OPTIMAL DESIGN OF STRUCTURES (MAP 562)

CHAPTER VI

GEOMETRIC OPTIMIZATION (second part)

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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

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

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 $\overline{u}(\theta, x)$

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

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

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

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. 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,

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

Proof. We write the integral in the reference domain

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

The result follows directly from the expansions

$$\det(I+\nabla\theta)=1+\,\mathrm{div}\theta+o(\theta),\qquad \lim_{\theta\to 0}\frac{\|o(\theta)\|_{L^\infty}}{\|\theta\|_{W^{1,\infty}}}=0;$$

$$\begin{aligned}u((\,\mathrm{Id}+\theta)\Omega_0)\circ(\,\mathrm{Id}+\theta)&=\bar{u}(\theta)\\&=\bar{u}(0)+Y(\theta)+o(\theta),\qquad \lim_{\theta\to 0}\frac{\|o(\theta)\|_{L^1}}{\|\theta\|_{W^{1,\infty}}}=0.\end{aligned}$$

Shape derivation of an equation

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

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. 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

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

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 $A(\theta) = |\det(I + \nabla\theta)| (I + \nabla\theta)^{-1} \left((I + \nabla\theta)^{-1}\right)^t$.
The differentiability of $\bar{u}$ is a consequence of the implicit function theorem.

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 that the right hand side is differentiable.
Furthermore, the map $\theta\to A(\theta)$ is differentiable too because

$$A(\theta) = (1+\,\mathrm{div}\theta)I - \nabla\theta - (\nabla\theta)^t + o(\theta)$$

$$\text{with } \lim_{\theta\to 0}\frac{\|o(\theta)\|_{L^\infty(\mathbb{R}^N;\mathbb{R}^{N^2})}}{\|\theta\|_{W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)}} = 0.$$

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

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

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

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

leads to the final result.

Shape derivative U

Corollary. 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

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

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

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. 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

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

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 as done before.

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

$$\int_{\Omega_0} (\nabla Y \cdot \nabla \psi + Y\psi)\, dy + \int_{\Omega_0} \left(\mathrm{div}\theta\, I - \nabla\theta - (\nabla\theta)^t \right) \nabla \overline{u} \cdot \nabla \psi\, dy$$
$$+ \int_{\Omega_0} \overline{u}\psi\, \mathrm{div}\theta\, dy = \int_{\Omega_0} \mathrm{div}(f\theta)\psi\, dy$$
$$+ \int_{\partial\Omega_0} \left(\nabla g \cdot \theta + g\left(\mathrm{div}\theta - \nabla\theta n \cdot n \right) \right) \psi ds.$$

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

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

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

Corollary. 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.

Derivation of shape functions

Combining the above results to the derivation of integrals and solutions of boundary value problems, **we retrieve the shape derivatives of cost functions stated in the first part.**

Numerical algorithms in the elasticity setting

Free boundary Γ. Fixed boundary Γ_N and Γ_D.

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

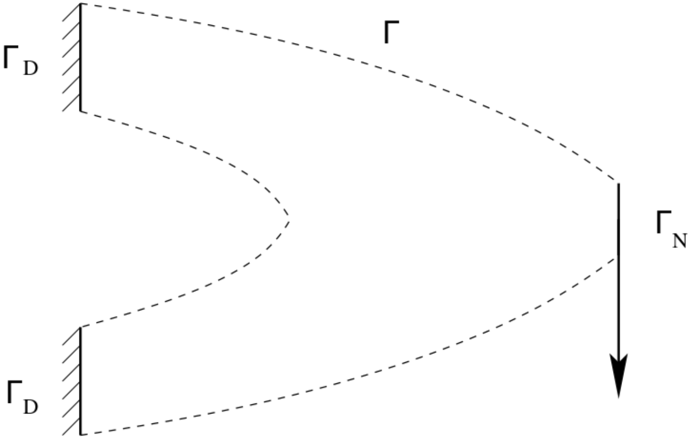
with $e(u) = (\nabla u + (\nabla u)^t)/2$. Compliance is minimized

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

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 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 $V'(\Omega_k)(\theta) = \displaystyle\int_{\Gamma_k} \theta \cdot n$.

Algorithm

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

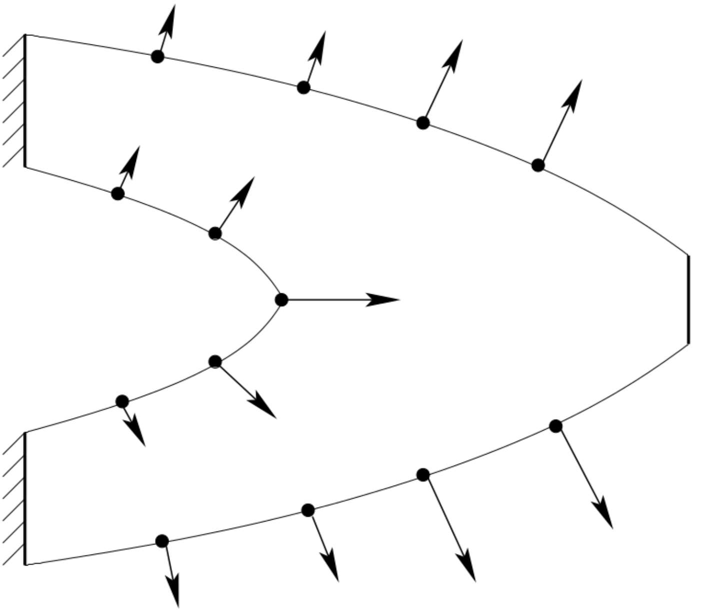
1. Initialization of the shape Ω_0.
2. Iterations until convergence, for $k \geq 0$:

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

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.

1. Displacement field θ proportional to n (normal to the boundary), merely defined on the boundary.
2. We prefer to deform the mesh (it is less costly).
3. In such a case we have to extend θ inside the shape.
4. We need to check that the displaced boundaries do not cross...
5. Nevertheless, in case of large shape deformations we must remesh (it is computationally costly).

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 by

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

We rather take this opportunity to (further) 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

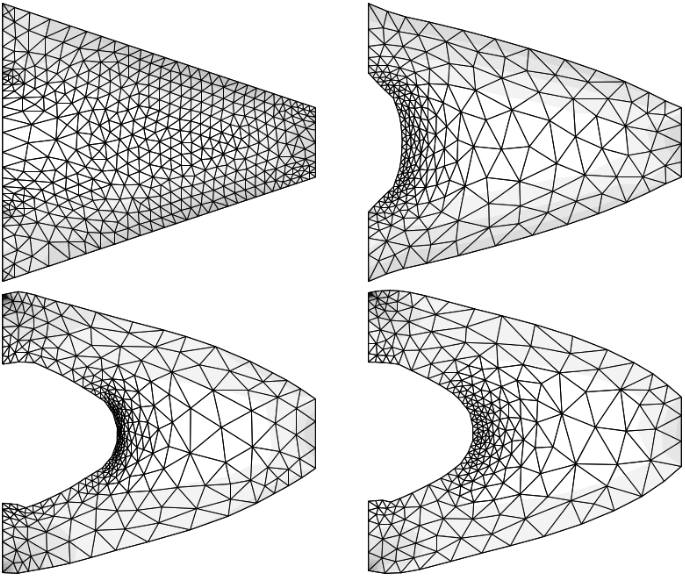
$$-\int_\Omega |\nabla\theta|^2 dx = t\int_\Gamma (\ell - j)\,\theta\cdot n\,ds \le 0.$$

Technical details

1. 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.
2. We step back and diminish the descent step $t > 0$ when $J(\Omega)$ increases.
3. To obtain a precise evaluation of u and p, we adapt the mesh, after its displacement.

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

Numerical results: initialization and iterations 5, 10, 20



Influence of the initial topology