

OPTIMAL DESIGN OF STRUCTURES (MAP 562)

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CHAPTER V

PARAMETRIC (OR SIZING) OPTIMIZATION (end)

Numerical algorithms

Reminder: membrane model problem

Fixed membrane $\Omega \subset \mathbb{R}^N$, forces $f \in L^2(\Omega)$, displacement $u \in H_0^1(\Omega)$

$$\begin{cases} -\operatorname{div}(h\nabla u) = f & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega. \end{cases}$$

$$\inf_{h \in \mathcal{U}_{ad}} J(h) = \int_{\Omega} j(u) dx$$

Admissible set of thicknesses

$$\mathcal{U}_{ad} = \left\{ h \in L^\infty(\Omega), \quad h_{max} \geq h(x) \geq h_{min} > 0 \text{ in } \Omega, \int_{\Omega} h(x) dx = h_0 |\Omega| \right\}.$$

Theorem 5.19. The cost function $J(h)$ is **differentiable** on \mathcal{U}_{ad} and

$$J'(h) = \nabla u \cdot \nabla p$$

where p is the **adjoint state**, unique solution in $H_0^1(\Omega)$ of

$$\begin{cases} -\operatorname{div}(h\nabla p) = -j'(u) & \text{in } \Omega \\ p = 0 & \text{on } \partial\Omega. \end{cases}$$

5.3.2 Numerical algorithm

Projected gradient

1. **Initialization** of the thickness $h_0 \in \mathcal{U}_{ad}$ (by example, a constant function which satisfies the constraints).
2. **Iterations** until convergence, for $n \geq 0$:

$$h_{n+1} = P_{\mathcal{U}_{ad}} \left(h_n - \mu J'(h_n) \right),$$

where $\mu > 0$ is a descent step, $P_{\mathcal{U}_{ad}}$ is the projection operator on the closed convex set \mathcal{U}_{ad} and the derivative is given by

$$J'(h_n) = \nabla u_n \cdot \nabla p_n$$

with the state u_n and the adjoint p_n (associated to the thickness h_n).

To make the algorithm fully explicit, we have to precise what is the projection operator $P_{\mathcal{U}_{ad}}$.

We characterize the projection operator $P_{\mathcal{U}_{ad}}$

$$\left(P_{\mathcal{U}_{ad}}(h)\right)(x) = \max(h_{min}, \min(h_{max}, h(x) + \ell))$$

where ℓ is the unique Lagrange multiplier such that

$$\int_{\Omega} P_{\mathcal{U}_{ad}}(h) dx = h_0 |\Omega|.$$

The determination of the constant ℓ is not explicit: we must use an iterative algorithm based on the property of the function

$$\ell \rightarrow F(\ell) = \int_{\Omega} \max(h_{min}, \min(h_{max}, h(x) + \ell)) dx$$

which is **strictly increasing** on the interval $[\ell^-, \ell^+]$, reciprocal image of $[h_{min}|\Omega|, h_{max}|\Omega|]$. Thanks to this monotonicity property, we propose a simple iterative algorithm: we first bracket the root by an interval $[\ell^1, \ell^2]$ such that

$$F(\ell^1) \leq h_0 |\Omega| \leq F(\ell^2),$$

then we proceed by **dichotomy** to find the root ℓ .

- ☞ In practice, we rather use a projected gradient algorithm with a **variable step** (not optimal) which guarantees the decrease of the functional $J(h_{n+1}) < J(h_n)$.
- ☞ The algorithm is rather slow. A possible acceleration is based on the quasi-Newton algorithm.
- ☞ The overhead generated by the adjoint computation is very modest : one has to build a new right-hand-side (using the state) and solve the corresponding linear system (with the same rigidity matrix).
- ☞ Convergence is detected when the optimality condition is satisfied with a threshold $\epsilon > 0$

$$|h_n - \max(h_{min}, \min(h_{max}, h_n - \mu_n J'(h_n) + \ell_n))| \leq \epsilon \mu_n h_{max}.$$

5.4.3 Numerical algorithm for the compliance

When $j(u) = fu$, we find $p = -u$ since $j'(u) = f$. This particular case is said to be **self-adjoint**.

We use **the dual or complementary energy**

$$J(h) = \int_{\Omega} fu \, dx = \min_{\substack{\tau \in L^2(\Omega)^N \\ -\operatorname{div} \tau = f \text{ in } \Omega}} \int_{\Omega} h^{-1} |\tau|^2 \, dx .$$

We can rewrite the optimization problem as a **double minimization**

$$\inf_{h \in \mathcal{U}_{ad}} \min_{\substack{\tau \in L^2(\Omega)^N \\ -\operatorname{div} \tau = f \text{ in } \Omega}} \int_{\Omega} h^{-1} |\tau|^2 \, dx ,$$

and the order of minimization is irrelevant.

The problem is convex and admits a minimizer.

Lemma 5.25 (optimality conditions). For a given $\tau \in L^2(\Omega)^N$, the problem

$$\min_{h \in \mathcal{U}_{ad}} \int_{\Omega} h^{-1} |\tau|^2 dx$$

admits a minimizer $h(\tau)$ in \mathcal{U}_{ad} given by

$$h(\tau)(x) = \begin{cases} h^*(x) & \text{if } h_{min} < h^*(x) < h_{max} \\ h_{min} & \text{if } h^*(x) \leq h_{min} \\ h_{max} & \text{if } h^*(x) \geq h_{max} \end{cases} \quad \text{with } h^*(x) = \frac{|\tau(x)|}{\sqrt{\ell}},$$

where $\ell \in \mathbb{R}^+$ is the Lagrange multiplier such that $\int_{\Omega} h(x) dx = h_0 |\Omega|$.

Optimality criteria method

1. Initialization of the thickness $h_0 \in \mathcal{U}_{ad}$.
2. Iterations until convergence, for $n \geq 0$:
 - (a) Computation of the state τ_n , unique solution of

$$\min_{\substack{\tau \in L^2(\Omega)^N \\ -\operatorname{div} \tau = f \text{ in } \Omega}} \int_{\Omega} h_n^{-1} |\tau|^2 dx ,$$

with the previous thickness h_n .

- (b) Update of the thickness :

$$h_{n+1} = h(\tau_n),$$

where $h(\tau)$ is the minimizer defined by the optimality condition. The Lagrange multiplier is computed by dichotomy.

Remark that minimizing in τ is equivalent to solving the equation

$$\begin{cases} -\operatorname{div}(h_n \nabla u_n) = f & \text{in } \Omega \\ u_n = 0 & \text{on } \partial\Omega, \end{cases}$$

and we recover τ_n by the formula

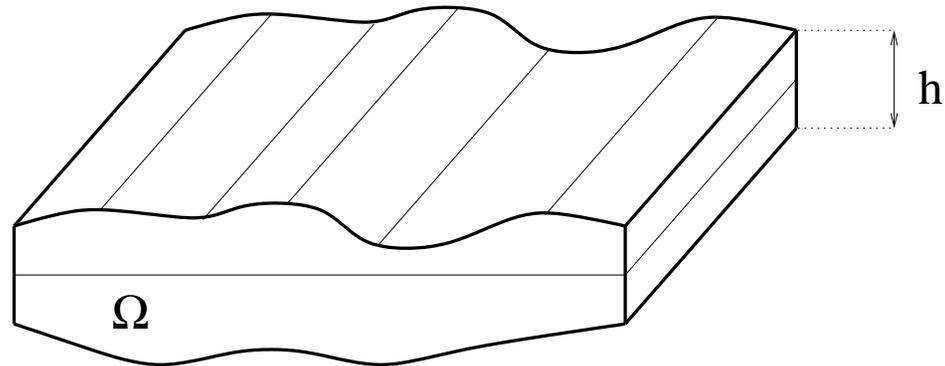
$$\tau_n = h_n \nabla u_n.$$

This algorithm can be interpreted as an alternate minimization in τ and h of the objective function. In particular, we deduce that the objective function **always decreases** through the iterations

$$J(h_{n+1}) = \int_{\Omega} h_{n+1}^{-1} |\tau_{n+1}|^2 dx \leq \int_{\Omega} h_{n+1}^{-1} |\tau_n|^2 dx \leq \int_{\Omega} h_n^{-1} |\tau_n|^2 dx = J(h_n).$$

This algorithm can also be interpreted as an **optimality criteria** method.

5.6 Thickness optimization of an elastic plate



$$\left\{ \begin{array}{ll} -\operatorname{div} \sigma = f & \text{in } \Omega \\ \sigma = 2\mu h e(u) + \lambda h \operatorname{tr}(e(u)) \operatorname{Id} & \text{in } \Omega \\ u = 0 & \text{on } \Gamma_D \\ \sigma n = g & \text{on } \Gamma_N \end{array} \right.$$

with the strain tensor $e(u) = \frac{1}{2}(\nabla u + (\nabla u)^t)$.

Set of admissible thicknesses:

$$\mathcal{U}_{ad} = \left\{ h \in L^\infty(\Omega) , \quad h_{max} \geq h(x) \geq h_{min} > 0 \text{ in } \Omega, \int_{\Omega} h(x) dx = h_0 |\Omega| \right\}.$$

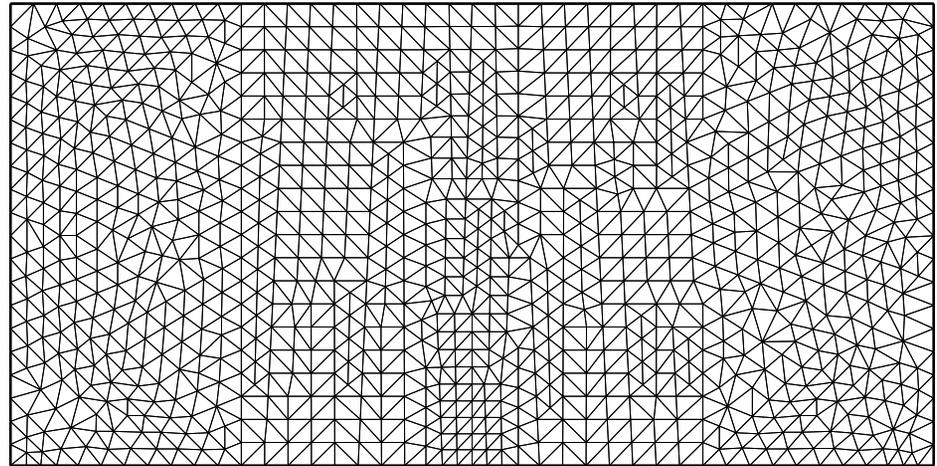
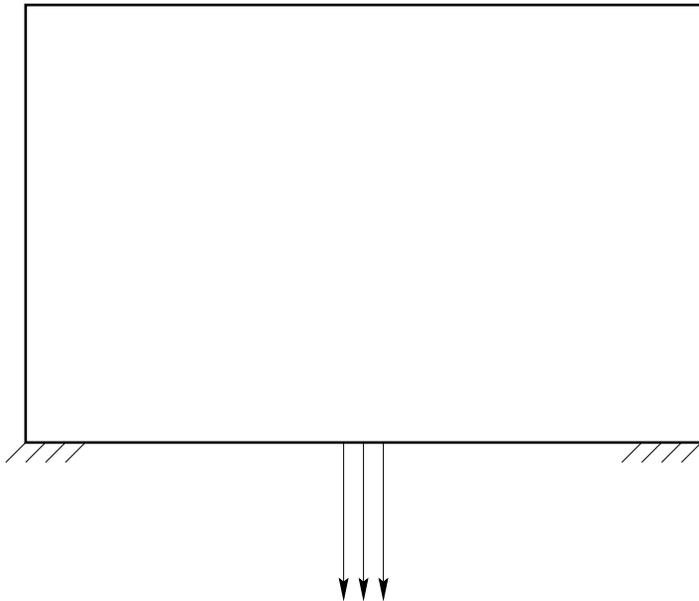
The compliance optimization can be written

$$\inf_{h \in \mathcal{U}_{ad}} J(h) = \int_{\Omega} f \cdot u dx + \int_{\Gamma_N} g \cdot u ds.$$

The theoretical results are the same.

We apply the optimality criteria method.

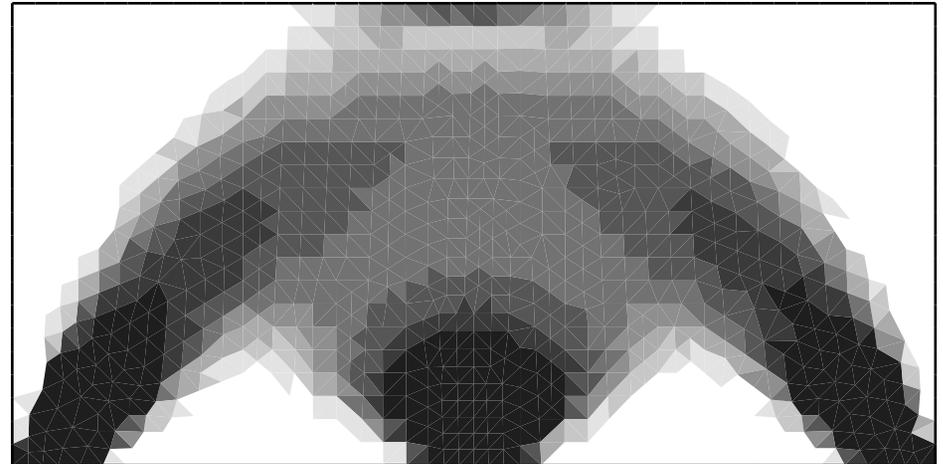
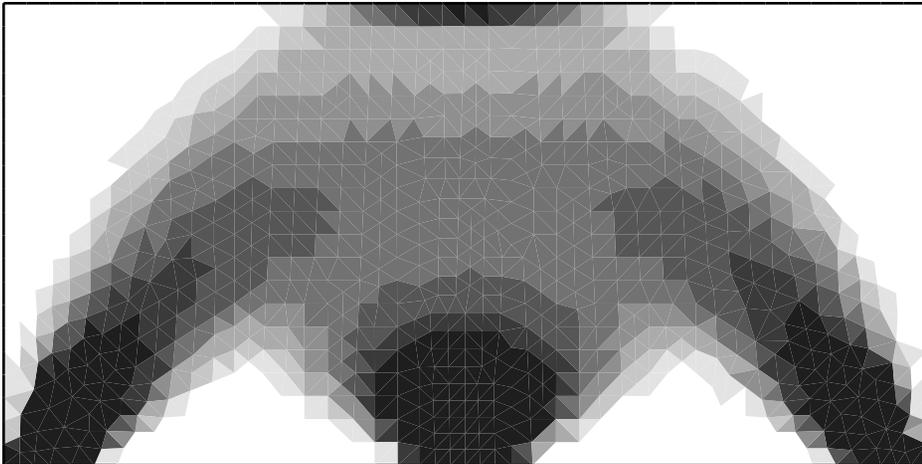
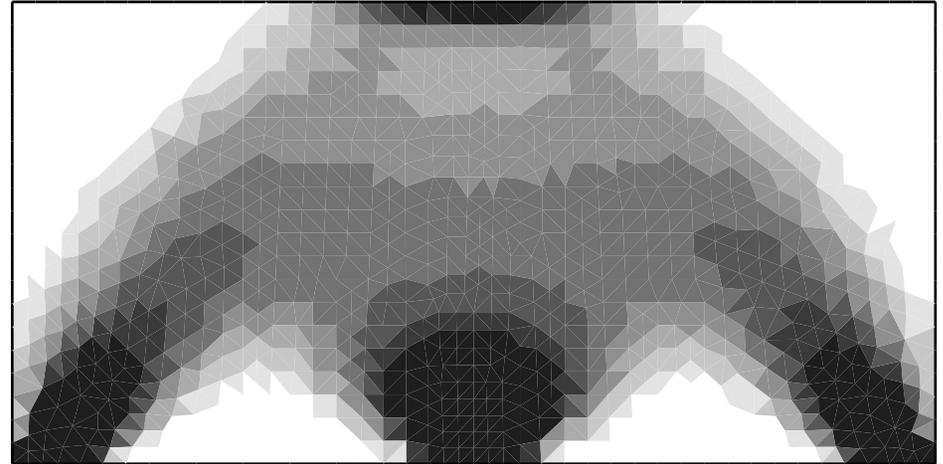
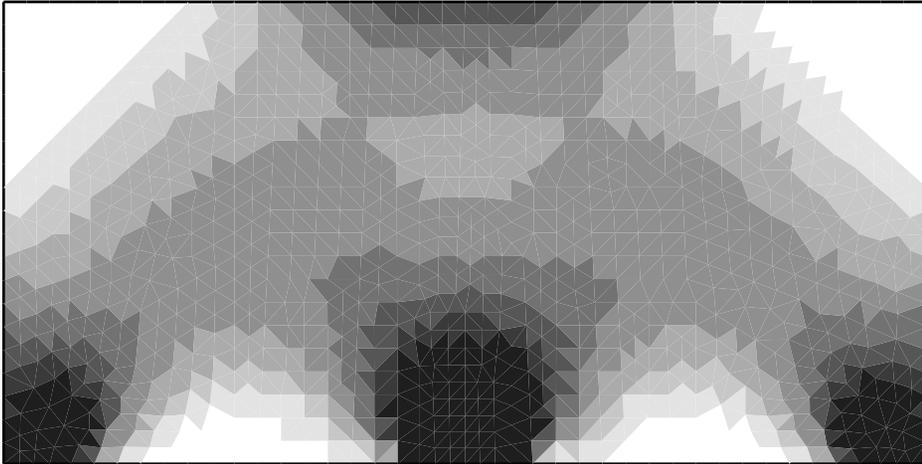
Boundary conditions and mesh for an elastic plate



FreeFem++ computations ; scripts available on the web page

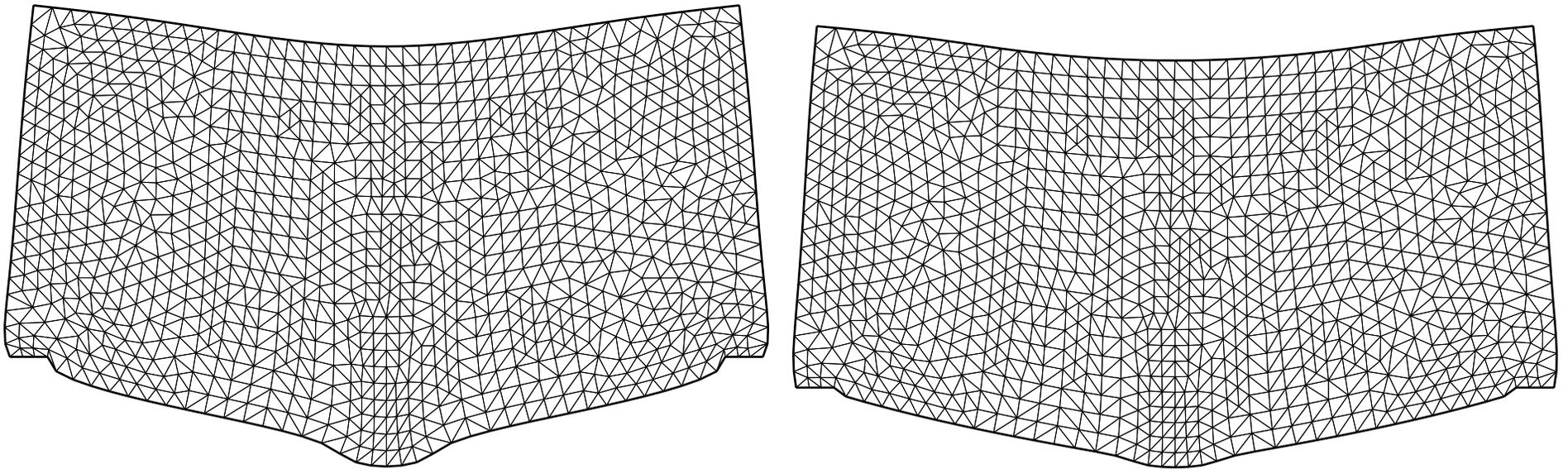
http://www.cmap.polytechnique.fr/~allaire/cours_X_annee3.html

Thickness at iterations 1, 5, 10, 30 (uniform initialization).

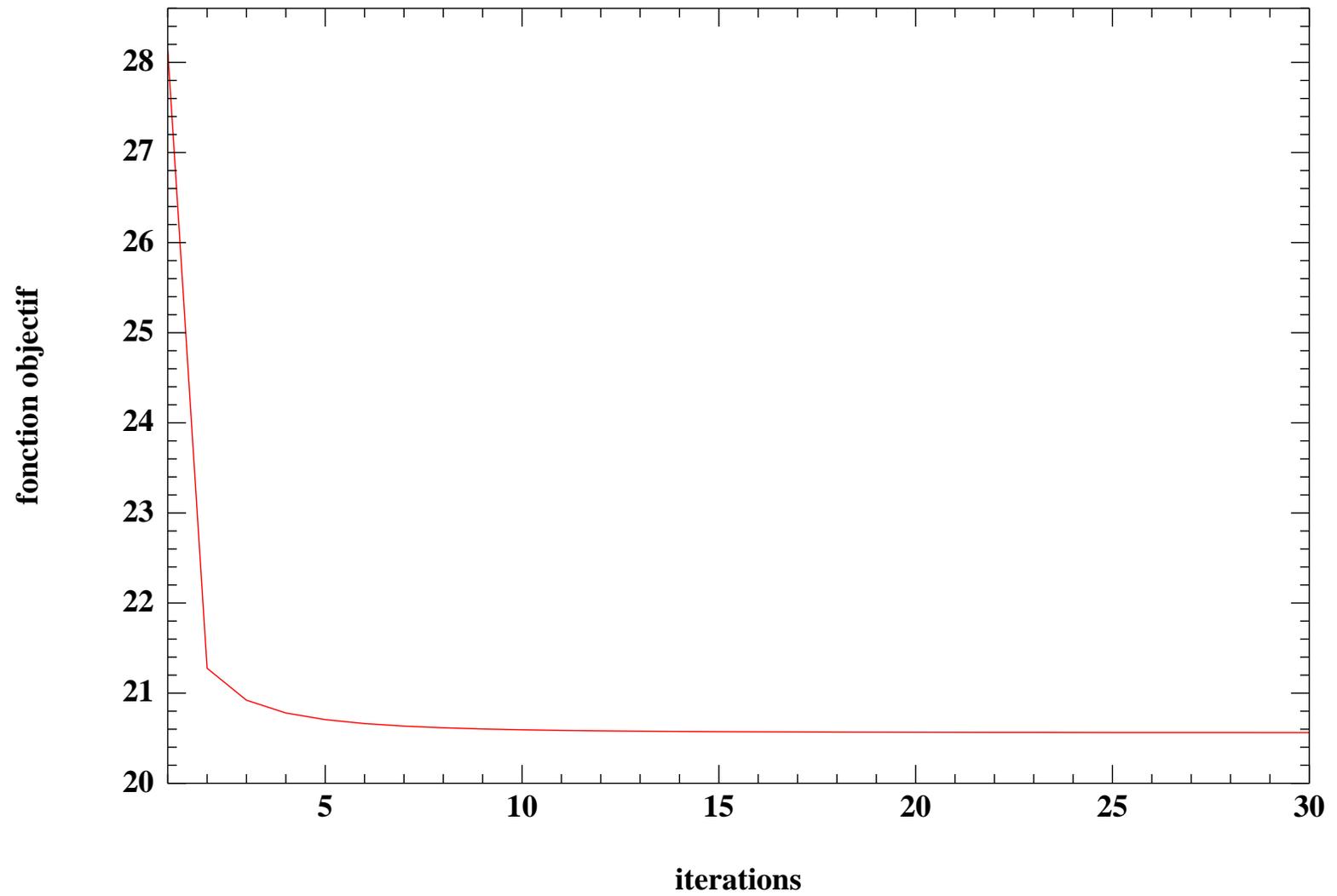


$h_{min} = 0.1, h_{max} = 1.0, h_0 = 0.5$ (increasing thickness from white to black)

Comparing the initial and final deformed shapes

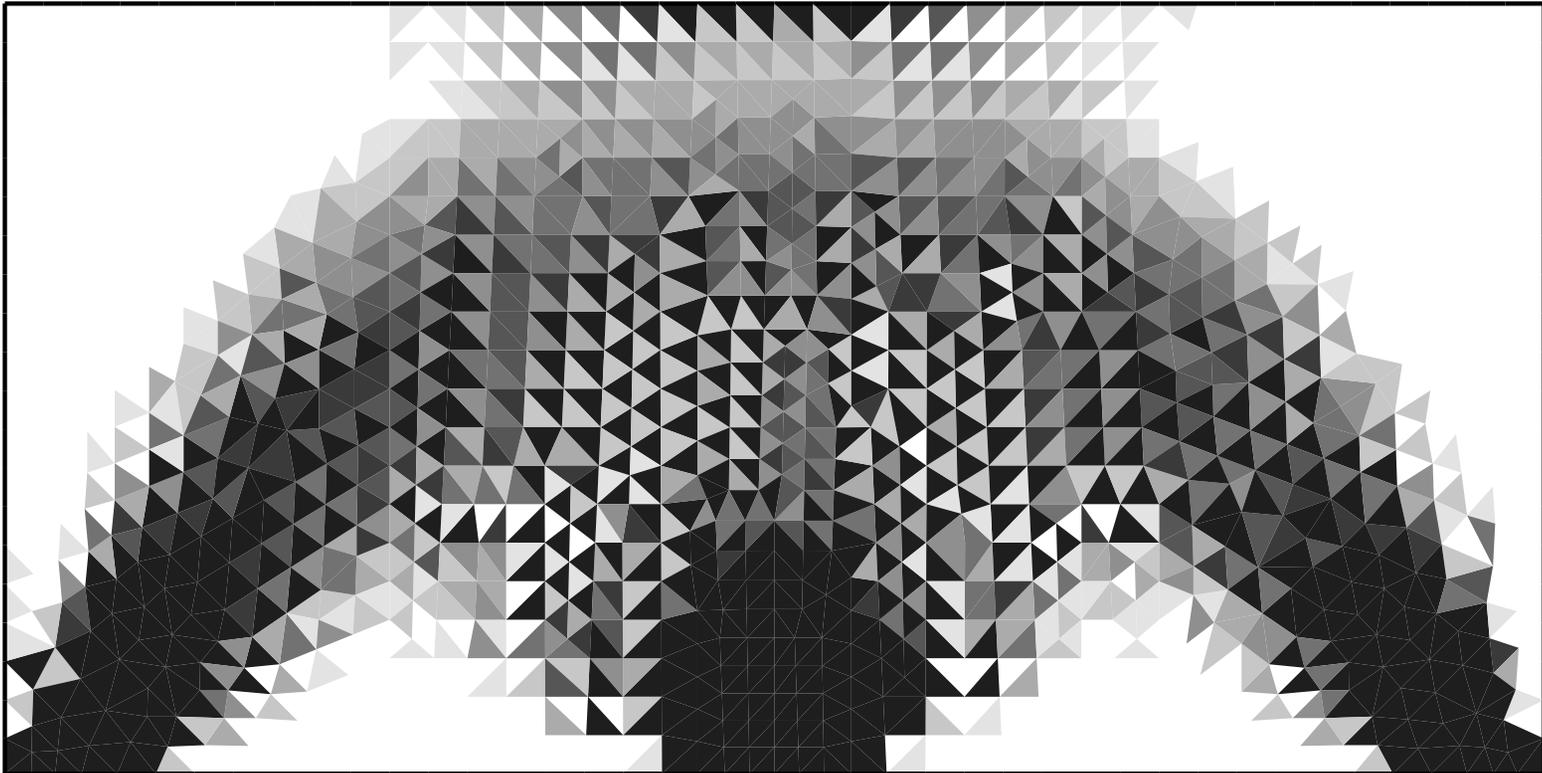


Convergence history



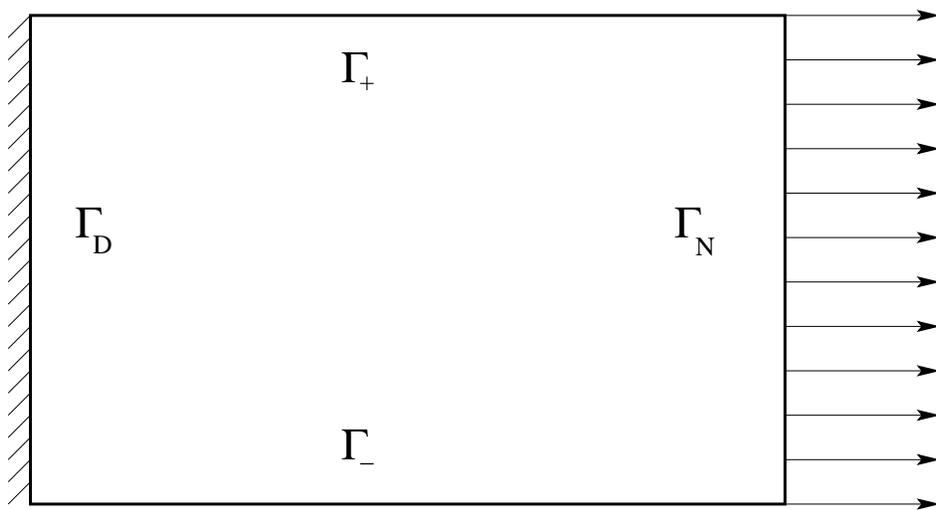
Numerical instabilities (checkerboards)

- ➔ Finite elements $P2$ for u and $P0$ for $h \Rightarrow$ OK
- ➔ Finite elements $P1$ for u and $P0$ for $h \Rightarrow$ unstable !

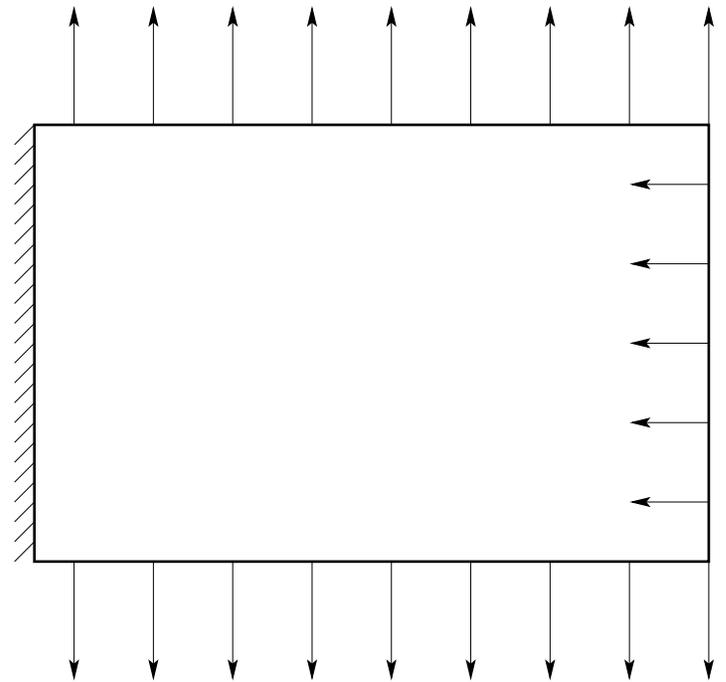


Numerical counter-example of non-existence of an optimal shape (in elasticity)

We look for the design which horizontally is less deformed and vertically more deformed.

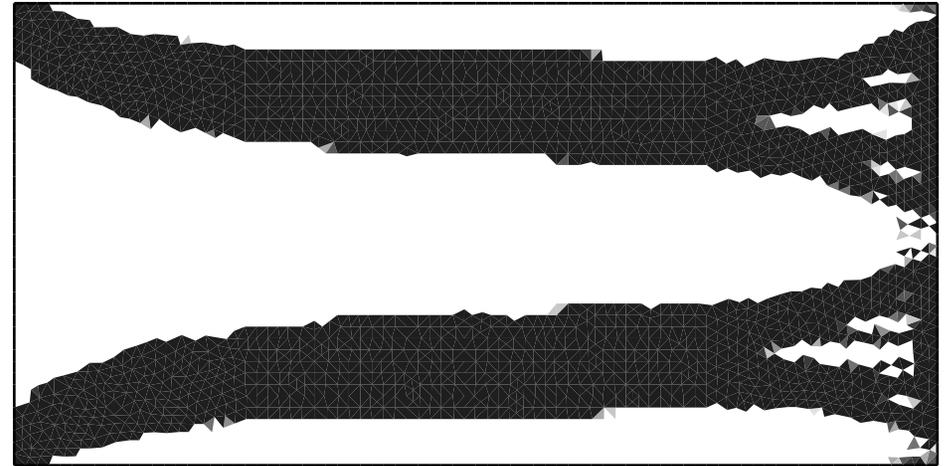
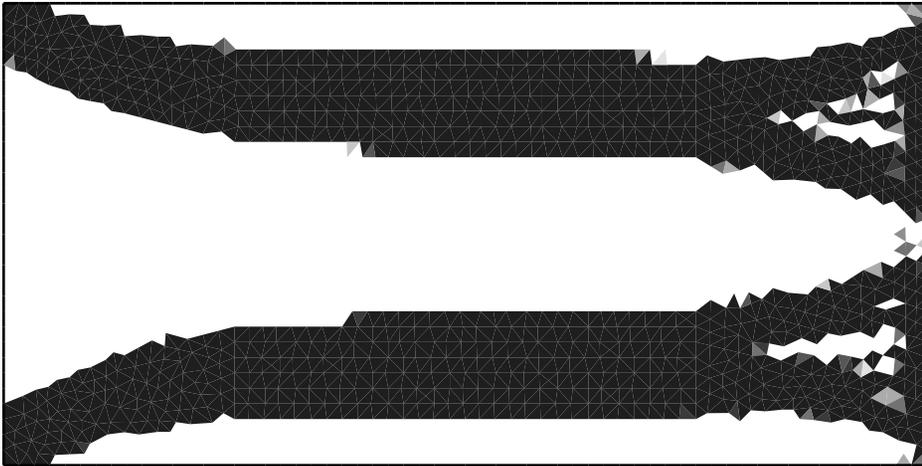
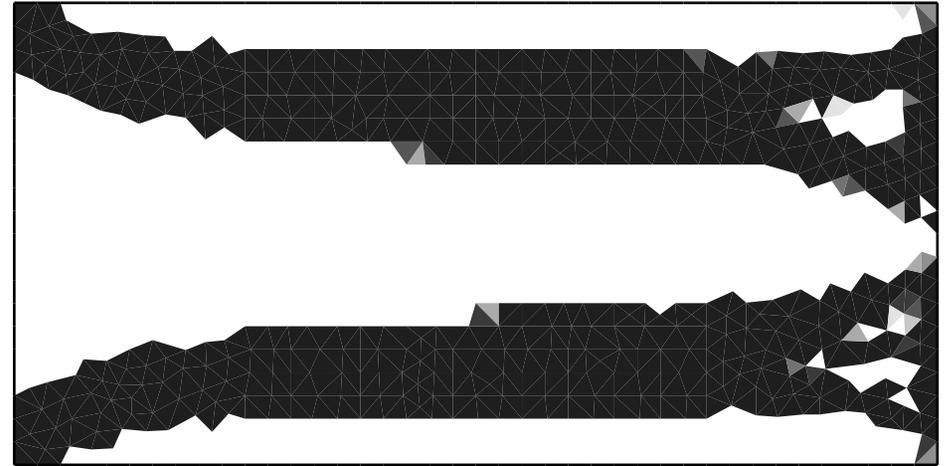
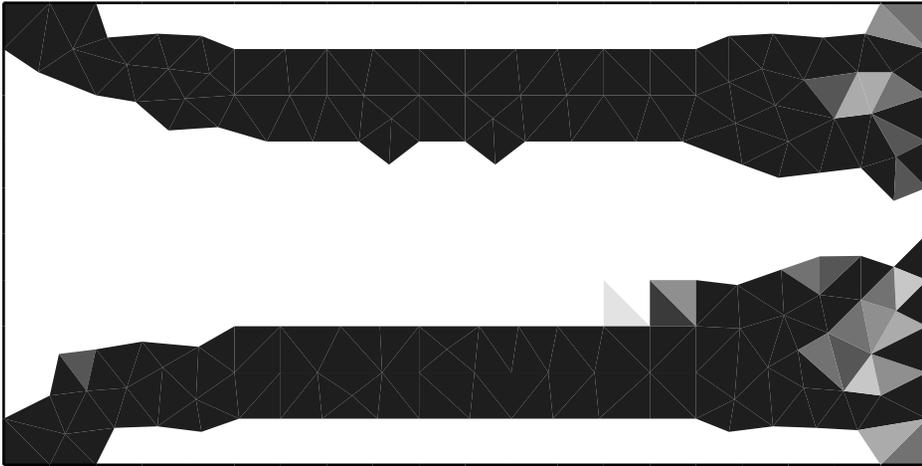


boundary conditions



target displacement

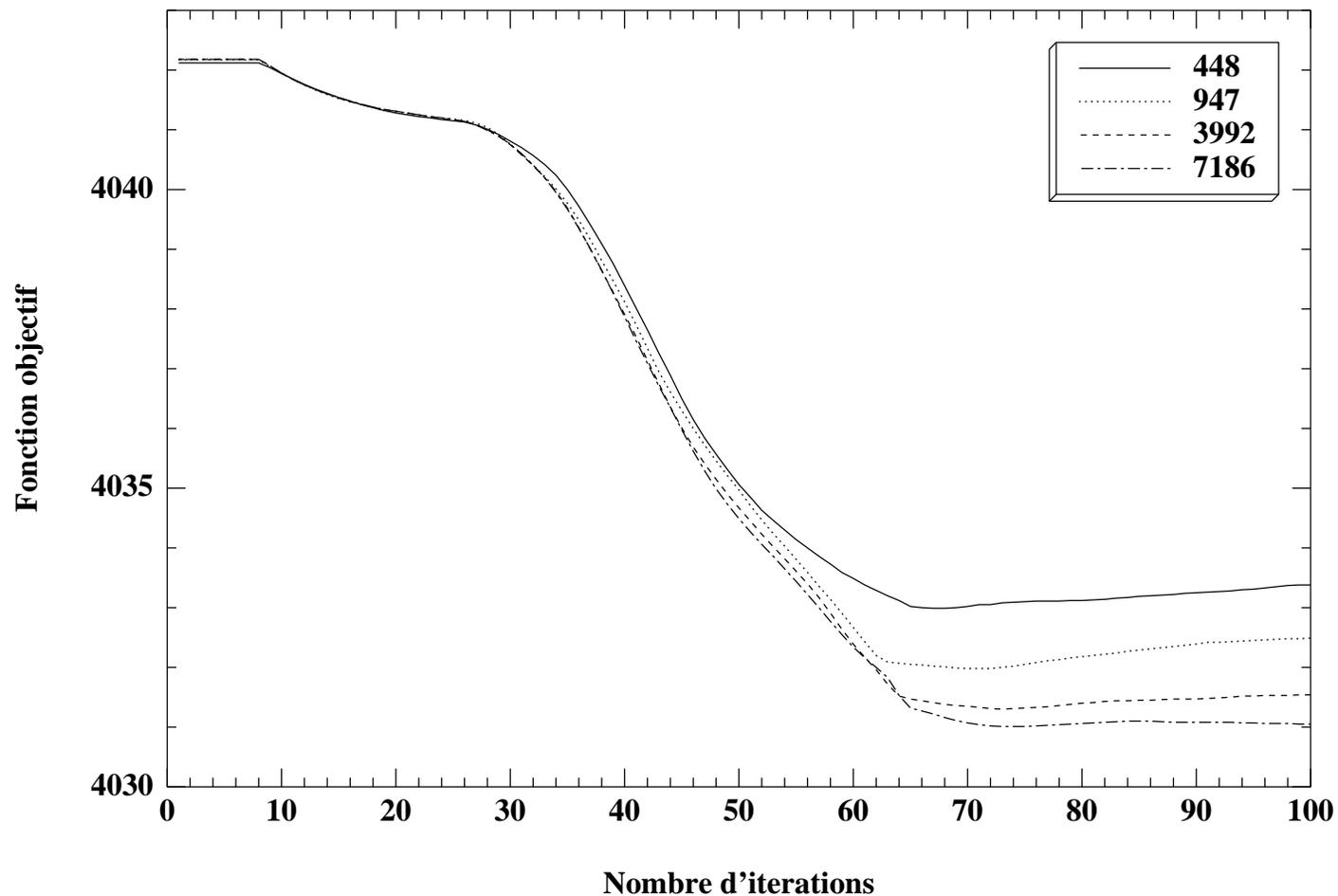
Optimal shapes for meshes with 448, 947, 3992, 7186 triangles



No convergence under mesh refinement !

More and more details appear when the mesh size is decreased.

The value of the objective function decreases with the mesh size.



5.6.4 Regularization

Triple motivation:

- ➡ To avoid instabilities when using $P1$ finite elements for u and $P0$ for h (less expensive than $P2-P0$).
- ➡ To obtain an algorithm which converges by mesh refinement.
- ➡ To adhere to the “regularized” framework of section 5.2.3 (with **existence** of optimal solutions).

Main idea: we change the scalar product

$$\langle J'(h), k \rangle = \int_{\Omega} k \nabla u \cdot \nabla p \, dx \quad \forall k \in \mathcal{U}_{ad}.$$

Previously we identified \mathcal{U}_{ad} to a subspace of $L^2(\Omega)$, thus

$$\langle J'(h), k \rangle = \int_{\Omega} J'(h) k \, dx \quad \Rightarrow \quad J'(h) = \nabla u \cdot \nabla p .$$

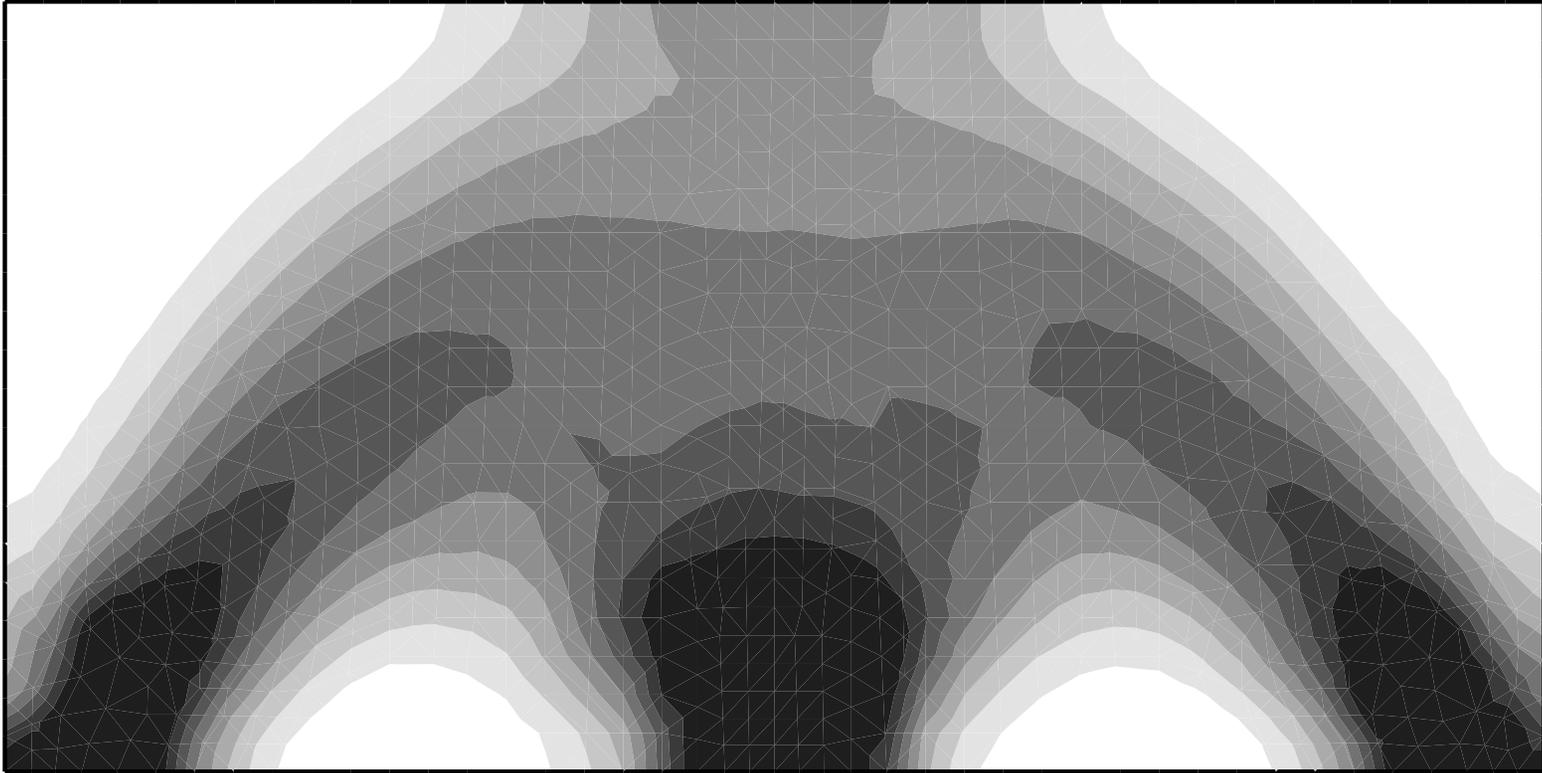
Now, we identify a “regularized” admissible set \mathcal{U}_{ad}^{reg} to a subspace $H^1(\Omega)$, thus

$$\langle J'(h), k \rangle = \int_{\Omega} (\nabla J'(h) \cdot \nabla k + J'(h)k) \, dx ,$$

and we deduce a new formula for the gradient

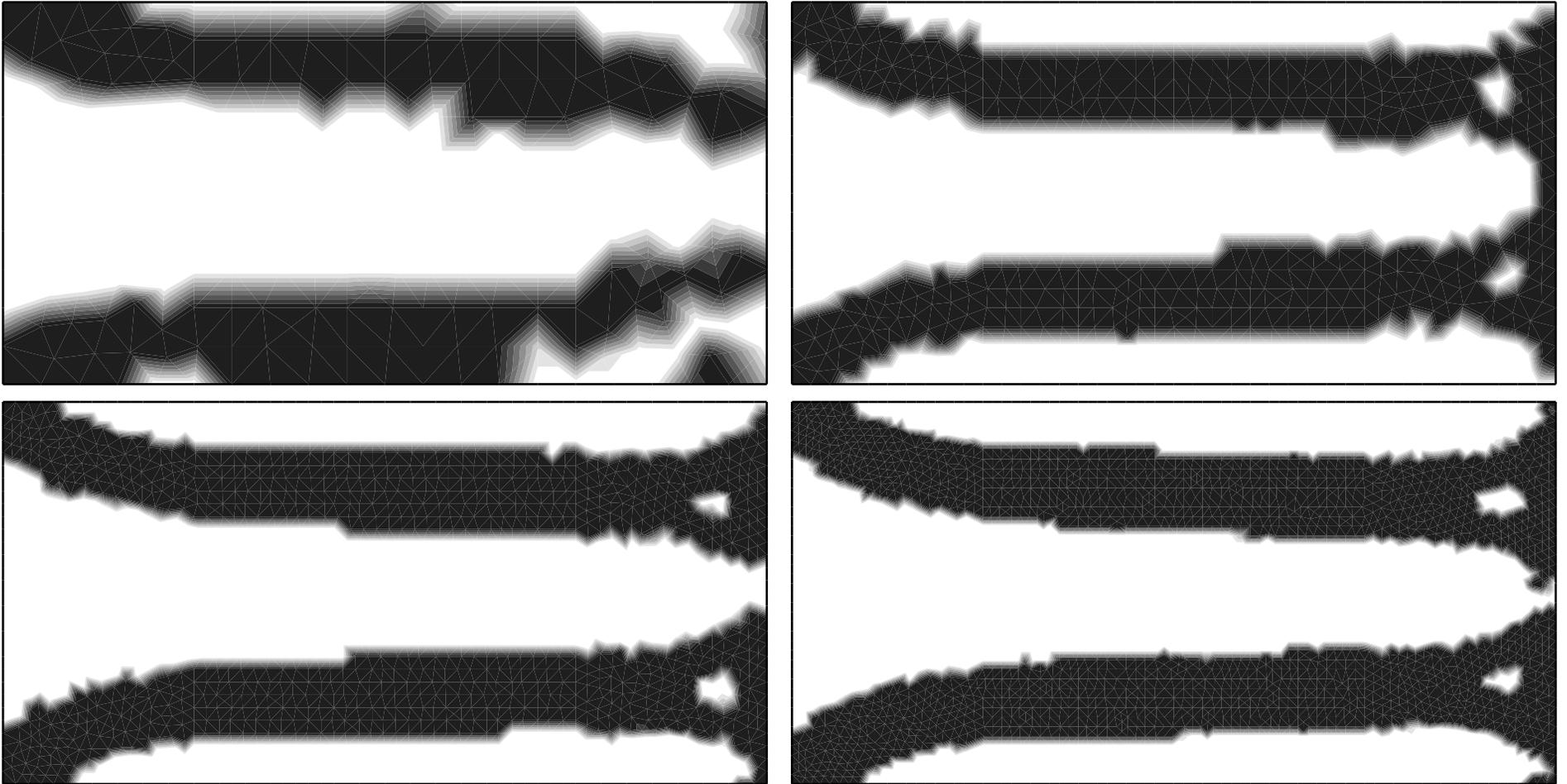
$$\begin{cases} -\Delta J'(h) + J'(h) = \nabla u \cdot \nabla p & \text{in } \Omega, \\ \frac{\partial J'(h)}{\partial n} = 0 & \text{on } \partial\Omega. \end{cases}$$

Regularized optimal shape



Finite elements P_1 - P_0 . Compliance minimization. Alternate directions algorithm.

Convergence by mesh refinement



Same case as the “numerical counter-examples” (meshes 448, 947, 3992, 7186).

Conclusion

- ➡ Regularization works !
- ➡ It costs a bit more (solving an additional Laplacian to compute the gradient).
- ➡ Difficulty in choosing the regularization parameter $\epsilon > 0$ (which can be interpreted as a lengthscale)

$$-\epsilon^2 \Delta J'(h) + J'(h) = \nabla u \cdot \nabla p \quad \text{in } \Omega$$

- ➡ It has a tendency to smooth the geometric details.

CHAPTER VI

GEOMETRIC OPTIMIZATION (First Part)

Geometric optimization of a membrane

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

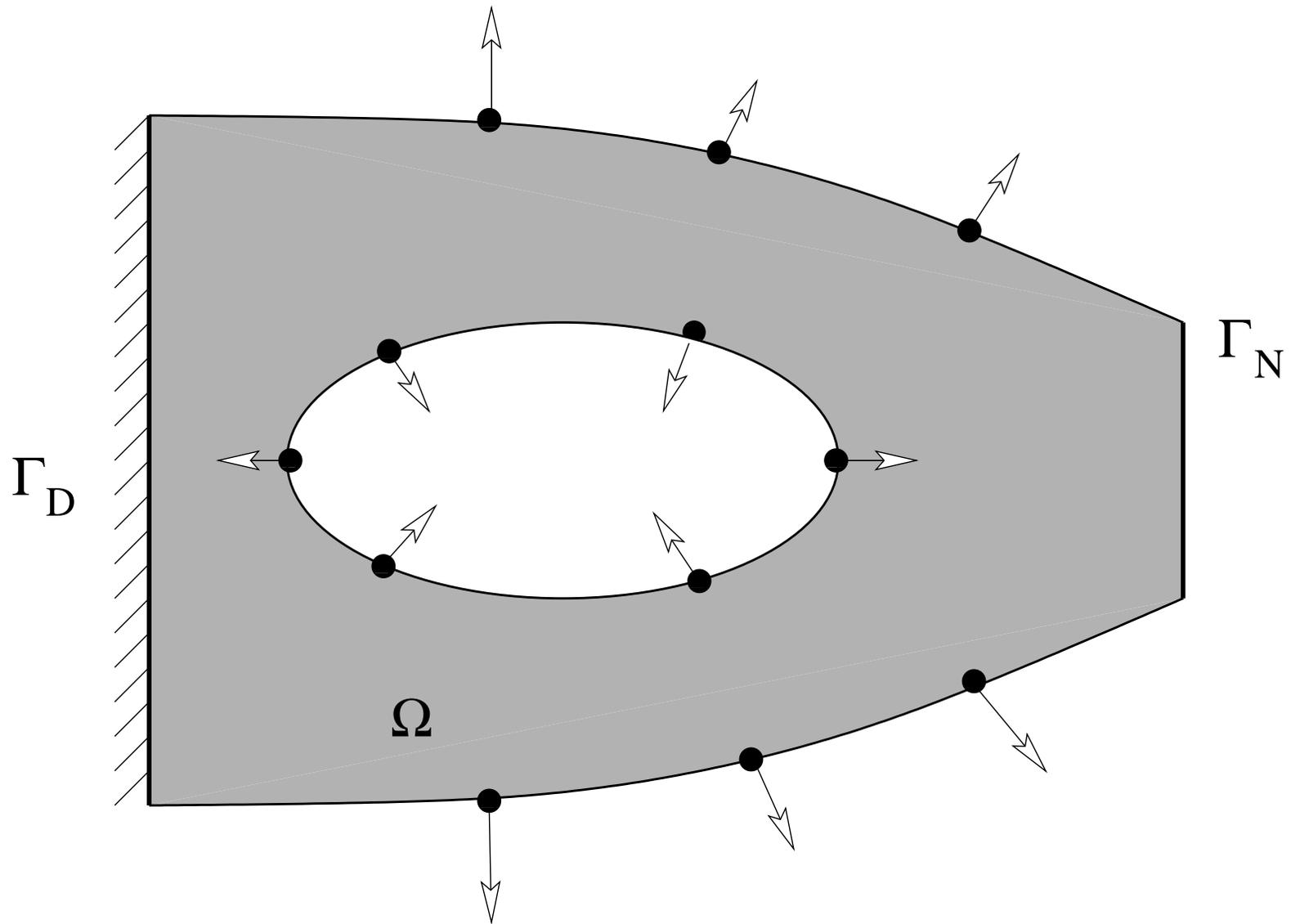
$$\partial\Omega = \Gamma \cup \Gamma_N \cup \Gamma_D,$$

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.

$$\left\{ \begin{array}{ll} -\Delta u = 0 & \text{in } \Omega \\ u = 0 & \text{on } \Gamma_D \\ \frac{\partial u}{\partial n} = g & \text{on } \Gamma_N \\ \frac{\partial u}{\partial n} = 0 & \text{on } \Gamma \end{array} \right.$$

(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 define 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

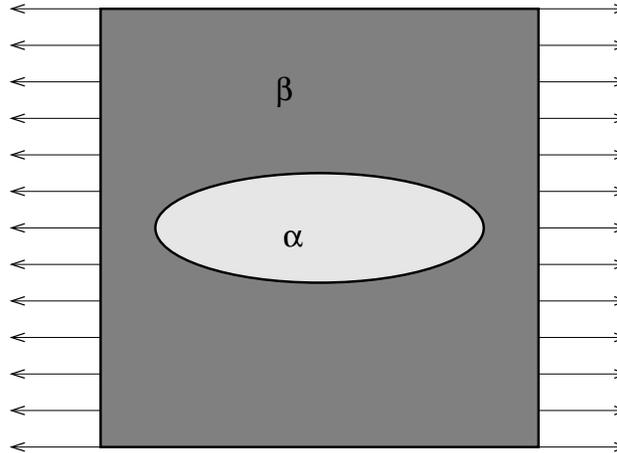
In full generality, there does not exist any optimal shape !

- ➡ 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 $\beta \gg \alpha > 0$. 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 preferred !

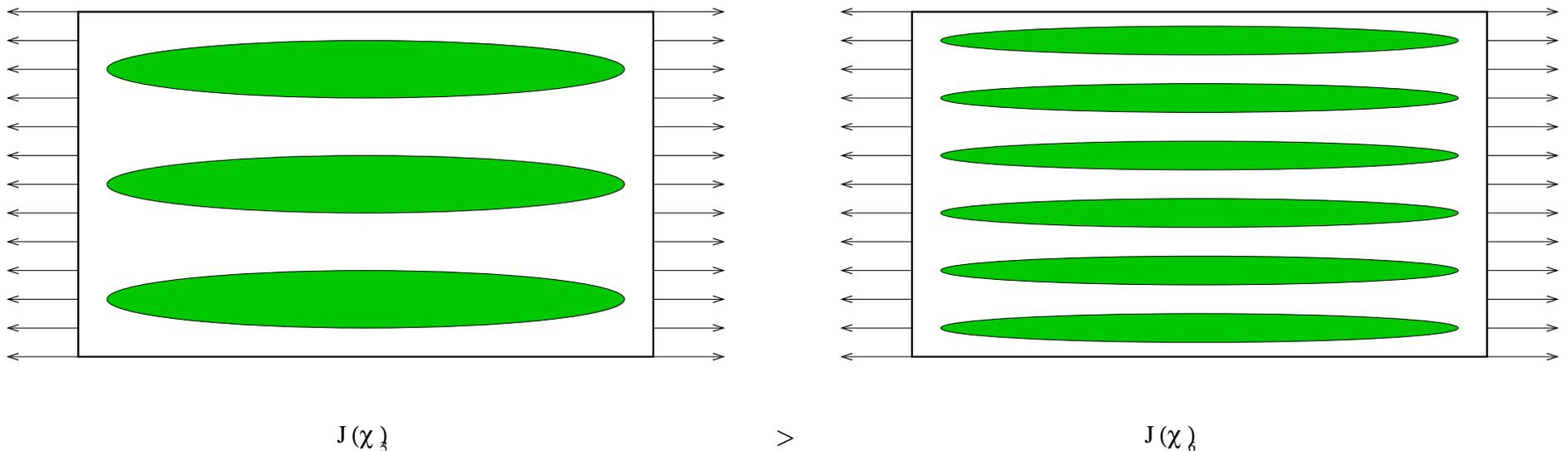
The shape optimization problem is:

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

Non-existence

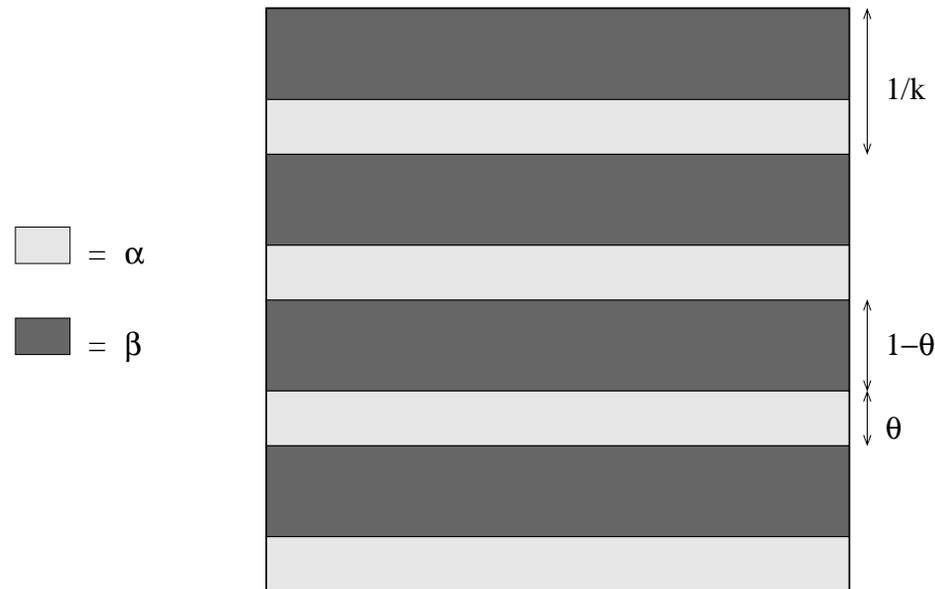
Proposition 6.2. If $0 < \theta < 1$, there does not exist an optimal shape in the set \mathcal{U}_{ad} .

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 $k \rightarrow +\infty$: 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.

6.2.2 Existence under a geometric condition

Let D be a given working domain. We define

$$\mathcal{U}_{ad} = \left\{ \Omega \subset D \text{ such that } \begin{array}{l} (i) \ \Omega \text{ satisfies the uniform cone property} \\ (ii) \ \Gamma_D \cup \Gamma_N \subset \partial\Omega \text{ and } |\Omega| = V_0 \end{array} \right\}$$

where V_0 is a fixed volume.

Theorem 6.6 (D. Chenais). The shape optimization problem

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

admits at least one minimizer.

Remark. Condition (i) implies a bound on the boundary curvature radius and prevents the creation of small holes.

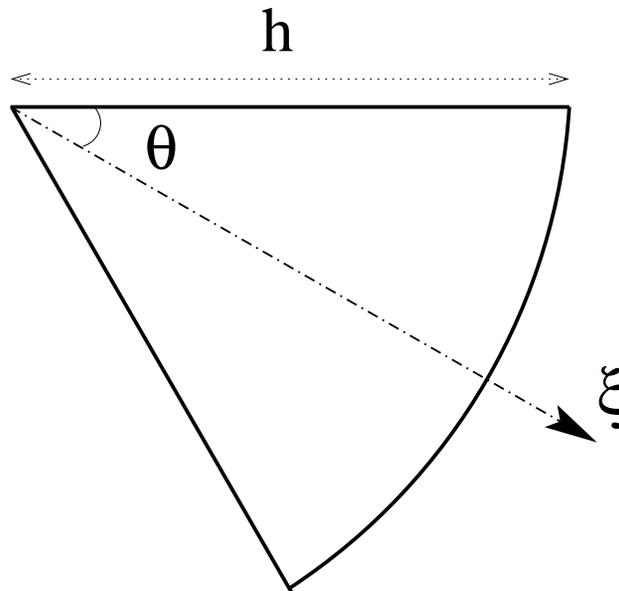
Definition of a cone

Let $\theta \in]0, \pi/2[$ be an angle, $h > 0$ a height, and $\xi \in \mathbb{R}^N$ a unit direction. A **cone** of angle θ , height h and direction ξ is the open set

$$C(\theta, h, \xi) = \{x \in \mathbb{R}^N \text{ such that } x \cdot \xi > \|x\| \cos \theta \text{ et } \|x\| < h\}.$$

For $y \in \mathbb{R}^N$, the cone of vertex y is defined by

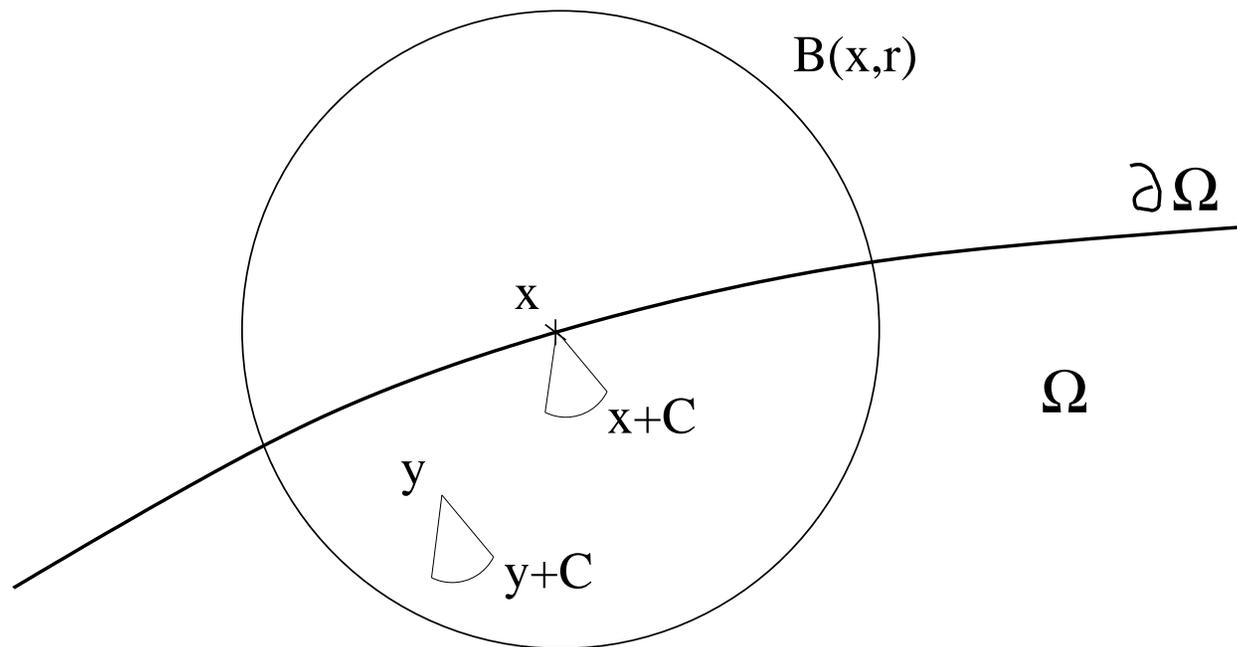
$$y + C(\theta, h, \xi) = \{y + x \text{ such that } x \in C(\theta, h, \xi)\}.$$



Uniform cone property

Let θ be an angle, $h > 0$ a height, and $r > 0$ a radius. An open set Ω is said to “**satisfy the uniform cone property**” if, for any $x \in \partial\Omega$, there exists a unit vector ξ_x such that

$$\forall y \in B(x, r) \cap \Omega \quad y + C(\theta, h, \xi_x) \subset \Omega.$$



6.2.3 Existence under a topological condition (in dimension $N = 2$)

A working domain $D \subset \mathbb{R}^2$ is fixed. For any shape $\Omega \subset D$ we define its **holes number**, or more precisely, the number of connected components of its complementary

$$\#cc(D \setminus \Omega).$$

For a given integer k and a volume V_0 , we define

$$\mathcal{U}_{ad} = \left\{ \Omega \subset D \text{ such that } \begin{array}{l} (i) \#cc(D \setminus \Omega) \leq k \\ (ii) \Gamma_D \cup \Gamma_N \subset \partial\Omega \text{ and } |\Omega| = V_0 \end{array} \right\}$$

Theorem 6.9 (V. Sverak, A. Chambolle). The shape optimization problem

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

admits at least one minimizer.

Remark. Condition (i) prevents the creation of too many holes.

6.2.4 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

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

(They are perturbations of the identity $\text{Id}: x \rightarrow x$.)

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

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

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

Remark: ϕ is continuous but its gradient is just 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 $\mathcal{D}(\Omega_0)$

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

- ➡ 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

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

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

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

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

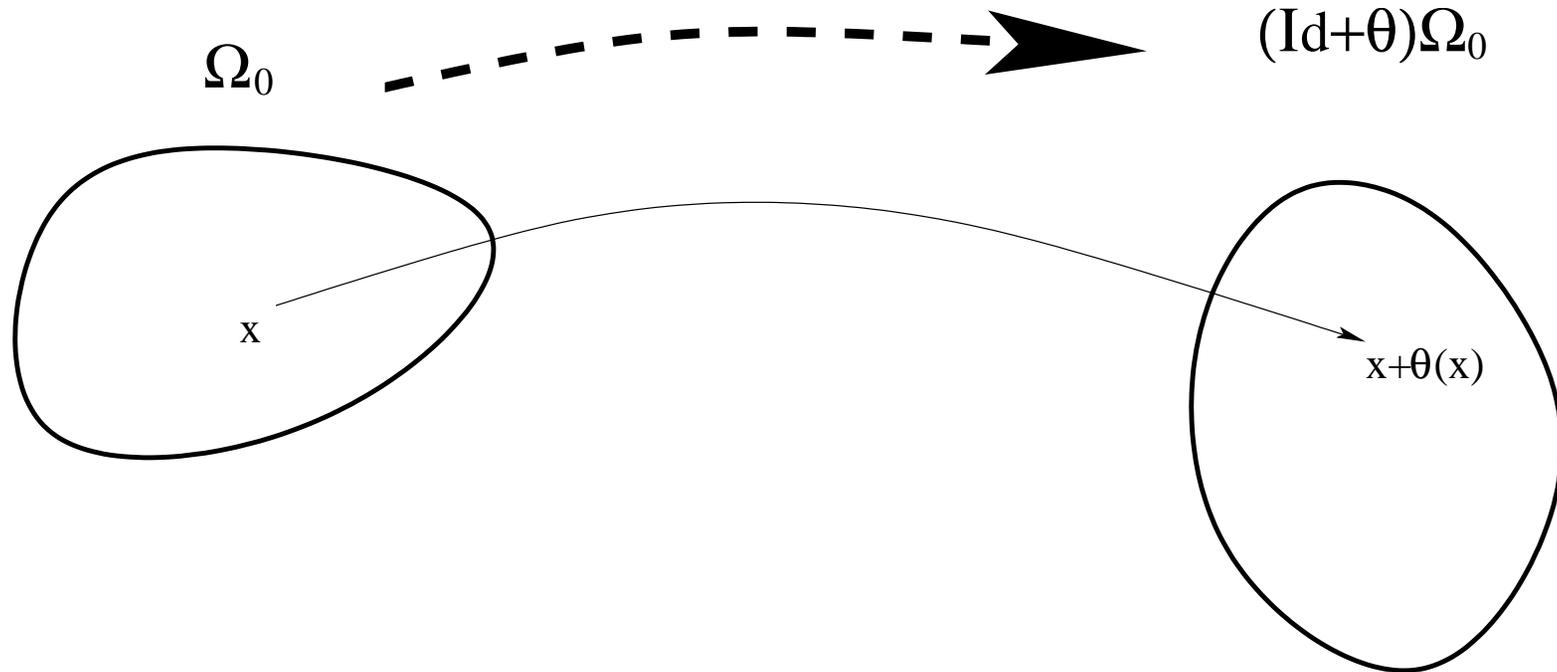
$$T = \text{Id} + \theta \quad \text{with} \quad \theta \in W^{1,\infty}(\mathbb{R}^N; \mathbb{R}^N)$$

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

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

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

with a given incremental function g .



The shape $\Omega = (\text{Id} + \theta)(\Omega_0)$ 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 $T = \text{Id} + \theta$ is one-to-one into \mathbb{R}^N and belongs to the set \mathcal{T} .

Proof. Based on the formula

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

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

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

$$\theta \rightarrow J((\text{Id} + \theta)(\Omega_0))$$

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

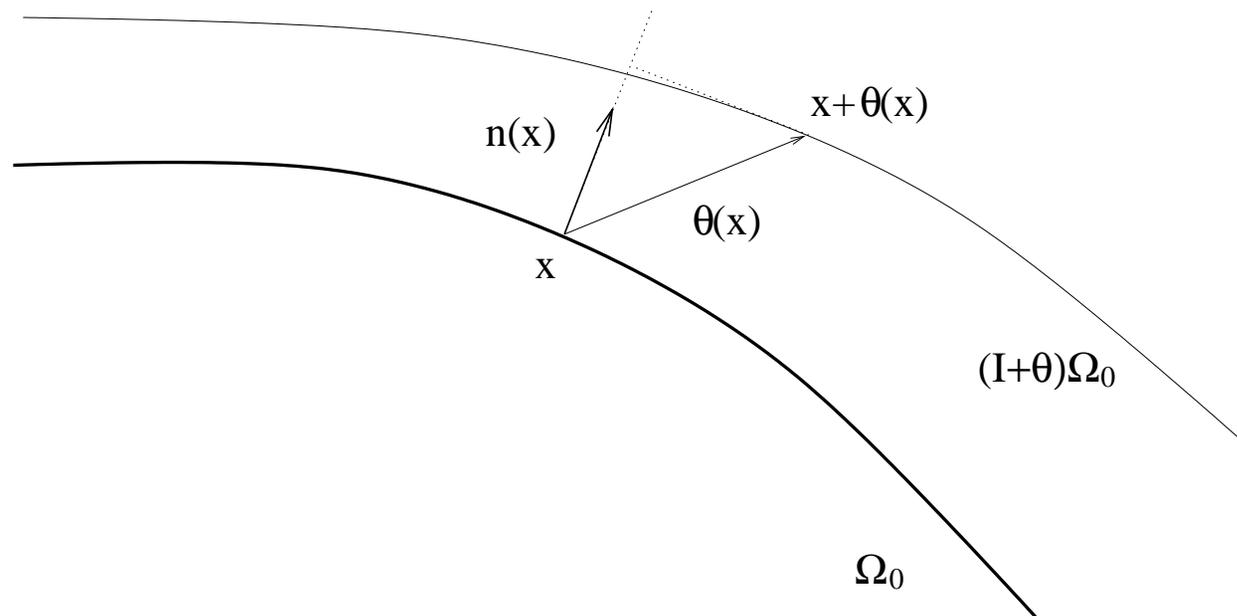
$$J((\text{Id} + \theta)(\Omega_0)) = J(\Omega_0) + L(\theta) + o(\theta) \quad , \quad \text{with} \quad \lim_{\theta \rightarrow 0} \frac{|o(\theta)|}{\|\theta\|} = 0 .$$

$J'(\Omega_0)$ 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.,

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



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

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

which satisfies

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

$$y(\lambda t, x, \theta) = y(t, x, \lambda\theta) \quad \text{for any } \lambda \in \mathbb{R}$$

Then we define the one-to-one map from \mathbb{R}^N into \mathbb{R}^N , $x \rightarrow e^\theta(x) = y(1, x, \theta)$, the inverse of which is $e^{-\theta}$, $e^0 = \text{Id}$, and $t \rightarrow e^{t\theta}(x)$ 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 $t \geq t_0$,

$$\frac{d}{dt} \left(\phi(\tilde{y}(t, x_0)) \right) = \frac{d\tilde{y}}{dt} \cdot \nabla\phi(\tilde{y}) = \tilde{\theta}(\tilde{y}) \cdot n|n_0| = 0$$

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

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

By the chain rule lemma we deduce

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

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 $f \in L^p(T(\Omega_0))$ 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, $f \in W^{1,p}(T(\Omega_0))$ if and only if $f \circ T \in W^{1,p}(\Omega_0)$, and

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

(^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 $f \in L^1(\partial T(\Omega_0))$. Then $f \circ T \in L^1(\partial\Omega_0)$, and we have

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

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

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

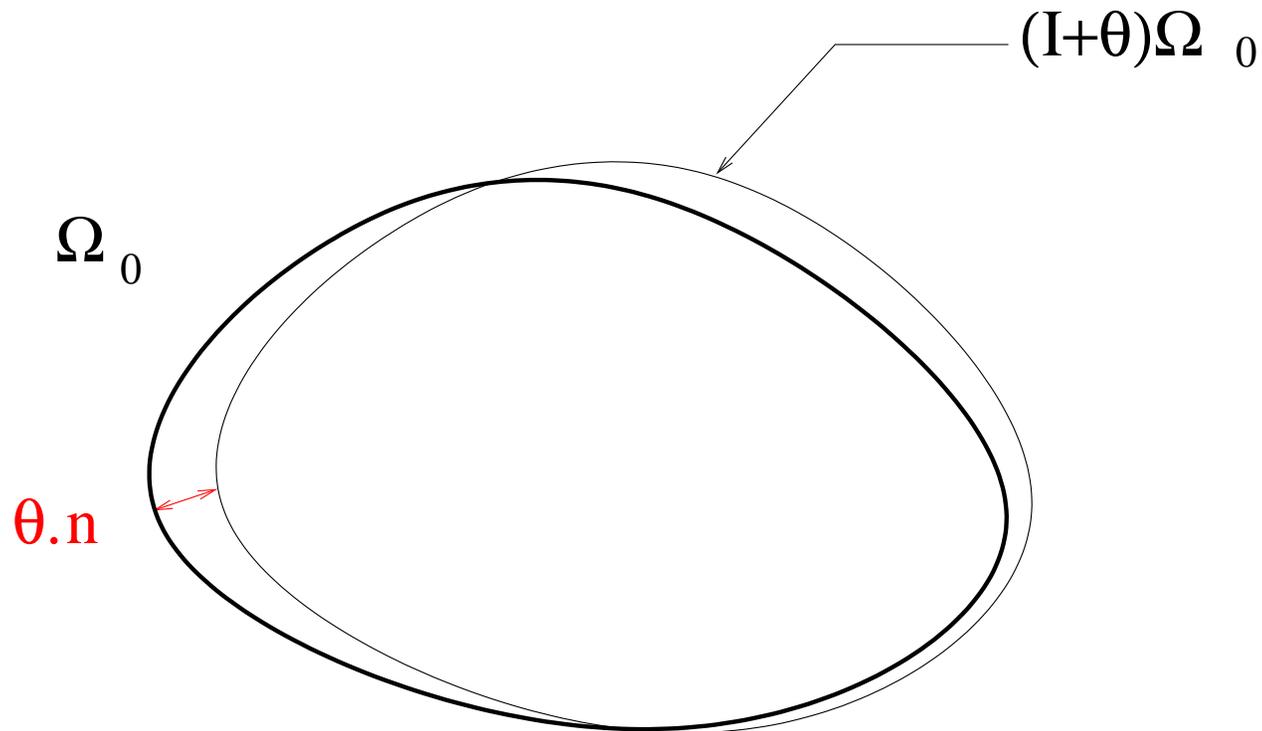
Then J is shape differentiable at Ω_0 and

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

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 $(\text{Id} + \theta)\Omega_0$ and Ω_0
 $\approx \partial\Omega_0 \times (\theta \cdot n)$. Thus

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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