# OPTIMAL DESIGN OF STRUCTURES (MAP 562)

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CHAPTER VI

## GEOMETRIC OPTIMIZATION (Continued)

## 6.3.3. Derivation of a function depending on the shape

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

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 $\Omega_0$ 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 $\Omega$... 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 $\Omega_0$ 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 $\Omega_0$ 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 $U$,

$$J'(\Omega_0)(\theta) = \int_{\Omega_0} U(\theta)\,dx + \int_{\partial\Omega_0} u(\Omega_0)\,\theta\cdot n\,ds$$

## 6.3.4 Shape derivation of an equation

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

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

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

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 $u(\Omega) \in H^1_0(\Omega)$ be the solution and $\overline{u}(\theta) \in H^1_0(\Omega_0)$ 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 $\theta$, called Lagrangian derivative is

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

where $Y \in H^1_0(\Omega_0)$ 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

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

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 $\overline{u} \in H^1_0(\Omega_0)$ such that, for any $\psi \in H^1_0(\Omega_0)$,

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

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

We differentiate with respect to $\theta$ 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 $\psi$ is a function which does not depend on $\theta$.

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

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

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

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

Since $\overline{u}(\theta)\in H^1_0(\Omega_0)$, its derivative $Y$ belongs to $H^1_0(\Omega_0)$ too. Thus $Y$ is a solution of

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

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

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

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 $\phi$ 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 $\Omega$, neither the test function, nor the domain of integration depend on $\Omega$. 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

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

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

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 $\theta$, 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 $\theta$ 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 $\Omega_0$ and $\frac{\partial u}{\partial n} = g$ on $\partial\Omega_0$, and the identity

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

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.

# 6.5 Numerical algorithms in the elasticity setting

Free boundary $\Gamma$. Fixed boundary $\Gamma_N$ and $\Gamma_D$.

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

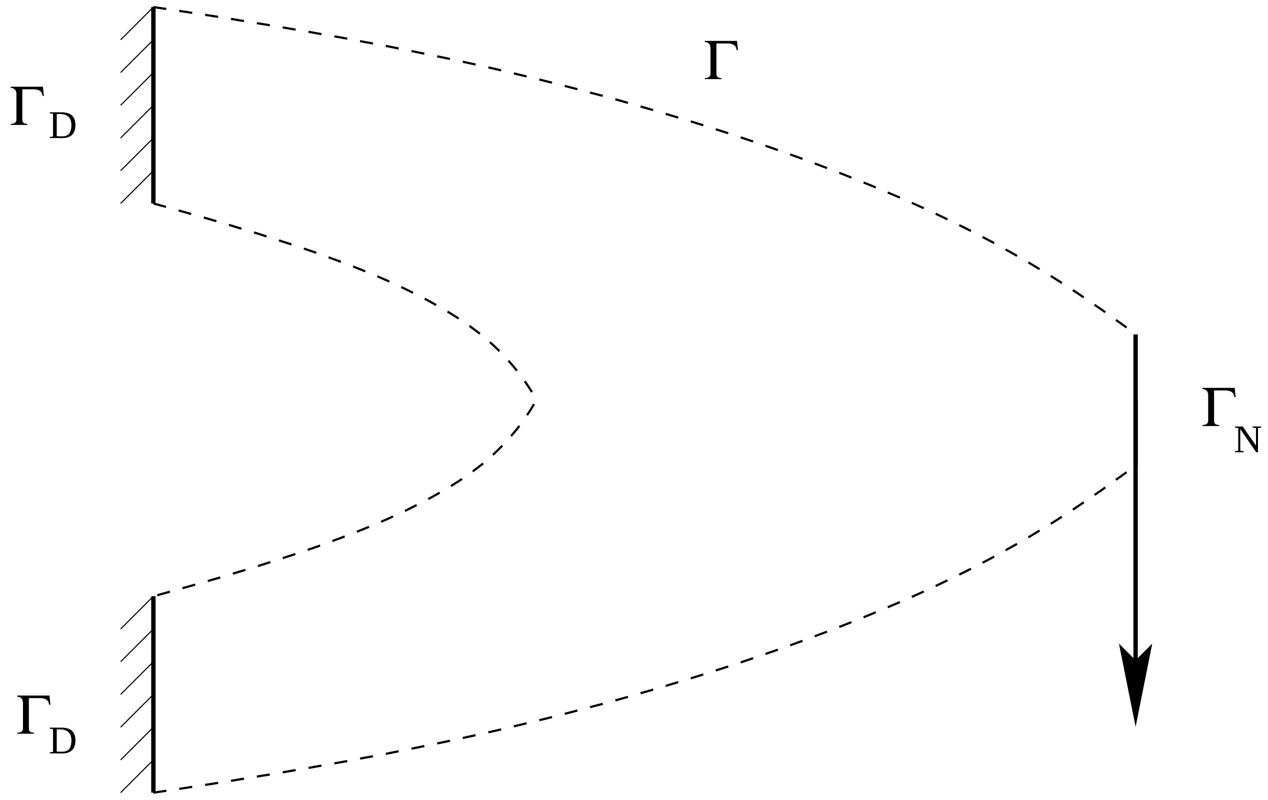
with $e(u) = (\nabla u + (\nabla u)^t)/2$. Compliance is minimized

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

In such a (self-adjoint) case we get

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

Boundary conditions for an elastic cantilever: $\Gamma_D$ is the left vertical side, $\Gamma_N$ is the right vertical side, and $\Gamma$ (dashed line) is the remaining boundary.



## Main idea of the algorithm

Given an inital design $\Omega_0$ we compute a sequence of iterative shapes $\Omega_k$, satisfying the following constraints

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

where $\Gamma_N$ and $\Gamma_D$ 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 $\Gamma$ 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 $V'(\Omega_k)(\theta) = \displaystyle\int_{\Gamma_k} \theta \cdot n.$

## Algorithm

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

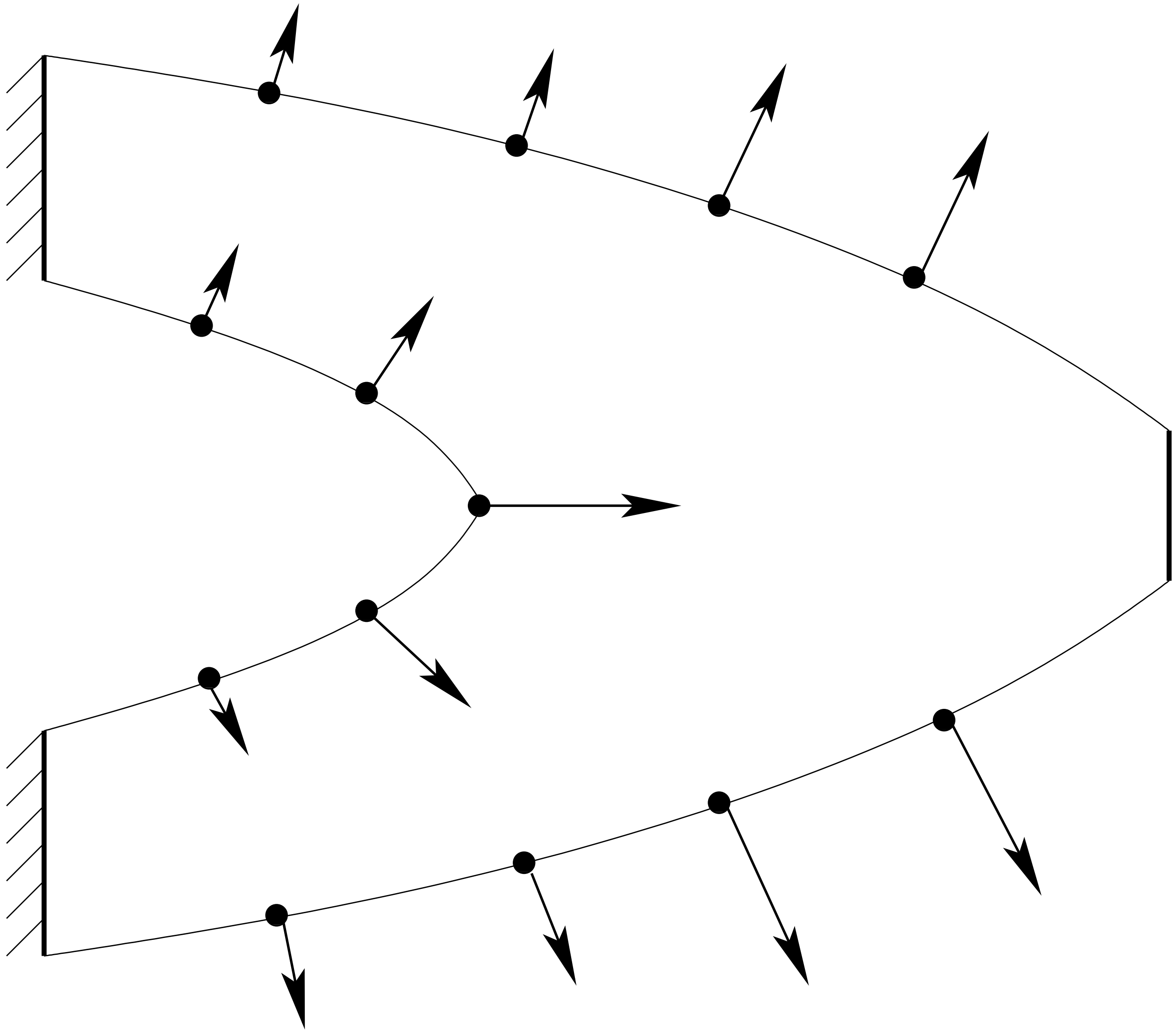
1. Initialization of the shape $\Omega_0$.
2. Iterations until convergence, for $k \geq 0$:

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

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



## 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 $\theta$ 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 $\theta$ 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, $\theta$ admits one order of derivation more than $j$ and one can check that it is actually a descent direction because

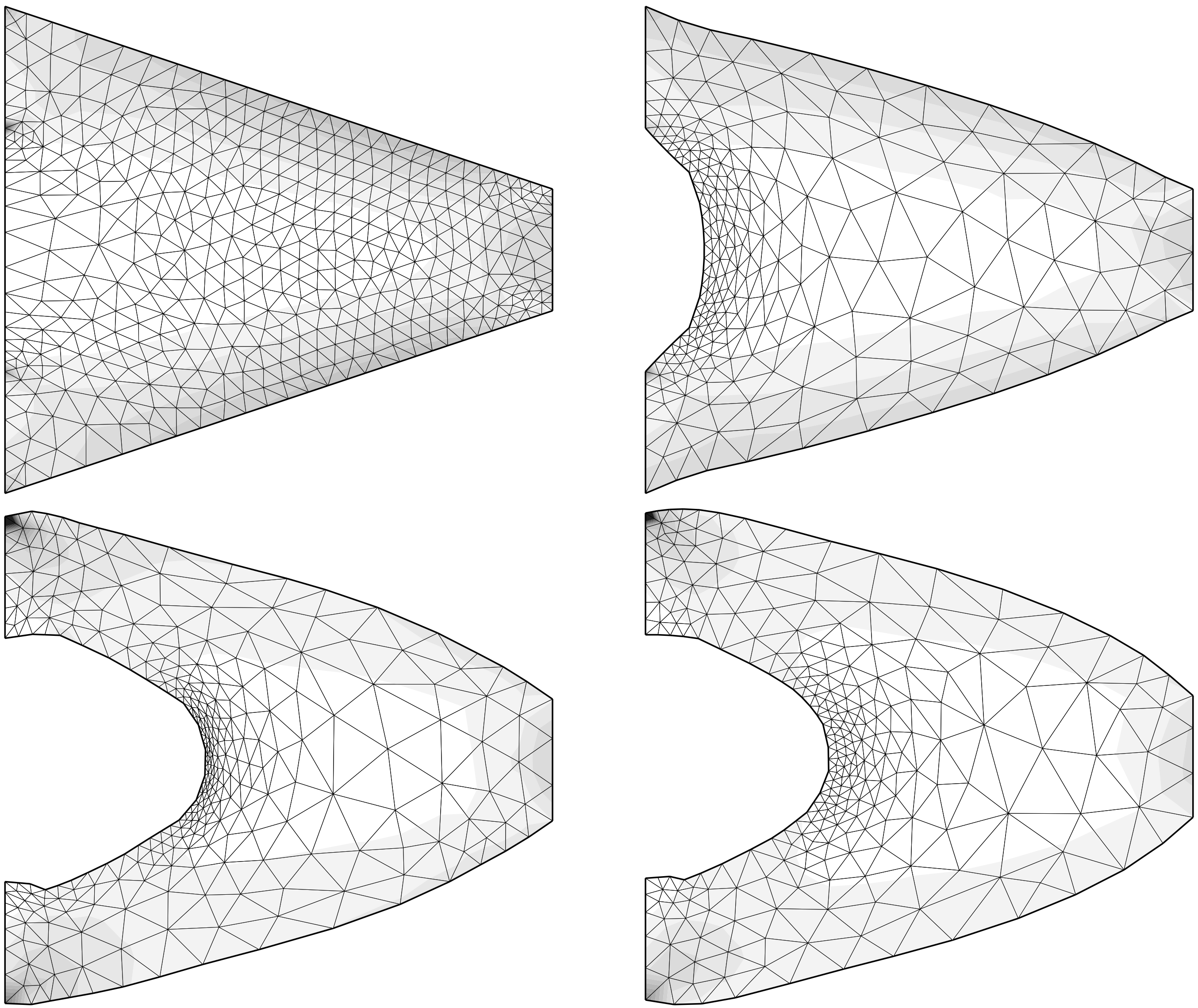
$$-\int_\Omega |\nabla\theta|^2 dx = t\int_\Gamma (\ell - j)\,\theta\cdot n\,ds$$

## 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