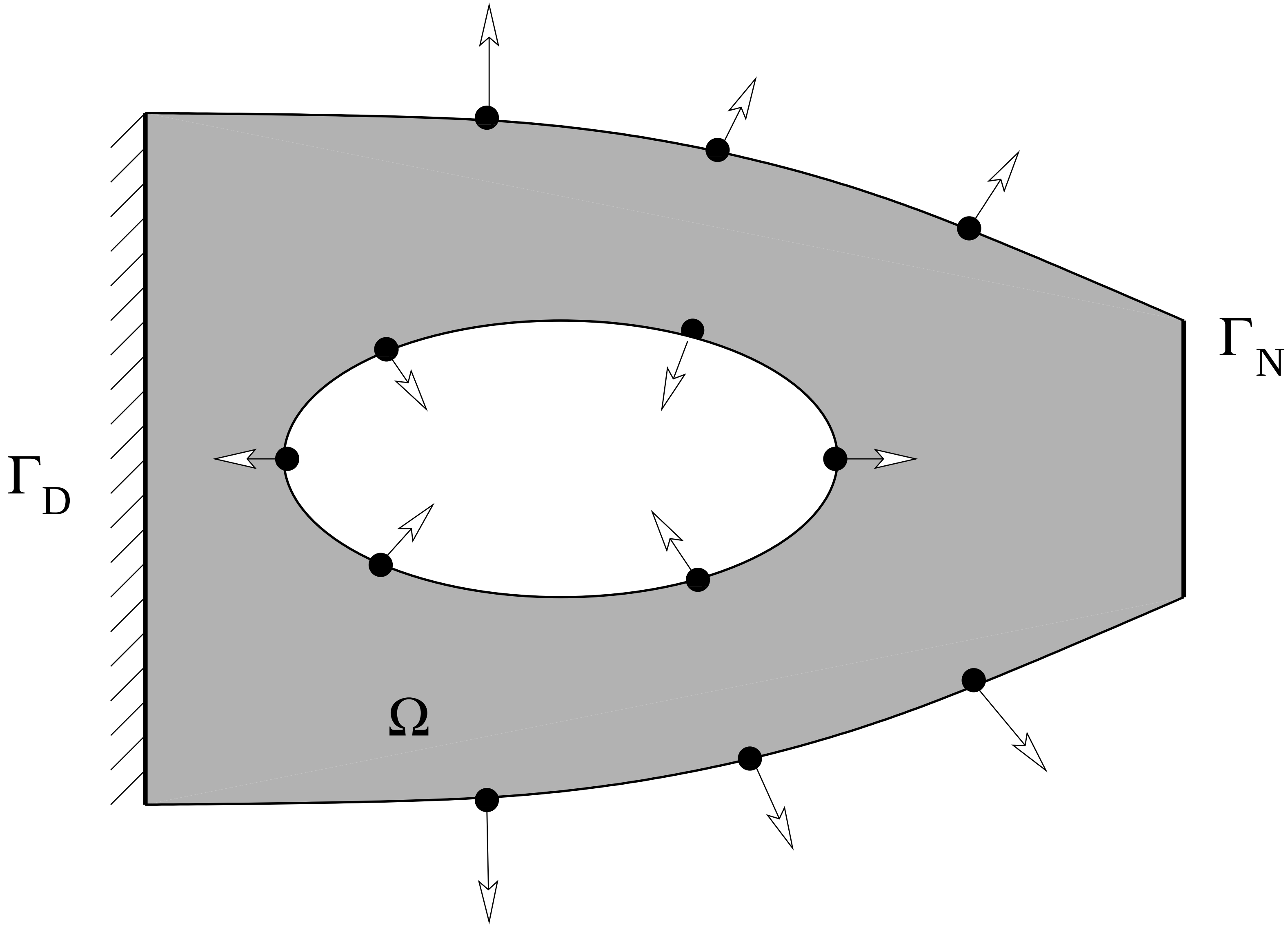
$$\partial\Omega = \Gamma \cup \Gamma_N \cup \Gamma_D,$$

where $\Gamma \neq \emptyset$ is the variable part of the boundary, $\Gamma_D \neq \emptyset$ is a fixed part of the boundary where the membrane is clamped, and $\Gamma_N \neq \emptyset$ is another fixed part of the boundary where the loads $g \in L^2(\Gamma_N)$ are applied.

$$\begin{cases} -\Delta u = 0 & \text{in } \Omega \\ u = 0 & \text{on } \Gamma_D \\ \frac{\partial u}{\partial n} = g & \text{on } \Gamma_N \\ \frac{\partial u}{\partial n} = 0 & \text{on } \Gamma \end{cases}$$

(No bulk forces to simplify)

Boundary variation in geometric optimization



Shape optimization of a membrane

Geometric shape optimization problem

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

We must defined the set of admissible shapes $\mathcal{U}_{ad}$. That is the main difficulty.

Examples:

☞ Compliance or work done by the load (rigidity measure)

$$J(\Omega) = \int_{\Gamma_N} g u \, ds$$

☞ Least square criterion for a target displacement $u_0 \in L^2(\Omega)$

$$J(\Omega) = \int_{\Omega} |u - u_0|^2 dx$$

where u depends on Ω through the state equation.

6.2 Existence results

In full generality, there does not exist any optimal shape !

☞ Existence under a geometric constraint.

☞ Existence under a topological constraint.

☞ Existence under a regularity constraint.

☞ Counter-example in the absence of these conditions.

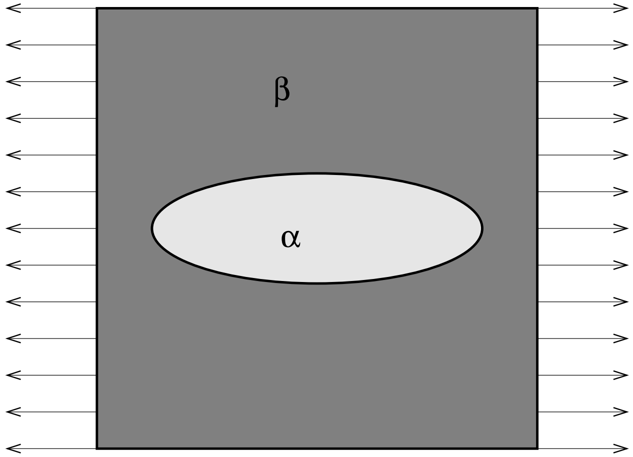
related questions:

☞ How to pose the problem ? How to parametrize shapes ?

☞ Calculus of variations for shapes.

☞ Mathematical framework for establishing numerical algorithms.

6.2.1 Counter-example of non-existence



Let $D =]0;1[\times]0;L[$ be a rectangle in $\mathbb{R}^2$. We fill D with a mixture of two materials, homogeneous isotropic, characterized by an elasticity coefficient β for the strong material, and α for the weak material (almost like void) with $\beta >> \alpha > 0$. We denote by $\chi(x) = 0, 1$ the **characteristic function** of the weak phase α, and we define

$$a_\chi(x) = \alpha\chi(x) + \beta(1 - \chi(x)).$$

(Other possible interpretation: variable thickness which can take only two values.)

State equation:

$$\begin{cases} -\operatorname{div}(a_\chi \nabla u_\chi) = 0 & \text{in } D \\ a_\chi \nabla u_\chi \cdot n = e_1 \cdot n & \text{on } \partial D \end{cases}$$

Uniform horizontal loading.

Objective function: compliance

$$J(\chi) = \int_{\partial D} (e_1 \cdot n) u_\chi ds$$

Admissible set: **no geometric or smoothness constraint, i.e.** $\chi \in L^\infty(D; \{0,1\})$. There is however a volume constraint

$$\mathcal{U}_{ad} = \left\{ \chi \in L^\infty(D; \{0,1\}) \text{ such that } \frac{1}{|D|} \int_D \chi(x)\, dx = \theta \right\},$$

otherwise the strong phase would always be prefered !

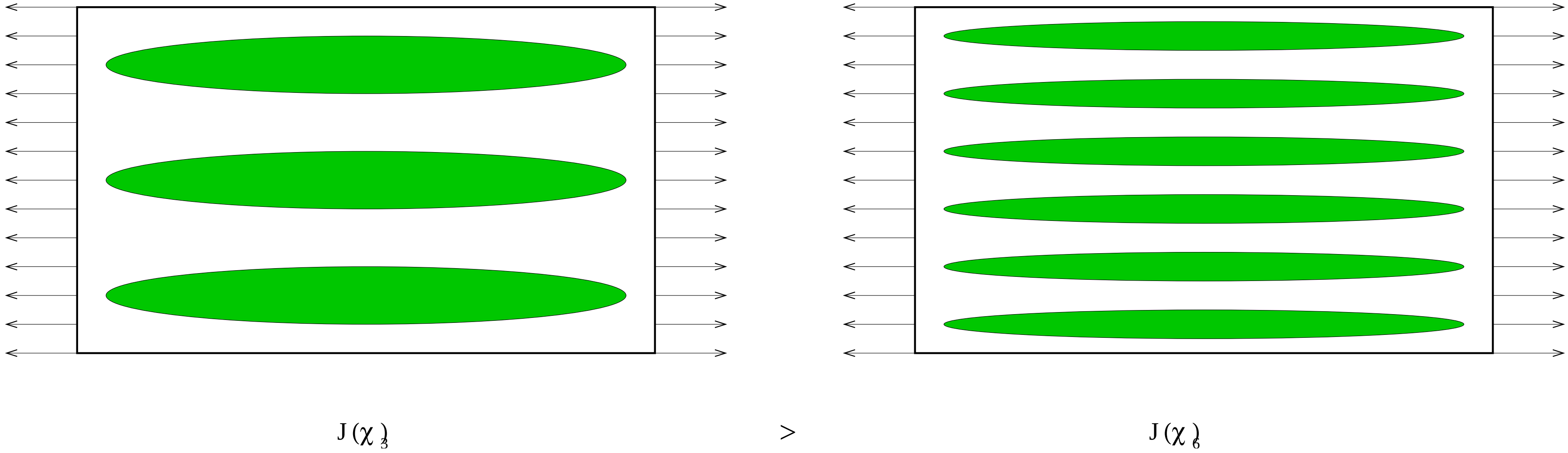
The shape optimization problem is:

$$\inf_{\chi \in \mathcal{U}_{ad}} J(\chi).$$

Non-existence

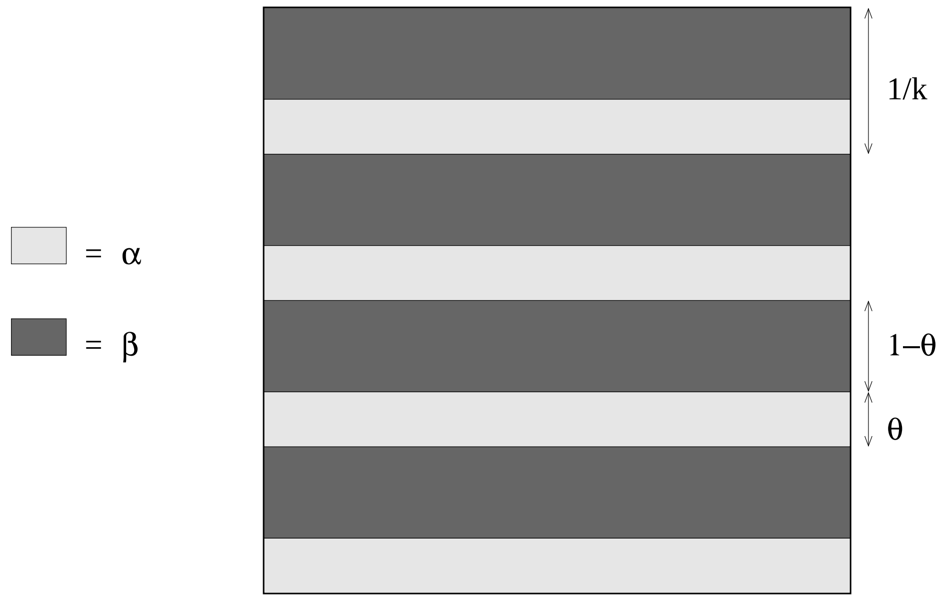
Proposition 6.2. If $0 < \theta < 1$, there does not exist an optimal shape in the set $\mathcal{U}_{ad}$.

Remark. Cause of non-existence = lack of geometric or smoothness constraint on the shape boundary.



Many small holes are better than just a few bigger holes !

Mechanical intuition



Minimizing sequence $k \to +\infty$: k rigid fibers, aligned in the principal stress e_1, and uniformly distributed. To achieve a uniform boundary condition, the fibers must be finer and finer and alternate more and more weak and strong ones.

This is the main idea of a minimizing sequence which never achieves the minimum.

Existence theories under a geometric condition

One can prove existence theorems underr various regularity or topological constraints.

1. Uniform cone condition (D. Chenais).
2. Uniform bound on the number of holes in 2-d (V. Sverak, A. Chambolle).
3. Uniform regularity.

In each case the goal is to prevent the oscillating behavior of minimizing sequences.

Existence under a regularity condition

Mathematical framework for shape deformation based on diffeomorphisms applied to a reference domain Ω_0 (useful to compute a gradient too).

A space of diffeomorphisms (or smooth one-to-one map) in $\mathbb{R}^N$

$$\mathcal{T} = \left\{ T \text{ such that } (T - \text{ Id}) \text{ and } (T^{-1} - \text{ Id}) \in W^{1,\infty}(\mathbb{R}^N; \mathbb{R}^N) \right\}.$$

(They are perturbations of the identity Id: $x \to x$.)

Definition of $W^{1,\infty}(\mathbb{R}^N; \mathbb{R}^N)$. Space of Lipschitzian vectors fields:

$$\phi : \begin{cases} \mathbb{R}^N & \to & \mathbb{R}^N \\ x & \to & \phi(x) \end{cases}$$

$$\|\phi\|_{W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)} = \sup_{x \in \mathbb{R}^N} \left(|\phi(x)|_{\mathbb{R}^N} + |\nabla\phi(x)|_{\mathbb{R}^{N\times N}} \right) < \infty$$

Remark: ϕ is continuous but its gradient is jut bounded. Actually, one can replace $W^{1,\infty}(\mathbb{R}^N; \mathbb{R}^N)$ by $C_b^1(\mathbb{R}^N; \mathbb{R}^N)$.

Space of admissible shapes

Let Ω_0 be a reference smooth open set.

$$\mathcal{C}(\Omega_0) = \{\Omega \text{ such that there exists } T \in \mathcal{T}, \Omega = T(\Omega_0)\}\,.$$

☞ Each shape Ω is parametrized by a diffeomorphism T (not unique !).

☞ All admissible shapes have the same topology.

☞ We define a pseudo-distance on $\mathcal{D}(\Omega_0)$

$$d(\Omega_1, \Omega_2) = \inf_{T \in \mathcal{T} | T(\Omega_1) = \Omega_2} \left(\|T - \mathrm{Id}\| + \|T^{-1} - \mathrm{Id}\| \right)_{W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)}\,.$$

☞ If Ω_0 is bounded, it is possible to use $C^1(\mathbb{R}^N;\mathbb{R}^N)$ instead of $W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$.

Existence theory

Space of admissible shapes

$$\mathcal{U}_{ad} = \left\{ \Omega \in \mathcal{C}(\Omega_0) \text{ such that } \Gamma_D \bigcup \Gamma_N \subset \partial\Omega \text{ and } |\Omega| = V_0 \right\}.$$

For a fixed constant $R > 0$, we introduce the smooth subspace

$$\mathcal{U}_{ad}^{reg} = \{ \Omega \in \mathcal{U}_{ad} \text{ such that } d(\Omega, \Omega_0) \leq R, \ \} \, .$$

Interpretation: in practice, it is a “feasability” constraint.

Theorem 6.11. The shape optimization problem

$$\inf_{\Omega \in \mathcal{U}_{ad}^{reg}} J(\Omega)$$

admits at least one optimal solution.

Remark. All shapes share the same topology in $\mathcal{U}_{ad}$. Furthermore, the shape boundaries in $\mathcal{U}_{ad}^{reg}$ cannot oscillate too much.

6.3 Shape differentiation

Goal: to compute a derivative of $J(\Omega)$ by using the parametrization based on diffeomorphisms T.

We restrict ourselves to diffeomorphisms of the type

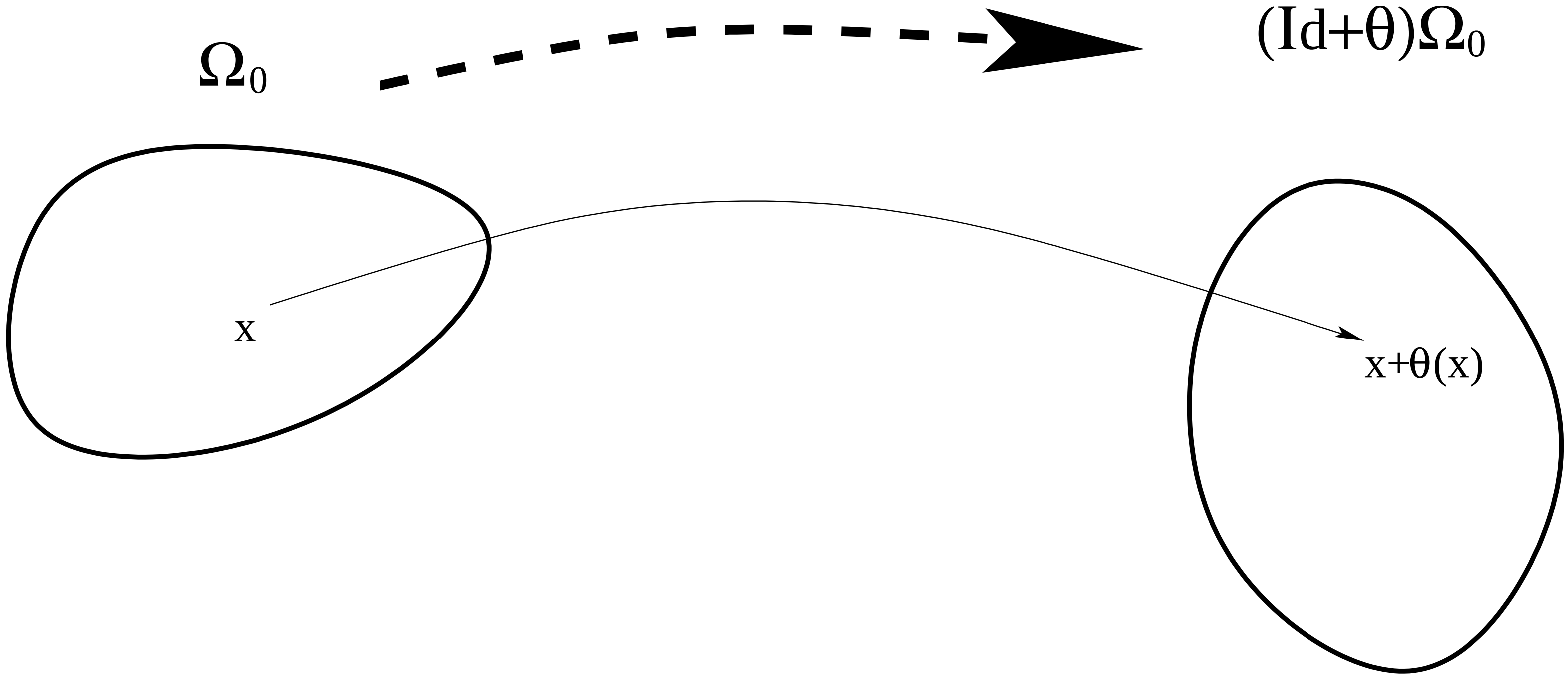
$$T = \text{Id} + \theta \quad \text{with} \quad \theta \in W^{1,\infty}(\mathbb{R}^N; \mathbb{R}^N)$$

Idea: we differentiate $\theta \to J\big((\text{Id} + \theta)\Omega_0\big)$ at 0.

Remark. This approach generalizes the Hadamard method of boundary shape variations along the normal: $\Omega_0 \to \Omega_t$ for $t \geq 0$

$$\partial\Omega_t = \left\{ x_t \in \mathbb{R}^N \mid \exists x_0 \in \partial\Omega_0 \mid x_t = x_0 + t\, g(x_0)\, n(x_0) \right\}$$

with a given incremental function g.



The shape $\Omega = (\,\mathrm{Id} + \theta)(\Omega_0)$ is defined by

$$\Omega = \{x + \theta(x) \mid x \in \Omega_0\}\,.$$

Thus $\theta(x)$ is a vector field which plays the role of the **displacement** of the reference domain Ω_0.

Lemma 6.13. For any $\theta \in W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$ satisfying $\|\theta\|_{W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)} < 1$, the map $T = \mathrm{Id} + \theta$ is one-to-one into $\mathbb{R}^N$ and belongs to the set $\mathcal{T}$.

Proof. Based on the formula

$$\theta(x) - \theta(y) = \int_0^1 (x-y)\cdot\nabla\theta\big(y + t(x-y)\big)\,dt\,,$$

we deduce that $|\,\theta(x) - \theta(y)\,| \leq \|\theta\|_{W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)}\,|\,x-y\,|$ and θ is a strict contraction. Thus, $T = \mathrm{Id} + \theta$ is one-to-one into $\mathbb{R}^N$.

Indeed, $\forall b \in \mathbb{R}^N$ the map $K(x) = b - \theta(x)$ is a contraction and thus admits a unique fixed point y, i.e., $b = T(y)$ and T is therefore one-to-one into $\mathbb{R}^N$.

Since $\nabla T = I + \nabla\theta$ (with $I = \nabla\,\mathrm{Id}$) and the norm of the matrix $\nabla\theta$ is strictly smaller than 1 ($\|I\| = 1$), the map ∇T is invertible. We then check that $(T^{-1} - \mathrm{Id}) \in W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$.

Definition of the shape derivative

Definition 6.15. Let $J(\Omega)$ be a map from the set of admissible shapes $\mathcal{C}(\Omega_0)$ into $\mathbb{R}$. We say that J is shape differentiable at Ω_0 if the function

$$\theta \to J\big((\,\mathrm{Id} + \theta)(\Omega_0)\big)$$

is Fréchet differentiable at 0 in the Banach space $W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$, i.e., there exists a linear continuous form $L = J'(\Omega_0)$ on $W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$ such that

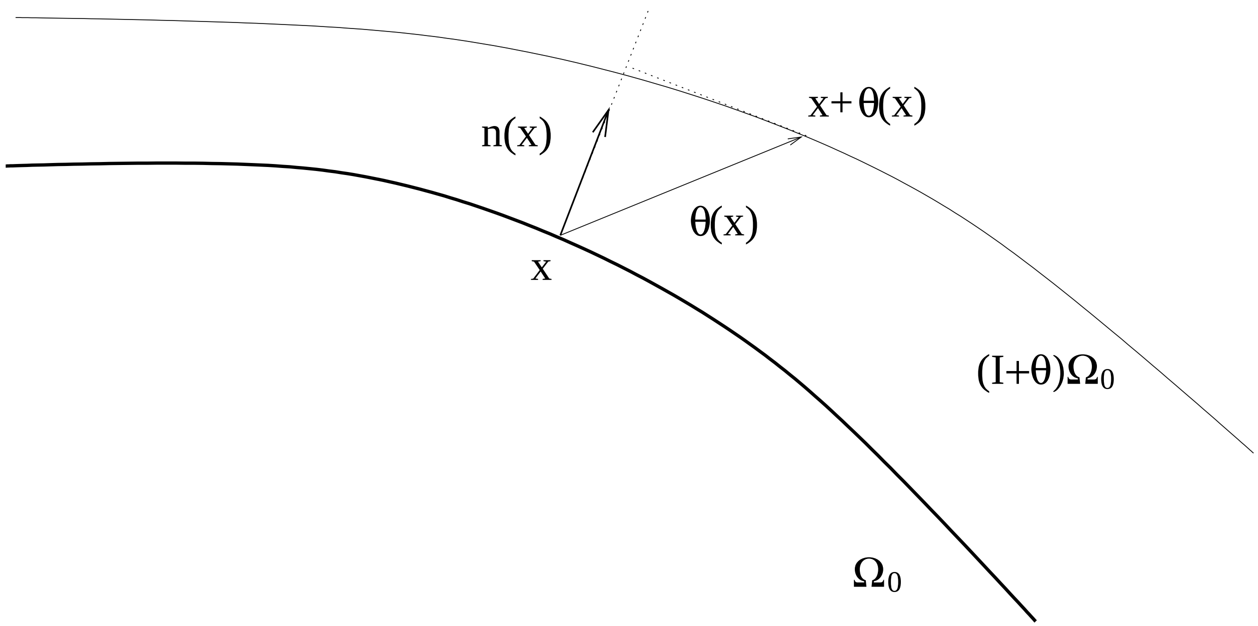
$$J\big((\,\mathrm{Id} + \theta)(\Omega_0)\big) = J(\Omega_0) + L(\theta) + o(\theta) \quad , \quad \text{with} \quad \lim_{\theta \to 0} \frac{|o(\theta)|}{\|\theta\|} = 0\,.$$

$J'(\Omega_0)$ is called the shape derivative and $J'(\Omega_0)(\theta)$ is a directional derivative.

The directional derivative $J'(\Omega_0)(\theta)$ depends only on the **normal component of θ on the boundary** of Ω_0.

This surprising property is linked to the fact that the internal variations of the field θ does not change the shape Ω, i.e.,

$$\theta \in C_c^1(\Omega)^N \text{ and } \|\theta\| << 1 \ \Rightarrow (\,\mathrm{Id} + \theta)\Omega = \Omega.$$



Proposition 6.15. Let Ω_0 be a smooth bounded open set of $\mathbb{R}^N$. Let J be a differentiable map at Ω_0 from $\mathcal{C}(\Omega_0)$ into $\mathbb{R}$. Its directional derivative $J'(\Omega_0)(\theta)$ depends only on the normal trace on the boundary of θ, i.e.

$$J'(\Omega_0)(\theta_1) = J'(\Omega_0)(\theta_2)$$

if $\theta_1, \theta_2 \in C^1(\mathbb{R}^N; \mathbb{R}^N)$ satisfy

$$\theta_1 \cdot n = \theta_2 \cdot n \quad \text{on } \partial\Omega_0.$$

Proof. Take $\theta = \theta_2 - \theta_1$ and introduce the solution of

$$\begin{cases} \frac{dy}{dt}(t) = \theta\big(y(t)\big) \\ y(0) = x \end{cases}$$

which satisfies

$$y(t+t', x, \theta) = y(t, y(t', x, \theta), \theta) \quad \text{for any } t, t' \in \mathbb{R}$$
$$y(\lambda t, x, \theta) = y(t, x, \lambda\theta) \quad \text{for any } \lambda \in \mathbb{R}$$

The we define the one-to-one map from $\mathbb{R}^N$ into $\mathbb{R}^N$, $x \to e^{\theta}(x) = y(1, x, \theta)$, the inverse of which is $e^{-\theta}$, $e^0 = \text{Id}$, and $t \to e^{t\theta}(x)$ is the solution of the o.d.e.

Lemma 6.20. Let $\theta \in W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$ be such that $\theta \cdot n = 0$ on $\partial\Omega_0$. Then $e^{t\theta}(\Omega_0) = \Omega_0$ for all $t \in \mathbb{R}$.

Proof (by contradiction). Assume $\exists x \in \Omega_0$ such that the trajectory $y(t,x)$ escapes from Ω_0 (or conversely). Thus $\exists t_0 > 0$ such that $x_0 = y(t_0,x) \in \partial\Omega_0$.

Locally the boundary $\partial\Omega_0$ is parametrized by an equation $\phi(x) = 0$ and the normal is $n = n_0/|n_0|$ with $n_0 = \nabla\phi$ (defined around $\partial\Omega_0$).

We modify the vector field as $\tilde{\theta} = \theta - (\theta \cdot n)n$ to obtain a modified trajectory $\tilde{y}(t,x_0)$ such that, for any $t \geq t_0$,

$$\frac{d}{dt}\Big(\phi(\tilde{y}(t,x))\Big) = \frac{d\tilde{y}}{dt} \cdot \nabla\phi(\tilde{y}) = \tilde{\theta}(\tilde{y}) \cdot n|n_0| = 0$$

Since $\phi(\tilde{y}(t_0,x_0)) = 0$, we deduce $\phi(\tilde{y}(t,x_0)) = 0$, i.e., the trajectory $\tilde{y}$ stays on $\partial\Omega_0$. Since $\theta \cdot n = 0$ on $\partial\Omega_0$, $\tilde{y}$ is **also** a trajectory for the vector field θ. Uniqueness of the o.d.e.'s solution yields $\tilde{y}(t) = y(t) \in \partial\Omega_0$ for any t which is a contradiction with $x \in \Omega_0$.

Remark. The crucial point is that θ is tangent to the boundary $\partial\Omega_0$.

Proof of Proposition 6.15 (Ctd.)

Since $e^{t\theta}(\Omega_0) = \Omega_0$ for any $t \in \mathbb{R}$, the function J is constant along this path and

$$\frac{dJ\big(e^{t\theta}(\Omega_0)\big)}{dt}(0) = 0.$$

By the chain rule lemma we deduce

$$\frac{dJ\big(e^{t\theta}(\Omega_0)\big)}{dt}(0) = J'(\Omega_0)\left(\frac{de^{t\theta}}{dt}\right)(0) = J'(\Omega_0)\,(\theta) = 0,$$

because the path $e^{t\theta}(x)$ satisfies

$$\frac{de^{t\theta}(x)}{dt}(0) = \theta(x),$$

which yields the result by linearity in θ.

Review of known formulas

To compute shape derivatives we need to recall how to change variables in integrals.

Lemma 6.21. Let Ω_0 be an open set of $\mathbb{R}^N$. Let $T \in \mathcal{T}$ be a diffeomorphism and $1 \leq p \leq +\infty$. Then $f \in L^p\big(T(\Omega_0)\big)$ if and only if $f \circ T \in L^p(\Omega_0)$, and

$$\int_{T(\Omega_0)} f\,dx = \int_{\Omega_0} f \circ T \,|\det \nabla T\,|\,dx$$

$$\int_{T(\Omega_0)} f\,|\det(\nabla T)^{-1}\,|\,dx = \int_{\Omega_0} f \circ T\,dx.$$

On the other hand, $f \in W^{1,p}\big(T(\Omega_0)\big)$ if and only if $f \circ T \in W^{1,p}(\Omega_0)$, and

$$\big(\nabla f\big) \circ T = \big((\nabla T)^{-1}\big)^t\,\nabla(f \circ T).$$

(^{t} = adjoint or transposed matrix)

Change of variables in a boundary integral.

Lemma 6.23. Let Ω_0 be a smooth bounded open set of $\mathbb{R}^N$. Let $T \in \mathcal{T} \cap C^1(\mathbb{R}^N; \mathbb{R}^N)$ be a diffeomorphism and $f \in L^1\big(\partial T(\Omega_0)\big)$. Then $f \circ T \in L^1(\partial\Omega_0)$, and we have

$$\int_{\partial T(\Omega_0)} f\, ds = \int_{\partial\Omega_0} f \circ T \,|\det \nabla T\,| \; \left|\left((\nabla T)^{-1}\right)^t n\right|_{\mathbb{R}^N} ds,$$

where n is the exterior unit normal to $\partial\Omega_0$.

Examples of shape derivatives

Proposition 6.22. Let Ω_0 be a smooth bounded open set of $\mathbb{R}^N$, $f(x) \in W^{1,1}(\mathbb{R}^N)$ and J the map from $\mathcal{C}(\Omega_0)$ into $\mathbb{R}$ defined by

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

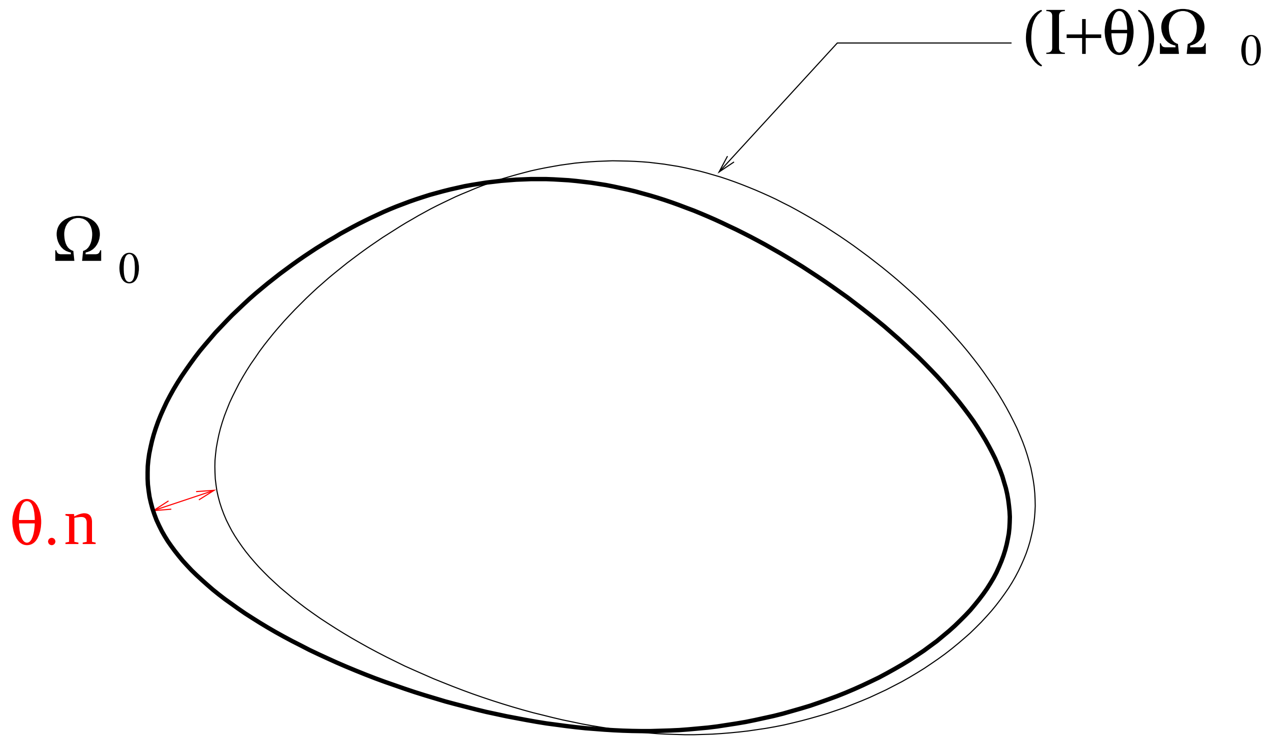
Then J is shape differentiable at Ω_0 and

$$J'(\Omega_0)(\theta) = \int_{\Omega_0} \operatorname{div}\big(\theta(x)\, f(x)\big)\, dx = \int_{\partial\Omega_0} \theta(x)\cdot n(x)\, f(x)\, ds$$

for any $\theta \in W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$.

Remark. To make sure the result is right, the safest way (but not the easiest) is to make a change of variables to get back to the reference domain Ω_0.

Intuitive proof



Surface swept by the transformation: difference between $(\,\mathrm{Id}+\theta)\Omega_0$ and Ω_0 $\approx \partial\Omega_0 \times \Big(\theta \cdot n\Big)$. Thus

$$\int_{(\,\mathrm{Id}+\theta)\Omega_0} f(x)\,dx = \int_{\Omega_0} f(x)\,dx + \int_{\partial\Omega_0} f(x)\theta\cdot n\,ds + o(\theta).$$

Proof. We rewrite $J(\Omega)$ as an integral on the reference domain Ω_0

$$J\big((\mathrm{Id}+\theta)\Omega_0\big) = \int_{\Omega_0} f\circ(\mathrm{Id}+\theta)\,|\det(\mathrm{Id}+\nabla\theta)|\,dx.$$

The functional $\theta \to \det(\mathrm{Id}+\nabla\theta)$ is differentiable from $W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$ into $L^\infty(\mathbb{R}^N)$ because

$$\det(\mathrm{Id}+\nabla\theta) = \det \mathrm{Id} + \mathrm{div}\theta + o(\theta) \quad \text{with} \quad \lim_{\theta\to 0} \frac{\|o(\theta)\|_{L^\infty(\mathbb{R}^N;\mathbb{R}^N)}}{\|\theta\|_{W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)}} = 0.$$

On the other hand, if $f(x)\in W^{1,1}(\mathbb{R}^N)$, the functional $\theta \to f\circ(\mathrm{Id}+\theta)$ is differentiable from $W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$ into $L^1(\mathbb{R}^N)$ because

$$f\circ(\mathrm{Id}+\theta)(x) = f(x) + \nabla f(x)\cdot\theta(x) + o(\theta) \quad \text{with} \quad \lim_{\theta\to 0} \frac{\|o(\theta)\|_{L^1(\mathbb{R}^N)}}{\|\theta\|_{W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)}} = 0.$$

By composition of these two derivatives we obtain the result.

Proposition 6.24. Let Ω_0 be a smooth bounded open set of $\mathbb{R}^N$, $f(x) \in W^{2,1}(\mathbb{R}^N)$ and J the map from $\mathcal{C}(\Omega_0)$ into $\mathbb{R}$ defined by

$$J(\Omega) = \int_{\partial\Omega} f(x)\, ds.$$

Then J is shape differentiable at Ω_0 and

$$J'(\Omega_0)(\theta) = \int_{\partial\Omega_0} \left(\nabla f \cdot \theta + f \big(\mathrm{div}\theta - \nabla\theta n \cdot n \big) \right) ds$$

for any $\theta \in W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$. By a (boundary) integration by parts this formula is equivalent to

$$J'(\Omega_0)(\theta) = \int_{\partial\Omega_0} \theta \cdot n \left(\frac{\partial f}{\partial n} + H f \right) ds,$$

where H is the mean curvature of $\partial\Omega_0$ defined by $H = \mathrm{div} n$.

Interpretation

Two simple examples:

- ☞ If $\partial\Omega_0$ is an hyperplane, then $H = 0$ and the variation of the boundary integral is proportional to the normal derivative of f.
- ☞ If $f \equiv 1$, then $J(\Omega)$ is the perimeter (in 2-D) or the surface (in 3-D) of the domain Ω and its variation is proportional to the mean curvature.

Proof. A change of variable yields

$$J\big((\mathrm{Id}+\theta)\Omega_0\big) = \int_{\partial\Omega_0} f\circ(\mathrm{Id}+\theta)|\det(\mathrm{Id}+\nabla\theta)|\ \left|\big((\mathrm{Id}+\nabla\theta)^{-1}\big)^t n\right|_{\mathbb{R}^N} ds.$$

We already proved that $\theta \to \det(\mathrm{Id}+\nabla\theta)$ and $\theta \to f\circ(\mathrm{Id}+\theta)$ are differentiables.

On the other hand, $\theta \to \big((\mathrm{Id}+\nabla\theta)^{-1}\big)^t n$ is differentiable from $W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$ into $L^\infty(\partial\Omega_0;\mathbb{R}^N)$ because

$$\big((\mathrm{Id}+\nabla\theta)^{-1}\big)^t n = n - (\nabla\theta)^t n + o(\theta) \quad \text{with} \quad \lim_{\theta\to 0}\frac{\|o(\theta)\|_{L^\infty(\partial\Omega_0;\mathbb{R}^N)}}{\|\theta\|_{W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)}} = 0.$$

By composition with the derivative of $g \to |g|_{\mathbb{R}^N}$, we deduce

$$\left|\big((\mathrm{Id}+\nabla\theta)^{-1}\big)^t n\right|_{\mathbb{R}^N} = 1-(\nabla\theta)^t n\cdot n+o(\theta) \quad \text{with} \quad \lim_{\theta\to 0}\frac{\|o(\theta)\|_{L^\infty(\partial\Omega_0)}}{\|\theta\|_{W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)}} = 0.$$

Composing these three derivatives leads to the result. The formula, including the mean curvature, is obtained by an integration by parts on the surface $\partial\Omega_0$.

"Strategy" of the course

Computing the shape derivative of the solution of a p.d.e. is not easy !

- We explain **once** the rigorous method for computing a shape derivative.
- It is a bit involved and quite calculus-intensive...
- At the end we shall introduce a formal simpler method which is the one to be used **in practice**.
- This formal method is called the Lagrangian method and you should learn how to use it !

6.3.3. Derivation of a function depending on the shape

Let $u(\Omega, x)$ be a function defined on the domain Ω.

There exist two notions of derivative:

1) Eulerian (or shape) derivative U

$$u((\mathrm{Id} + \theta)\Omega_0, x) = u(\Omega_0, x) + U(\theta, x) + o(\theta) \quad , \quad \text{with} \quad \lim_{\theta \to 0} \frac{\|o(\theta)\|}{\|\theta\|} = 0$$

OK if $x \in \Omega_0 \cap (\mathrm{Id} + \theta)\Omega_0$ (local definition, makes no sense on the boundary).

2) Lagrangian (or material) derivative Y

We define the **transported** function $\overline{u}(\theta)$ on Ω_0 by

$$\overline{u}(\theta, x) = u \circ (\mathrm{Id} + \theta) = u\Big((\mathrm{Id} + \theta)\Omega_0, x + \theta(x)\Big) \quad \forall\, x \in \Omega_0.$$

The Lagrangian derivative Y is obtained by differentiating $\overline{u}(\theta, x)$

$$\overline{u}(\theta, x) = \overline{u}(0, x) + Y(\theta, x) + o(\theta) \quad , \quad \text{with} \quad \lim_{\theta \to 0} \frac{\|o(\theta)\|}{\|\theta\|} = 0 \, ,$$

Differentiating $\overline{u} = u \circ (\,\mathrm{Id} + \theta)$, one can check that

$$Y(\theta, x) = U(\theta, x) + \theta(x) \cdot \nabla u(\Omega_0, x).$$

The Eulerian derivative, although being simpler, is very delicate to use and often not rigorous. For example, if $u \in H_0^1(\Omega)$, the space of definition varies with Ω... Equivalently what boundary condition should the derivative satisfy ?

We recommend to use the Lagrangian derivative to avoid mistakes.

Remark. Computations will be made with Y but the final result is stated with U (which is simpler).

Composed shape derivative

Proposition 6.28. Let Ω_0 be a smooth bounded open set of $\mathbb{R}^N$, and $u(\Omega) \in L^1(\mathbb{R}^N)$. We assume that the transported function $\overline{u}$ is differentiable at 0 from $W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$ into $L^1(\mathbb{R}^N)$, with derivative Y. Then

$$J(\Omega) = \int_\Omega u(\Omega)\, dx$$

is differentiable at Ω_0 and $\forall \theta \in W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$

$$J'(\Omega_0)(\theta) = \int_{\Omega_0} \big(u(\Omega_0)\, \mathrm{div}\theta + Y(\theta) \big)\, dx.$$

In other words, using the Eulerian derivative U,

$$J'(\Omega_0)(\theta) = \int_{\Omega_0} \big(U(\theta) + \mathrm{div}(u(\Omega_0)\theta) \big)\, dx.$$

Similarly, if $\overline{u}(\theta)$ is differentiable at 0 as a function from $W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$ into $L^1(\partial\Omega_0)$, then

$$J(\Omega) = \int_{\partial\Omega} u(\Omega)\, dx$$

is differentiable at Ω_0 and

$$J'(\Omega_0)(\theta) = \int_{\partial\Omega_0} \Big(u(\Omega_0)\left(\, \mathrm{div}\theta - \nabla\theta n \cdot n\right) + Y(\theta) \Big) ds.$$

In other words, using the Eulerian derivative U,

$$J'(\Omega_0)(\theta) = \int_{\partial\Omega_0} \left(U(\theta) + \theta \cdot n \left(\frac{\partial u(\Omega_0)}{\partial n} + H u(\Omega_0) \right) \right) dx.$$

6.3.4 Shape derivation of an equation

From now on, $u(\Omega)$ is the solution of a p.d.e. in the domain Ω.

Recall that

$$Y(\theta, x) = U(\theta, x) + \theta(x) \cdot \nabla u(\Omega_0, x).$$

The Eulerian derivative, although being simpler, is very delicate to use and often not rigorous. For example, if $u \in H^1_0(\Omega)$, the space of definition varies with Ω... Equivalently what boundary condition should the derivative satisfy ?

We recommend to use the Lagrangian derivative: after getting back to the fixed reference domain Ω_0 we differentiate with respect to θ. This is the safest and most rigorous way for computing the shape derivative of u, but the details can be tricky.

We shall later introduce a heuristic method which is simpler.

The results depend on the type of boundary conditions.

Dirichlet boundary conditions

For $f \in L^2(\mathbb{R}^N)$ we consider the boundary value problem

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

which admits a unique solution $u(\Omega) \in H_0^1(\Omega)$.

Its variational formulation is: find $u \in H_0^1(\Omega)$ such that

$$\int_\Omega \nabla u \cdot \nabla \phi \, dx = \int_\Omega f \phi \, dx \quad \forall \, \phi \in H_0^1(\Omega).$$

(Simplification with respect to the textbook since here $g = 0$.)

For $\Omega = (\,\mathrm{Id} + \theta)(\Omega_0)$ we define the change of variables

$$x = y + \theta(y) \quad y \in \Omega_0 \quad x \in \Omega.$$

Proposition 6.30. Let $u(\Omega) \in H_0^1(\Omega)$ be the solution and $\overline{u}(\theta) \in H_0^1(\Omega_0)$ be its transported function

$$\overline{u}(\theta)(y) = u(\Omega)(x) = u\Big((\,\mathrm{Id} + \theta)(\Omega_0)\Big) \circ (\,\mathrm{Id} + \theta)(y).$$

The functional $\theta \to \overline{u}(\theta)$, from $W^{1,\infty}(\mathbb{R}^N; \mathbb{R}^N)$ into $H^1(\Omega_0)$, is differentiable at 0, and its derivative in the direction θ, called Lagrangian derivative is

$$Y = \langle \overline{u}'(0), \theta \rangle$$

where $Y \in H_0^1(\Omega_0)$ is the unique solution of

$$\begin{cases} -\Delta Y = -\Delta\big(\theta \cdot \nabla u(\Omega_0)\big) & \text{in } \Omega_0 \\ Y = 0 & \text{on } \partial\Omega_0. \end{cases}$$

Proof. We perform the change of variables $x = y + \theta(y)$ with $y \in \Omega_0$ in the variational formulation

$$\int_\Omega \nabla u \cdot \nabla \phi \, dx = \int_\Omega f \phi \, dx \quad \forall \, \phi \in H_0^1(\Omega).$$

Take a test function $\phi = \psi \circ (\,\mathrm{Id} + \theta)^{-1}$, i.e., $\psi(y) = \phi(x)$. Recall that

$$\big(\nabla \phi\big) \circ (\,\mathrm{Id} + \theta) = \left((I + \nabla\theta)^{-1}\right)^t \nabla \Big(\phi \circ (\,\mathrm{Id} + \theta)\Big).$$

We obtain: find $\overline{u} \in H_0^1(\Omega_0)$ such that, for any $\psi \in H_0^1(\Omega_0)$,

$$\int_{\Omega_0} A(\theta) \nabla \overline{u} \cdot \nabla \psi \, dy = \int_{\Omega_0} f \circ (\,\mathrm{Id} + \theta)\, \psi \,|\det(\,\mathrm{Id} + \nabla\theta)| dy$$

with $A(\theta) = |\det(I + \nabla\theta)| (I + \nabla\theta)^{-1} \left((I + \nabla\theta)^{-1}\right)^t$.

We differentiate with respect to θ at 0 the variational formulation

$$\int_{\Omega_0} A(\theta)\nabla\overline{u}\cdot\nabla\psi\, dy = \int_{\Omega_0} f\circ(\,\mathrm{Id}+\theta)\,\psi\,|\,\det(\,\mathrm{Id}+\nabla\theta)|dy$$

where ψ is a function which does not depend on θ.

We already checked in the proof of Proposition 6.22 that the righ hand side is differentiable. Furthermore, the map $\theta \to A(\theta)$ is differentiable too because

$$A(\theta) = (1+\,\mathrm{div}\theta)I - \nabla\theta - (\nabla\theta)^t + o(\theta) \quad \text{with} \quad \lim_{\theta\to 0}\frac{\|o(\theta)\|_{L^\infty(\mathbb{R}^N;\mathbb{R}^{N^2})}}{\|\theta\|_{W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)}} = 0.$$

Since $\overline{u}(\theta = 0) = u(\Omega_0)$, we get

$$\int_{\Omega_0} \nabla Y \cdot \nabla \psi \, dy + \int_{\Omega_0} \Big(\operatorname{div}\theta \, I - \nabla\theta - (\nabla\theta)^t \Big) \nabla u(\Omega_0) \cdot \nabla \psi \, dy = \int_{\Omega_0} \operatorname{div}\Big(f\theta \Big) \psi \, dy$$

Since $\overline{u}(\theta) \in H_0^1(\Omega_0)$, its derivative Y belongs to $H_0^1(\Omega_0)$ too. Thus Y is a solution of

$$\begin{cases} -\Delta Y = \operatorname{div}\Big[\Big(\operatorname{div}\theta \, I - \nabla\theta - (\nabla\theta)^t \Big) \nabla u(\Omega_0) \Big] + \operatorname{div}\Big(f\theta \Big) & \text{in } \Omega_0 \\ Y = 0 & \text{on } \partial\Omega_0. \end{cases}$$

Recalling that $\Delta u(\Omega_0) = -f$ in Ω_0, and using the identity (true for any $v \in H^1(\Omega_0)$ such that $\Delta v \in L^2(\Omega_0)$)

$$\Delta \left(\nabla v \cdot \theta \right) = \operatorname{div}\Big((\Delta v)\theta - (\operatorname{div}\theta) \nabla v + \Big(\nabla\theta + (\nabla\theta)^t \Big) \nabla v \Big),$$

leads to the final result. (gotcha !)

Shape derivative U

Corollary 6.32. The Eulerian derivative U of the solution $u(\Omega)$, defined by formula

$$U = Y - \nabla u(\Omega_0) \cdot \theta,$$

is the solution in $H^1(\Omega_0)$ of

$$\begin{cases} -\Delta U = 0 & \text{in } \Omega_0 \\ U = -(\theta \cdot n) \frac{\partial u(\Omega_0)}{\partial n} & \text{on } \partial\Omega_0. \end{cases}$$

(Obvious proof starting from Y.)

We are going to recover **formally** this p.d.e. for U without using the knowledge of Y.

Let ϕ be a compactly supported test function in $\omega \subset \Omega$ for the variational formulation

$$\int_\omega \nabla u \cdot \nabla \phi \, dx = \int_\omega f \phi \, dx.$$

Differentiating with respect to Ω, neither the test function, nor the domain of integration depend on Ω. Thus it yields

$$\int_\omega \nabla U \cdot \nabla \phi \, dx = 0 \quad \Leftrightarrow \quad -\Delta U = 0.$$

To find the boundary condition we formally differentiate

$$\int_{\partial\Omega} u(\Omega)\psi \, ds = 0 \quad \forall \, \psi \in C^\infty(\mathbb{R}^N)$$

$$\Rightarrow \int_{\partial\Omega_0} U\psi \, ds + \int_{\partial\Omega_0} \left(\frac{\partial(u\psi)}{\partial n} + H u \psi \right) \theta \cdot n \, ds = 0$$

which leads to the correct result since $u = 0$ on $\partial\Omega_0$.

Remark. The direct computation of U is not always that easy !

Neumann boundary conditions

For $f \in H^1(\mathbb{R}^N)$ and $g \in H^2(\mathbb{R}^N)$ we consider the boundary value problem

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

which admits a unique solution $u(\Omega) \in H^1(\Omega)$.

Its variational formulation is: find $u \in H^1(\Omega)$ such that

$$\int_\Omega (\nabla u \cdot \nabla \phi + u\phi)\, dx = \int_\Omega f\phi\, dx + \int_{\partial\Omega} g\phi\, ds \quad \forall\, \phi \in H^1(\Omega).$$

Proposition 6.34. For $\Omega = (\,\mathrm{Id}+\theta)(\Omega_0)$ we define the change of variables

$$x = y + \theta(y) \quad y \in \Omega_0 \quad x \in \Omega.$$

Let $u(\Omega) \in H^1(\Omega)$ be the solution and $\overline{u}(\theta) \in H^1(\Omega_0)$ be its transported function

$$\overline{u}(\theta)(y) = u(\Omega)(x) = u\Big((\,\mathrm{Id}+\theta)(\Omega_0)\Big) \circ (\,\mathrm{Id}+\theta)(y).$$

The functional $\theta \to \overline{u}(\theta)$, from $W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$ into $H^1(\Omega_0)$, is differentiable at 0, and its derivative in the direction θ, called Lagrangian derivative is

$$Y = \langle \overline{u}'(0), \theta \rangle$$

where $Y \in H^1(\Omega_0)$ is the unique solution of

$$\begin{cases} -\Delta Y + Y = -\Delta(\nabla u(\Omega_0)\cdot\theta) + \nabla u(\Omega_0)\cdot\theta & \text{in } \Omega_0 \\ \dfrac{\partial Y}{\partial n} = (\nabla\theta + (\nabla\theta)^t)\nabla u(\Omega_0)\cdot n + \nabla g\cdot\theta - g(\nabla\theta n\cdot n) & \text{on } \partial\Omega_0. \end{cases}$$

Proof. We perform the change of variables $x = y + \theta(y)$ with $y \in \Omega_0$ in the variational formulation. Take a test function $\phi = \psi \circ (\,\mathrm{Id} + \theta)^{-1}$, i.e., $\psi(y) = \phi(x)$. We get

$$\begin{aligned}\int_{\Omega_0} A(\theta)\nabla\overline{u}\cdot\nabla\psi\,dy \quad & + \int_{\Omega_0} \overline{u}\psi|\det(I+\nabla\theta)|dy \\ & = \int_{\Omega_0} f\circ(\,\mathrm{Id}+\theta)\,\psi|\det(I+\nabla\theta)|dy \\ & + \int_{\partial\Omega_0} g\circ(\,\mathrm{Id}+\theta)\,\psi|\det(I+\nabla\theta)|\;|\,(I+\nabla\theta)^{-t}n\,|\,ds\end{aligned}$$

with $A(\theta) = |\det(I+\nabla\theta)|(I+\nabla\theta)^{-1}\left((I+\nabla\theta)^{-1}\right)^t$.

We differentiate with respect to θ at 0.

The only new term is the boundary integral which can be differentiated like in Proposition 6.24.

Defining $Y = \langle \overline{u}'(0), \theta \rangle$ we deduce

$$\int_{\Omega_0} (\nabla Y \cdot \nabla \psi + Y\psi)\, dy + \int_{\Omega_0} \big(\mathrm{div}\theta\, I - \nabla\theta - (\nabla\theta)^t \big) \nabla \overline{u} \cdot \nabla \psi \, dy$$

$$+ \int_{\Omega_0} \overline{u}\psi \, \mathrm{div}\theta \, dy = \int_{\Omega_0} \mathrm{div}(f\theta)\psi \, dy$$

$$+ \int_{\partial\Omega_0} \big(\nabla g \cdot \theta + g \big(\mathrm{div}\theta - \nabla\theta n \cdot n \big) \big) \psi ds$$

Then we recall that $\overline{u}(0) = u(\Omega_0) = u$, $\Delta u = u - f$ in Ω_0 and $\frac{\partial u}{\partial n} = g$ on $\partial\Omega_0$, and the identity

$$\Delta (\nabla v \cdot \theta) = \mathrm{div} \big((\Delta v)\theta - (\mathrm{div}\theta)\nabla v + (\nabla\theta + (\nabla\theta)^t)\nabla v \big) ,$$

to get the result. Simple in principle but computationally intensive...

Corollary 6.36. The Eulerian derivative U of the solution $u(\Omega)$, defined by

$$U = Y - \nabla u(\Omega_0) \cdot \theta,$$

is a solution in $H^1(\Omega_0)$ of

$$-\Delta U + U = 0 \quad \text{in } \Omega_0.$$

and satisfies the boundary condition

$$\frac{\partial U}{\partial n} = \theta \cdot n \left(\frac{\partial g}{\partial n} - \frac{\partial^2 u(\Omega_0)}{\partial n^2} \right) + \nabla_t(\theta \cdot n) \cdot \nabla_t u(\Omega_0) \quad \text{on} \quad \partial\Omega_0,$$

where $\nabla_t \phi = \nabla \phi - (\nabla \phi \cdot n) n$ denotes the tangential gradient on the boundary.

Proof. Easy but tedious computation.

6.4 Gradient and optimality condition

We consider the shape optimization problem

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

with $\mathcal{U}_{ad} = \left\{ \Omega = (\,\mathrm{Id} + \theta)(\Omega_0) \text{ and } \int_\Omega dx = V_0 \right\}$. The cost function $J(\Omega)$ is either the compliance, or a least square criterion for a target displacement $u_0(x) \in L^2(\mathbb{R}^N)$

$$J(\Omega) = \int_\Omega f u \, dx + \int_{\partial\Omega} g u \, ds \quad \text{or} \quad J(\Omega) = \int_\Omega |u - u_0|^2 dx.$$

The function $u(\Omega)$ is the solution in $H^1(\Omega)$ of

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

with $f \in H^1(\mathbb{R}^N)$ and $g \in H^2(\mathbb{R}^N)$.

Gradient and optimality condition

Theorem 6.38. The functional $J(\Omega) = \int_\Omega |u - u_0|^2 dx$ is shape differentiable

$$J'(\Omega_0)(\theta) = \int_{\partial\Omega_0} \theta \cdot n \left(|u - u_0|^2 + \nabla u \cdot \nabla p + p(u - f) - \frac{\partial (gp)}{\partial n} - Hgp \right) ds,$$

where p is the adjoint state, unique solution in $H^1(\Omega_0)$ of

$$\begin{cases} -\Delta p + p = -2\,(u - u_0) & \text{in } \Omega_0 \\ \frac{\partial p}{\partial n} = 0 & \text{on } \partial\Omega_0, \end{cases}$$

We recover the fact that the shape derivative depends only on the normal trace of θ on the boundary.

Proof. Applying Proposition 6.28 to the cost function yields

$$J'(\Omega_0)(\theta) = \int_{\Omega_0} \left(|u(\Omega_0) - u_0|^2 \,\mathrm{div}\theta + 2(u(\Omega_0) - u_0)(Y - \nabla u_0 \cdot \theta) \right) dx,$$

or equivalently, with $U = Y - \nabla u(\Omega_0) \cdot \theta$,

$$J'(\Omega_0)(\theta) = \int_{\Omega_0} \left[\mathrm{div} \left(\theta |u(\Omega_0) - u_0|^2 \right) + 2(u(\Omega_0) - u_0)U \right] dx.$$

Multiplying the adjoint equation by U

$$\int_{\Omega_0} (\nabla p \cdot \nabla U + pU)\, dy = -2 \int_{\Omega_0} (u(\Omega_0) - u_0)\, U\, dy,$$

then the equation for U by p

$$\int_{\Omega_0} (\nabla p \cdot \nabla U + pU)\, dy \; = \\ \int_{\partial\Omega_0} \theta \cdot n \left(-\nabla u(\Omega_0) \cdot \nabla p - p\Delta u(\Omega_0) + \frac{\partial (gp)}{\partial n} + Hgp \right) ds,$$

we deduce the result by comparison of the two equalities.

The compliance case (self-adjoint)

Theorem 6.40. The functional $J(\Omega) = \int_\Omega f u \, dx + \int_{\partial\Omega} g u \, ds$ is shape-differentiable

$$J'(\Omega_0)(\theta) = \int_{\partial\Omega_0} \theta \cdot n \left(-|\nabla u(\Omega_0)|^2 - |u(\Omega_0)|^2 + 2u(\Omega_0) f \right) ds$$

$$+ \int_{\partial\Omega_0} \theta \cdot n \left(2 \frac{\partial (g u(\Omega_0))}{\partial n} + 2 H g u(\Omega_0) \right) ds,$$

Interpretation: assume $f = 0$ and $g = 0$ where $\theta \cdot n \neq 0$. The formula simplifies in

$$J'(\Omega_0)(\theta) = - \int_{\partial\Omega_0} \theta \cdot n \left(|\nabla u|^2 + u^2 \right) ds \leq 0$$

It is always advantageous to increase the domain (i.e., $\theta \cdot n > 0$) for decreasing the compliance.

Proof. Applying Proposition 6.28 to the cost function yields

$$J'(\Omega_0)(\theta) = \int_{\Omega_0} (fu\,\mathrm{div}\theta + u\theta\cdot\nabla f + fY)\,dx$$
$$+ \int_{\partial\Omega_0} (gu\,(\,\mathrm{div}\theta - \nabla\theta n\cdot n) + u\theta\cdot\nabla g + gY)\,ds,$$

or equivalently, with $U = Y - \nabla u\cdot\theta$,

$$J'(\Omega_0)(\theta) = \int_{\Omega_0} (\,\mathrm{div}(fu\theta) + fU)\,dx + \int_{\partial\Omega_0} \left(\theta\cdot n\left(\frac{\partial(gu)}{\partial n} + Hgu\right) + gU\right) ds.$$

Multiplying the equation for u by U and that for U by u, then comparing, leads to the result.

Remark. Same type of result for a Dirichlet boundary condition (but different formulas).

6.4.3 Fast derivation: the Lagrangian method

- The previous computations are quite tedious... but there is a simpler and faster (albeit formal) method, called the Lagrangian method (proposed in this context by J. Céa).
- The Lagrangian allows us to find the correct definition of the adjoint state too.
- It is easy for Neumann boundary conditions, a little more involved for Dirichlet ones.
- That is the method to be known !

Fast derivation for Neumann boundary conditions

If the objective function is

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

the Lagrangian is defined as the sum of J and of the variational formulation of the state equation

$$\mathcal{L}(\Omega, v, q) = \int_{\Omega} j(v)\, dx + \int_{\Omega} \Big(\nabla v \cdot \nabla q + vq - fq \Big) dx - \int_{\partial\Omega} gq\, ds,$$

with v and $q \in H^1(\mathbb{R}^N)$. It is important to notice that the space $H^1(\mathbb{R}^N)$ does not depend on Ω and thus the three variables in $\mathcal{L}$ are clearly independent.

The partial derivative of $\mathcal{L}$ with respect to q in the direction $\phi \in H^1(\mathbb{R}^N)$ is

$$\langle\frac{\partial \mathcal{L}}{\partial q}(\Omega, v, q), \phi\rangle = \int_\Omega \Big(\nabla v \cdot \nabla \phi + v\phi - f\phi\Big) dx - \int_{\partial\Omega} g\phi \, ds,$$

which, upon equating to 0, gives the variational formulation of the state.

The partial derivative of $\mathcal{L}$ with respect to v in the direction $\phi \in H^1(\mathbb{R}^N)$ is

$$\langle\frac{\partial \mathcal{L}}{\partial v}(\Omega, v, q), \phi\rangle = \int_\Omega j'(v)\phi \, dx + \int_\Omega \Big(\nabla \phi \cdot \nabla q + \phi q\Big) dx,$$

which, upon equating to 0, gives the variational formulation of the adjoint.

The partial derivative of $\mathcal{L}$ with respect to Ω in the direction θ is

$$\frac{\partial \mathcal{L}}{\partial \Omega}(\Omega_0, v, q)(\theta) = \int_{\partial\Omega} \theta \cdot n \left(j(v) + \nabla v \cdot \nabla q + vq - fq - \frac{\partial(gq)}{\partial n} - Hgq \right) ds.$$

When evaluating this derivative with the state $u(\Omega_0)$ and the adjoint $p(\Omega_0)$, we precisely find the derivative of the objective function

$$\boxed{\frac{\partial \mathcal{L}}{\partial \Omega}\Big(\Omega_0, u(\Omega_0), p(\Omega_0)\Big)(\theta) = J'(\Omega_0)(\theta)}$$

Indeed, if we differentiate the equality

$$\mathcal{L}(\Omega, u(\Omega), q) = J(\Omega) \quad \forall\, q \in H^1(\mathbb{R}^N),$$

the chain rule lemma yields

$$J'(\Omega_0)(\theta) = \frac{\partial \mathcal{L}}{\partial \Omega}(\Omega_0, u(\Omega_0), q)(\theta) + \langle \frac{\partial \mathcal{L}}{\partial v}(\Omega_0, u(\Omega_0), q), u'(\Omega_0)(\theta)\rangle$$

Taking $q = p(\Omega_0)$, the last term cancels since $p(\Omega_0)$ is the solution of the adjoint equation.

Thanks to this computation, the "correct" result can be guessed for $J'(\Omega_0)$ without using the notions of shape or material derivatives.

Nevertheless, in full rigor, this "fast" computation of the shape derivative $J'(\Omega_0)$ is valid only if we know that u is shape differentiable.

Fast derivation for Dirichlet boundary conditions

It is more involved ! Let $u \in H^1_0(\Omega)$ be the solution of

$$\int_\Omega \nabla u \cdot \nabla \phi \, dx = \int_\Omega f \phi \, dx \quad \forall \phi \in H^1_0(\Omega).$$

The "usual" Lagrangian is

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

for $v, q \in H^1_0(\Omega)$. The variables (Ω, v, q) are not independent !

Indeed, the functions v and q satisfy

$$v \ = \ q \ = \ 0 \quad \text{ on } \partial\Omega.$$

Another Lagrangian has to be introduced.

Lagrangian for Dirichlet boundary conditions

The Dirichlet boundary condition is penalized

$$\mathcal{L}(\Omega, v, q, \lambda) = \int_\Omega j(v)\,dx - \int_\Omega (\Delta v + f) q\,dx + \int_{\partial\Omega} \lambda v\,ds$$

where λ is the Lagrange multiplier for the boundary condition. It is now possible to differentiate since the 4 variables $v, q, \lambda \in H^1(\mathbb{R}^N)$ are independent.

Of course, we recover

$$\sup_{q,\lambda} \mathcal{L}(\Omega, v, q, \lambda) = \begin{cases} \int_\Omega j(u)\,dx = J(\Omega) & \text{if } v \equiv u, \\ +\infty & \text{otherwise.} \end{cases}$$

By definition of the Lagrangian:

the partial derivative of $\mathcal{L}$ with respect to q in the direction $\phi \in H^1(\mathbb{R}^N)$ is

$$\langle \frac{\partial \mathcal{L}}{\partial q}(\Omega, v, q, \lambda), \phi \rangle = -\int_\Omega \phi \Big(\Delta v + f \Big) dx,$$

which, upon equating to 0, gives the state equation,

the partial derivative of $\mathcal{L}$ with respect to λ in the direction $\phi \in H^1(\mathbb{R}^N)$ is

$$\langle \frac{\partial \mathcal{L}}{\partial \lambda}(\Omega, v, q, \lambda), \phi \rangle = \int_{\partial\Omega} \phi v \, dx,$$

which, upon equating to 0, gives the Dirichlet boundary condition for the state equation.

To compute the partial derivative of $\mathcal{L}$ with respect to v, we perform a first integration by parts

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

then a second integration by parts

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

We now can differentiate in the direction $\phi \in H^1(\mathbb{R}^N)$

$$\langle \frac{\partial \mathcal{L}}{\partial v}(\Omega, v, q), \phi \rangle = \int_\Omega j'(v)\phi\,dx - \int_\Omega \phi \Delta q\,dx + \int_{\partial\Omega} \left(-q \frac{\partial \phi}{\partial n} + \phi \left(\lambda + \frac{\partial q}{\partial n} \right) \right) ds$$

which, upon equating to 0, gives three relationships, the two first ones being the adjoint problem.

1. If ϕ has compact support in Ω_0, we get

$$-\Delta p = -j'(u) \quad \text{dans} \quad \Omega_0.$$

2. If $\phi = 0$ on $\partial\Omega_0$ with any value of $\frac{\partial \phi}{\partial n}$ in $L^2(\partial\Omega_0)$, we deduce

$$p = 0 \quad \text{sur} \quad \partial\Omega_0.$$

3. If ϕ is now varying in the full $H^1(\Omega_0)$, we find

$$\frac{\partial p}{\partial n} + \lambda = 0 \quad \text{sur} \quad \partial\Omega_0.$$

The adjoint problem has actually been recovered but furthermore the optimal Lagrange multiplier λ has been characterized.

Eventually, the shape partial derivative is

$$\frac{\partial \mathcal{L}}{\partial \Omega}(\Omega_0, u, p, \lambda)(\theta) = \int_{\partial \Omega_0} \theta \cdot n \Big(j(u) - (\Delta u + f)p + \frac{\partial (u\lambda)}{\partial n} + H u \lambda \Big) ds$$

Knowing that $u = p = 0$ on $\partial \Omega_0$ and $\lambda = -\frac{\partial p}{\partial n}$ we deduce

$$\frac{\partial \mathcal{L}}{\partial \Omega}(\Omega_0, u, p, \lambda)(\theta) = \int_{\partial \Omega_0} \theta \cdot n \Big(j(0) - \frac{\partial u}{\partial n} \frac{\partial p}{\partial n} \Big) ds = J'(\Omega_0)(\theta)$$

$$\boxed{J'(\Omega_0)(\theta) = \frac{\partial \mathcal{L}}{\partial \Omega}\Big(\Omega_0, u(\Omega_0), p(\Omega_0)\Big)(\theta)}$$

This formula is not a surprise because differentiating

$$\mathcal{L}(\Omega, u(\Omega), q, \lambda) = J(\Omega) \quad \forall q, \lambda$$

yields

$$J'(\Omega_0)(\theta) = \frac{\partial \mathcal{L}}{\partial \Omega}(\Omega_0, u(\Omega_0), q, \lambda)(\theta) + \langle \frac{\partial \mathcal{L}}{\partial v}(\Omega_0, u(\Omega_0), q, \lambda), u'(\Omega_0)(\theta)\rangle.$$

Then, taking $q = p(\Omega_0)$ (the adjoint state) and $\lambda = -\frac{\partial p}{\partial n}(\Omega_0)$, the last term cancels and we obtain the desired formula.

Application to compliance minimization

We minimize $J(\Omega) = \int_\Omega f u \, dx$ with $u \in H_0^1(\Omega)$ solution of

$$\int_\Omega \nabla u \cdot \nabla \phi \, dx = \int_\Omega f \phi \, dx \quad \forall \, \phi \in H_0^1(\Omega).$$

The adjoint state is just $p = -u$. The shape derivative is

$$J'(\Omega_0)(\theta) = \int_{\partial\Omega_0} \theta \cdot n \Big(f u - \frac{\partial u}{\partial n} \frac{\partial p}{\partial n} \Big) ds = \int_{\partial\Omega_0} \theta \cdot n \left(\frac{\partial u}{\partial n} \right)^2 ds \leq 0$$

It is always advantageous to shrink the domain (i.e., $\theta \cdot n < 0$) to decrease the compliance.

This is the opposite conclusion compared to Neumann b.c., but it is logical !

Another example: the drum

We optimize the shape of a drum (an elastic membrane) in order it produces the lowest possible tune. Let $\lambda(\Omega)$ be the eigenvalue (the square of the eigenfrequency) and $u(x)$ be the eigenmode

$$\begin{cases} -\Delta u = \lambda(\Omega) u & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega. \end{cases}$$

The fundamental mode is the smallest eigenvalue which is also characterized by

$$\lambda(\Omega) = \min_{u \in H_0^1(\Omega), u \neq 0} \frac{\int_\Omega |\nabla u|^2 dx}{\int_\Omega u^2 dx}.$$

Thus we study

$$\inf_{\Omega \subset \mathbb{R}^2} \left(\lambda(\Omega) + \ell \int_\Omega dx \right),$$

where $\ell \geq 0$ is a given Lagrange multiplier for a constraint on the membrane area.

Eulerian derivation

For a test function ϕ with compact support $\omega \subset \Omega$ we derive

$$\int_\omega \nabla u \cdot \nabla \phi \, dx = \lambda(\Omega) \int_\omega u\phi \, dx$$

$$\Rightarrow \quad \int_\omega \nabla U \cdot \nabla \phi \, dx = \lambda(\Omega) \int_\omega U\phi \, dx + \Lambda \int_\omega u\phi \, dx,$$

where $\Lambda = \lambda'(\Omega)(\theta)$ is the derivative of the eigenvalue (assumed to be simple).

$$\Rightarrow \quad -\Delta U - \lambda(\Omega) U = \Lambda u \quad \text{ in } \Omega.$$

To deduce the boundary condition for U we derive

$$\int_{\partial\Omega} u\psi \, ds = 0 \quad \forall \psi \in C^\infty(\mathbb{R}^2).$$

$$\Rightarrow \quad \int_{\partial\Omega} \left(U\psi + \theta \cdot n \left(\frac{\partial(u\psi)}{\partial n} + H u\psi \right) \right) ds = 0,$$

which yields $U = -\frac{\partial u}{\partial n} \theta \cdot n$ since $u = 0$ on $\partial\Omega$.

Multiplying the equation for U by u and integrating by parts leads to

$$\int_\Omega \nabla U \cdot \nabla u \, dx = \lambda \int_\Omega U u \, dx + \Lambda \int_\Omega u^2 \, dx.$$

Multiplying the equation for u by U and integrating by parts leads to

$$\int_\Omega \nabla U \cdot \nabla u \, dx = \lambda \int_\Omega U u \, dx + \int_{\partial\Omega} \frac{\partial u}{\partial n} U \, ds.$$

Thus, we deduce

$$\Lambda \int_\Omega u^2 dx = \int_{\partial\Omega} \frac{\partial u}{\partial n} U \, ds = - \int_{\partial\Omega} \left(\frac{\partial u}{\partial n} \right)^2 \theta \cdot n \, ds.$$

The derivative of the objective function is (self-adjoint problem)

$$J'(\Omega)(\theta) = \Lambda + \ell \int_{\partial\Omega} \theta \cdot n \, ds = \int_{\partial\Omega} \left(\ell - \frac{\left(\frac{\partial u}{\partial n}\right)^2}{\int_\Omega u^2 dx} \right) \theta \cdot n \, ds.$$

If $\ell = 0$ we have $J'(\Omega)(\theta) \leq 0$ as soon as $\theta \cdot n \geq 0$, i.e., we minimze $J(\Omega)$ if the domain Ω is enlarged.

Lagrangian method

For $\mu \in \mathbb{R}$, $v, q, z \in H^1(\mathbb{R}^N)$, we introduce the Lagrangian

$$\mathcal{L}(\Omega, \mu, v, q, z) = \mu - \int_\Omega (\Delta v + \mu v) q \, dx + \int_{\partial\Omega} z v \, ds$$

where z is the Lagrange multiplier for the boundary condition. Since the 5 variables are independent it is possible to differentiate.

The partial derivative $\frac{\partial \mathcal{L}}{\partial q} = 0$ gives the state equation.

The partial derivative $\frac{\partial \mathcal{L}}{\partial z} = 0$ gives the Dirichlet boundary condition for the state.

The partial derivative $\frac{\partial \mathcal{L}}{\partial v} = 0$ gives three relationships including the adjoint:

$$-\Delta p = \lambda p \quad \text{in} \quad \Omega, \quad p = 0 \quad \text{on} \quad \partial\Omega, \quad \frac{\partial p}{\partial n} + z = 0 \quad \text{on} \quad \partial\Omega.$$

The partial derivative $\frac{\partial \mathcal{L}}{\partial \mu} = 0$ yields

$$\int_\Omega up\,dx = 1$$

Since the eigenvalue λ is simple, p is a multiple of u. Thus

$$p = \frac{u}{\int_\Omega u^2 dx}.$$

Eventually, the shape partial derivative is

$$\frac{\partial \mathcal{L}}{\partial \Omega}(\Omega, \lambda, u, p, z)(\theta) = \int_{\partial\Omega} \theta \cdot n \Big(p\Delta u + \lambda p u + \frac{\partial (uz)}{\partial n} + H u z \Big) ds$$

Knowing that $u = p = 0$ on $\partial\Omega$ and $z = -\frac{\partial p}{\partial n}$ we deduce

$$\frac{\partial \mathcal{L}}{\partial \Omega}(\Omega, \lambda, u, p, z)(\theta) = \int_{\partial\Omega} \theta \cdot n \Big(- \frac{\partial u}{\partial n}\frac{\partial p}{\partial n} \Big) ds = J'(\Omega)(\theta)$$

6.5 Numerical algorithms in the elasticity setting

Free boundary Γ. Fixed boundary Γ_N and Γ_D.

$$\begin{cases} -\operatorname{div}\sigma = 0 & \text{in } \Omega \\ \sigma = 2\mu e(u) + \lambda \operatorname{tr}(e(u)) \operatorname{Id} & \text{in } \Omega \\ u = 0 & \text{on } \Gamma_D \\ \sigma n = g & \text{on } \Gamma_N \\ \sigma n = 0 & \text{on } \Gamma, \end{cases}$$

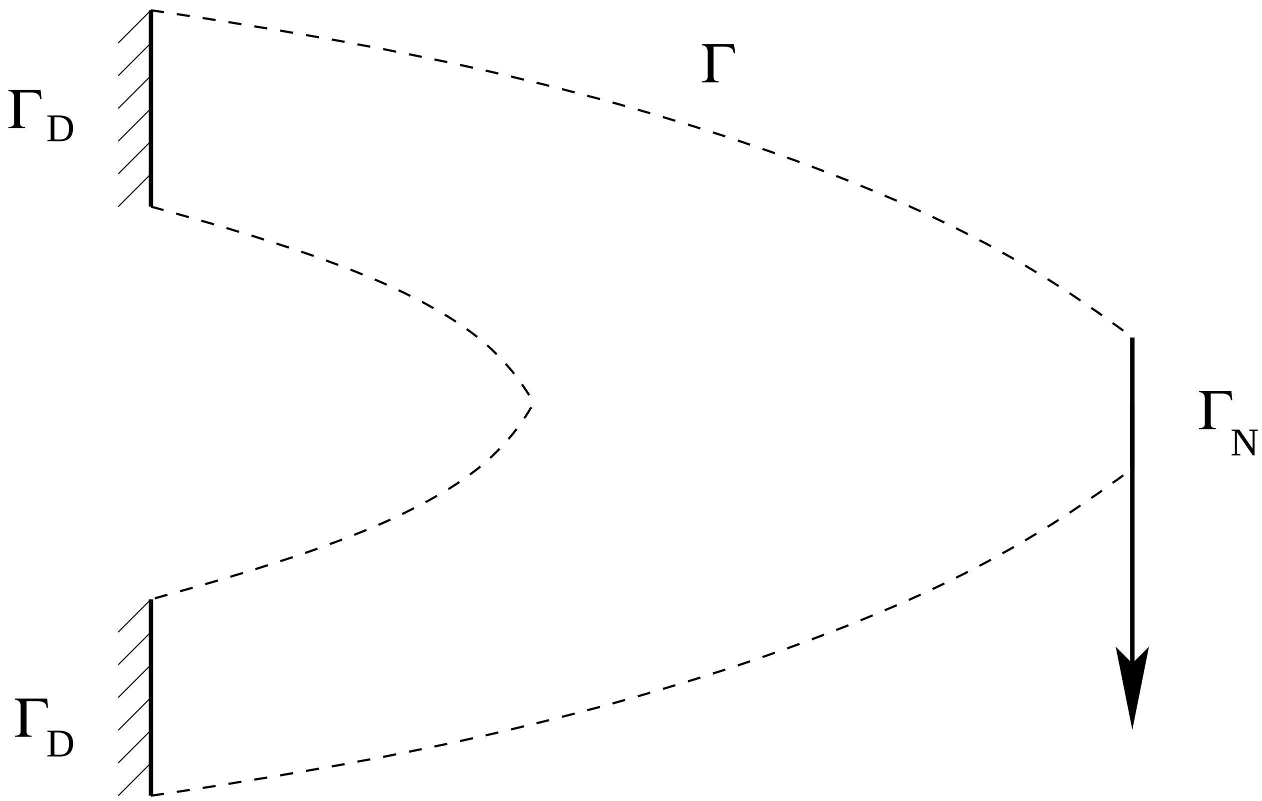
with $e(u) = (\nabla u + (\nabla u)^t)/2$. Compliance is minimized

$$J(\Omega) = \int_{\Gamma_N} g \cdot u \, dx.$$

In such a (self-adjoint) case we get

$$J'(\Omega_0)(\theta) = -\int_\Gamma \theta \cdot n \left(2\mu |e(u)|^2 + \lambda (\operatorname{tr} e(u))^2 \right) ds.$$

Boundary conditions for an elastic cantilever: Γ_D is the left vertical side, Γ_N is the right vertical side, and Γ (dashed line) is the remaining boundary.



Main idea of the algorithm

Given an inital design Ω_0 we compute a sequence of iterative shapes Ω_k, satisfying the following constraints

$$\partial\Omega_k = \Gamma_k \cup \Gamma_N \cup \Gamma_D$$

where Γ_N and Γ_D are fixed, and the volume (or weight) is fixed

$$V(\Omega_k) = \int_{\Omega_k} dx = V(\Omega_0).$$

To take into account the constraint that only Γ is allowed to move, it is enough to take $\theta \cdot n = 0$ on $\Gamma_N \cup \Gamma_D$.

Because of the volume constraint we rely on a projected gradient algorithm with a fixed step .

The derivative of the volume constraint is $V'(\Omega_k)(\theta) = \int_{\Gamma_k} \theta \cdot n.$

Algorithm

Let $t > 0$ be a given descent step. We compute a sequence $\Omega_k \in \mathcal{U}_{ad}$ by

1. Initialization of the shape Ω_0.

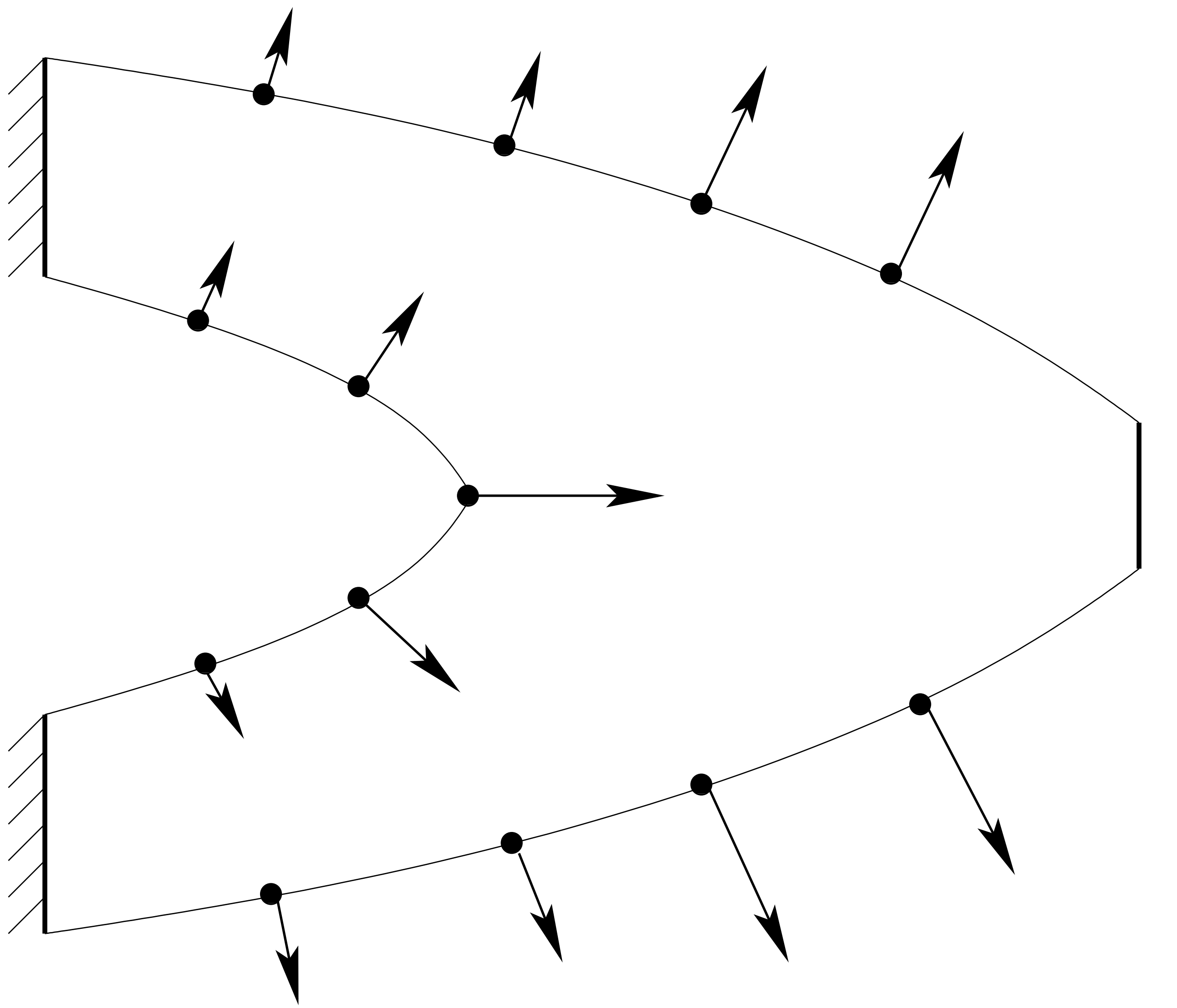
2. Iterations until convergence, for $k \geq 0$:

$$\Omega_{k+1} = (\,\mathrm{Id} + \theta_k)\Omega_k \quad \text{with} \quad \theta_k = t(j_k - \ell_k)n,$$

where n is the normal to the boundary $\partial\Omega_k$ and $\ell_k \in \mathbb{R}$ is the Lagrange multiplier such that Ω_{k+1} satisfies the volume constraint. The shape derivative is given on the boundary Γ_k by

$$J'(\Omega_k)(\theta) = -\int_\Gamma \theta \cdot n\, j_k\, ds \quad \text{with} \quad j_k = 2\mu|e(u_k)|^2 + \lambda(\,\mathrm{tr}\, e(u_k))^2$$

where u_k is the solution of the state equation posed in the domain Ω_k.



Mesh deformation

To change the shape we need to automatically remesh the new shape, or at least to deform the mesh at each iteration.

- ✘ Displacement field θ proportional to n (normal to the boundary), merely defined on the boundary.
- ✘ We prefer to deform the mesh (it is less costly).
- ✘ In such a case we have to extend θ inside the shape.
- ✘ We need to check that the displaced boundaries do not cross...
- ✘ Nevertheless, in case of large shape deformations we must remesh (it is computationally costly).
- ✘ Often the algorithm stops before convergence because of geometrical constraints.

Implementing geometric optimization on a computer is quite intricate, **especially in 3-d**.

Extension of the displacement field

$$J'(\Omega)(\theta) + \ell V'(\Omega)(\theta) = \int_\Gamma (\ell - j)\,\theta \cdot n\, ds$$

A first possibility to extend $(\ell - j)n$ inside the shape is

$$\begin{cases} -\Delta\theta = 0 & \text{in } \Omega \\ \theta = t(j-\ell)n & \text{on } \Gamma \\ \theta = 0 & \text{on } \Gamma_D \cup \Gamma_N \end{cases}$$

We rather take this opportunity to (furthermore) regularize by solving

$$\begin{cases} -\Delta\theta = 0 & \text{in } \Omega \\ \frac{\partial\theta}{\partial n} = t(j-\ell)n & \text{on } \Gamma \\ \theta = 0 & \text{on } \Gamma_D \cup \Gamma_N \end{cases}$$

Indeed, $j = 2\mu|e(u)|^2 + \lambda\,\mathrm{tr}(e(u))^2$ (for compliance) may be not smooth (not better than in $L^1(\Omega)$) although we always assumed that $\theta \in W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$).

It can cause boundary oscillations.

Typically, θ admits one order of derivation more than j and one can check that it is actually a descent direction because

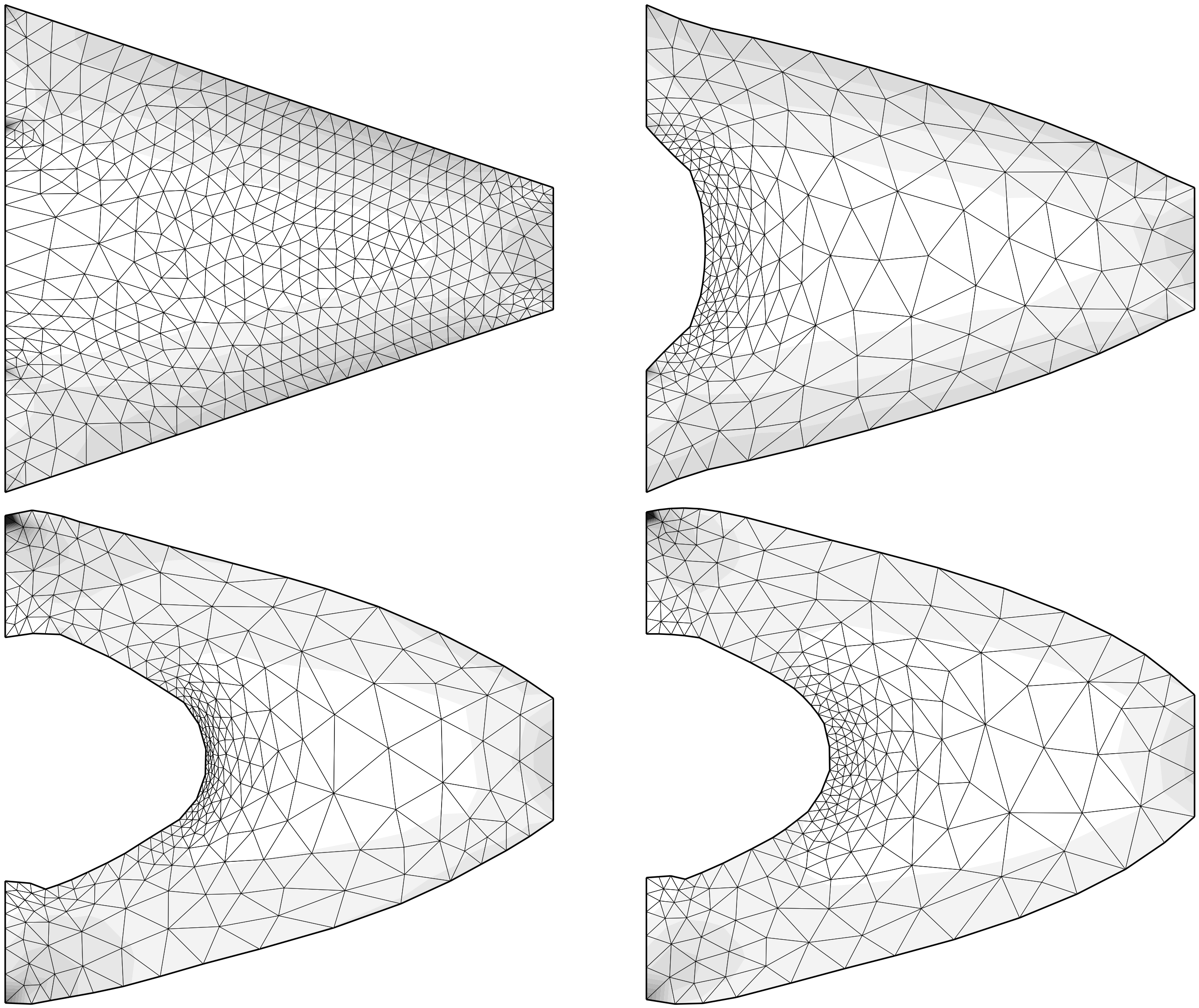
$$-\int_\Omega |\nabla\theta|^2 dx = t\int_\Gamma (\ell - j)\,\theta\cdot n\,ds$$

Technical details

- ☞ To check the volume constraint we update "a posteriori" the Lagrange multiplier $\ell_k \in \mathbb{R}$. The volume is thus not exact but it converges to the desired value.
- ☞ We step back and diminish the descent step $t > 0$ when $J(\Omega)$ increases.
- ☞ To avoid possible oscillations of the boundary, due to numerical instabilities, we use two meshes: a fine one to precisely evaluate u and p, a coarse one which is moved.

FreeFem++ computations ; scripts available on the web page
`http://www.cmap.polytechnique.fr/~allaire/cours_X_annee3.html`

Numerical results: initialization and iterations 5, 10, 20



Influence of the initial topology