Shape and topology optimization of structures built by additive manufacturing

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Outline of the course

- 1 - Introduction: a review of additive manufacturing
- 2 - Parametric optimization and the adjoint method
- 3 - Geometric optimization and Hadamard method
- 4 - Topology optimization and the level set method
- 5 - Typical constraints from additive manufacturing
- 6 - Optimization of lattice materials
- 7 - Coupled shape and laser path optimization

A "hot" topic with a lot of room for new ideas and modeling...

Chapter 2 - Parametric optimization and the adjoint method

- I - Introduction and motivation
- II - Thickness optimization
- III - Computation of a gradient
- IV - Self-adjoint case: the compliance
- V - Numerical algorithm and results

G. Allaire, *Conception optimale de structures*, Mathématiques et Applications, Vol. 58, Springer (2007).

G. Allaire, L. Cavallina, N. Miyake, T. Oka, T. Yachimura, *The homogenization method for topology optimization of structures: old and new*, Interdisciplinary Information Sciences, 25(2), pp.75-146 (2019).

A problem of optimal design (or shape optimization) for structures is defined by three ingredients:

- a **model** (typically a partial differential equation) to evaluate (or analyse) the mechanical behavior of a structure,
- an **objective function** which has to be minimized or maximized, or sometimes several objectives (also called cost functions or criteria),
- a **set of admissible designs** which precisely defines the optimization variables, including possible constraints.

Classification of optimal design problems

Optimal design problems can roughly be classified in three categories from the "easiest" ones to the "most difficult" ones:

- **parametric or sizing** optimization for which designs are parametrized by a few variables (for example, thickness or member sizes), implying that the set of admissible designs is considerably simplified,
- **geometric or shape** optimization for which all designs are obtained from an initial guess by moving its boundary (without changing its topology, i.e., its number of holes in 2-d),
- **topology** optimization where both the shape and the topology of the admissible designs can vary without any explicit or implicit restrictions.

Why studying parametric optimization ?

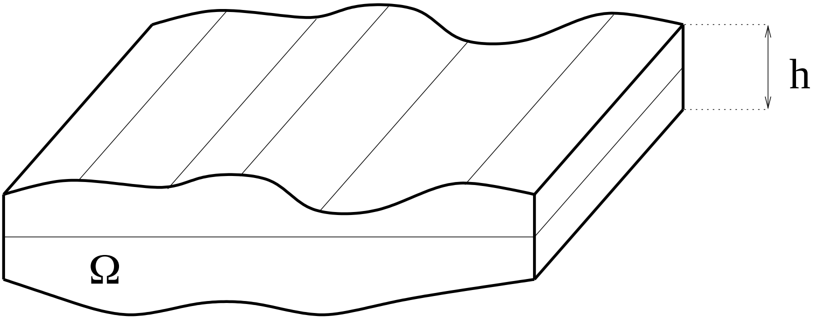
The three categories of optimal design problems (parametric, geometric, topology) share some common features in terms of:

- applications,
- sensitivities or gradients,
- adjoint method.

To simplify the exposition, we start with the simplest case of parametric optimization.

Remark: some topology optimization methods (like SIMP or homogenization) are very similar to parametric optimization...

One example of parametric optimization is thickness optimization of an elastic membrane.



- $\Omega =$ mean surface of a (plane) membrane
- $h =$ thickness in the normal direction to the mean surface

Membrane model

The membrane deformation is modeled by its vertical displacement $u(x) : \Omega \to \mathbb{R}$, solution of the following partial differential equation (p.d.e.), the so-called **membrane model**,

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

with the thickness h, bounded by minimum and maximum values

$$0 < h_{min} \leq h(x) \leq h_{max} < +\infty.$$

The thickness h is the optimization variable.

It is a **sizing or parametric** optimal design problem because the computational domain Ω does not change.

Variational formulation

We assume that Ω is bounded and Lipschitz and $f \in L^2(\Omega)$.

The variational formulation of the membrane model is: find $u \in H^1_0(\Omega)$ such that, for any $v \in H^1_0(\Omega)$

$$\int_\Omega h \nabla u \cdot \nabla v \, dx = \int_\Omega f v \, dx$$

By Lax-Milgram lemma, there exists a unique solution $u \in H^1_0(\Omega)$.

The set of admissible thicknesses is

$$\mathcal{U}_{ad} = \left\{ h(x) \in L^2(\Omega) \text{ such that } \begin{array}{l} 0 < h_{min} \le h(x) \le h_{max} \\ \int_\Omega h(x)\, dx = h_0 |\Omega| \end{array} \right\},$$

where h_0 is an imposed average thickness.

Possible additional "feasibility" constraints: according to the production process of membranes, the thickness $h(x)$ can be discontinuous, or on the contrary continuous ; its derivative $h'(x)$ can be uniformly bounded (molding-type constraint) or even its second-order derivative $h''(x)$, linked to the curvature radius (milling-type constraint).

The **optimization criterion** is linked to some mechanical property of the membrane, evaluated through its displacement u, solution of the p.d.e.,

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

where, of course, u depends on h. For example, the global rigidity of a structure is often measured by its **compliance**, or work done by the load: the smaller the work, the larger the rigidity (be careful ! compliance = - rigidity). In such a case,

$$j(u) = fu.$$

Another example amounts to achieve (at least approximately) a **target displacement** $u_0(x)$, which means

$$j(u) = |u - u_0|^2.$$

Conditions on the objective function

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

To ensure that the criterion $J(h)$ is well-defined and will be differentiable, we assume:

- j is a C^1 function from $\mathbb{R}$ to $\mathbb{R}$,
- $|j(u)| \leq C(u^2 + 1)$,
- $|j'(u)| \leq C(|u| + 1)$.

Since $u \in H^1_0(\Omega)$, we have

$$J(h) < +\infty \quad \text{and} \quad j'(u) \in L^2(\Omega).$$

Continuity of the cost function

Proposition. The application

$$h \to J(h) = \int_\Omega j(u)\, dx$$

is continuous from $\mathcal{U}_{ad}$ into $\mathbb{R}$.

Proof. Exercise !

Non-existence theory

In full generality, there does not exist a solution of the optimization problem

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

where u depends on h as the solution in $H^1_0(\Omega)$ of

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

- There are precise mathematical counter-examples (based on homogenization).
- It shows up numerically: non convergence, instabilities...
- Compliance is a miracle: existence of solutions.

For a given positive constant R, replace $\mathcal{U}_{ad}$ by

$$\mathcal{U}_{ad}^R = \left\{ h \in \mathcal{U}_{ad} \cap H^1(\Omega) \, , \quad \|h\|_{H^1(\Omega)} \leq R \right\} .$$

Theorem. There exists a solution h^R of the optimization problem

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

where u depends on h as the solution in $H_0^1(\Omega)$ of

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

Proof. Exercise by using a compactness argument.

Remark. The bound R is the same for all elements of $\mathcal{U}_{ad}^R$.

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

$$\mathcal{U} = \{h \in L^\infty(\Omega)\,, \quad \exists h_* > 0 \text{ such that } h(x) \geq h_* \text{ in } \Omega\}\,.$$

Lemma. The application $h \to u(h)$, which gives the solution $u(h) \in H_0^1(\Omega)$ for $h \in \mathcal{U}$, is differentiable and its directional derivative at h in the direction $k \in L^\infty(\Omega)$ is given by

$$\langle u'(h), k\rangle = v,$$

where v is the unique solution in $H_0^1(\Omega)$ of

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

Proof of differentiability

Proof. Formally, one simply computes the directional derivative. Define $h(t) = h + tk$ for $t > 0$. Let $u(t)$ be the solution for the thickness $h(t)$. Deriving with respect to t leads to

$$\begin{cases} -\operatorname{div}\left(h(t)\nabla u'(t)\right) = \operatorname{div}\left(h'(t)\nabla u(t)\right) & \text{in } \Omega \\ u'(t) = 0 & \text{on } \partial\Omega, \end{cases}$$

and, since $h'(0) = k$, we deduce $u'(0) = v$.
More rigorously, one could use an implicit function theorem for the variational formulation.

Directional derivative of the objective function

Lemma. For $h \in \mathcal{U}$, let $u(h)$ be the state in $H^1_0(\Omega)$ and

$$J(h) = \int_\Omega j\big(u(h)\big)\, dx \; .$$

The application $J(h)$, from $\mathcal{U}$ into $\mathbb{R}$, is differentiable and its directional derivative at h in the direction $k \in L^\infty(\Omega)$ is given by

$$\langle J'(h), k\rangle = \int_\Omega j'\big(u(h)\big) v\, dx \; ,$$

where $v = \langle u'(h), k\rangle$ is the unique solution in $H^1_0(\Omega)$ of

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

Proof. By simple composition of differentiable applications.

This formula is useless because v is implicit in k !

We introduce an adjoint state p defined as the unique solution in $H_0^1(\Omega)$ of

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

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

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

Remark. Here, the full gradient is explicitly given !

Proof. To make explicit $J'(h)$, we must eliminate $v = \langle u'(h), k\rangle$. We use the adjoint state for that: multiplying the equation for v by p and that for p by v, we integrate by parts

$$\int_\Omega h\nabla p \cdot \nabla v \, dx = -\int_\Omega j'(u)v \, dx$$

$$\int_\Omega h\nabla v \cdot \nabla p \, dx = -\int_\Omega k\nabla u \cdot \nabla p \, dx$$

Comparing these two equalities we deduce

$$\langle J'(h), k\rangle = \int_\Omega j'(u)v \, dx = \int_\Omega k\nabla u \cdot \nabla p \, dx,$$

for any $k \in L^\infty(\Omega)$. Since $\nabla u \cdot \nabla p$ belongs to $L^1(\Omega)$, we check that $J'(h)$ is continuous on $L^\infty(\Omega)$.

We explain that the adjoint is not a trick but it comes naturally as the Lagrange multiplier of a constrained optimization problem.

Recall the definition of a Lagrangian for the following simple optimization problem

$$\inf_{x\in\mathbb{R}^n, C(x)=0} F(x)$$

where C, F are two functions from $\mathbb{R}^n$ into $\mathbb{R}$.
The Lagrangian $\mathcal{L}(x,\lambda)$ is defined from $\mathbb{R}^n\times$ into $\mathbb{R}$ by

$$\mathcal{L}(x,\lambda) = F(x) + \lambda C(x)$$

A simple computation yields

$$\inf_{x\in\mathbb{R}^n} \sup_{\lambda\in\mathbb{R}} \mathcal{L}(x,\lambda) = \inf_{x\in\mathbb{R}^n, C(x)=0} F(x)$$

Lagrangian for thickness optimization

Here, the constraint is the variational formulation of the state equation.

Definition. For independent variables $(h, \hat{u}, \hat{p}) \in L^\infty(\Omega) \times H^1_0(\Omega) \times H^1_0(\Omega)$, the Lagrangian is defined by

$$\mathcal{L}(h, \hat{u}, \hat{p}) = \int_\Omega j(\hat{u})\, dx + \int_\Omega \hat{p} \left(-\operatorname{div}(h \nabla \hat{u}) - f \right) dx,$$

where $\hat{p}$ is a Lagrange multiplier (a function) for the constraint which connects u to h.

By integration by parts we get

$$\mathcal{L}(h, \hat{u}, \hat{p}) = \int_\Omega j(\hat{u})\, dx + \int_\Omega \left(h \nabla \hat{p} \cdot \nabla \hat{u} - f \hat{p} \right) dx.$$

By definition (because the Lagrangian is linear in $\hat{p}$), the partial derivative of $\mathcal{L}$ with respect to p in the direction $\phi \in H_0^1(\Omega)$ is

$$\langle \frac{\partial \mathcal{L}}{\partial p}(h, \hat{u}, \hat{p}), \phi \rangle = \int_\Omega \left(h \nabla \hat{u} \cdot \nabla \phi - f \phi \right) dx,$$

which, when it vanishes, is nothing else than the variational formulation of the state equation.

Definition. The adjoint $p \in H_0^1(\Omega)$ is defined as the solution of the variational formulation

$$\langle \frac{\partial \mathcal{L}}{\partial u}(h, \hat{u}, \hat{p}), \phi \rangle = 0 \quad \forall \phi \in H_0^1(\Omega).$$

Adjoint equation

A simple computation shows that

$$\langle \frac{\partial \mathcal{L}}{\partial u}(h, \hat{u}, \hat{p}), \phi \rangle = \int_\Omega j'(\hat{u})\phi \, dx + \int_\Omega (h \nabla \hat{p} \cdot \nabla \phi) \, dx.$$

Therefore,

$$\langle \frac{\partial \mathcal{L}}{\partial u}(h, \hat{u}, \hat{p}), \phi \rangle = 0 \quad \forall \phi \in H_0^1(\Omega).$$

is indeed equivalent to our previous variational formulation of the adjoint equation

$$\int_\Omega j'(\hat{u})\phi \, dx + \int_\Omega (h \nabla \hat{p} \cdot \nabla \phi) \, dx = 0 \quad \forall \phi \in H_0^1(\Omega).$$

Theorem. The differential of the objective function is given by

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

where u is the state and p is the adjoint.

Proof. Since u satisfies its variational formulation, we have

$$J(h) = \mathcal{L}(h, u, \hat{p}) \quad \forall \hat{p} \in H_0^1(\Omega).$$

Thus, if $u(h)$ is differentiable, we get

$$\langle J'(h), k \rangle = \langle \frac{\partial \mathcal{L}}{\partial h}(h, u, \hat{p}), k \rangle + \langle \frac{\partial \mathcal{L}}{\partial u}(h, u, \hat{p}), \frac{\partial u}{\partial h}(k) \rangle$$

Then, taking $\hat{p} = p$, the second term vanishes to yield

$$\langle J'(h), k \rangle = \langle \frac{\partial \mathcal{L}}{\partial h}(h, u, p), k \rangle$$

Conclusion

This approach is called the adjoint method.

- Introduce a Lagrangian $\mathcal{L}(h, \hat{u}, \hat{p})$ for independent variables.
- The notation $\hat{u}, \hat{p}$ indicates that these functions are not solutions of any equations...
- The partial derivative of $\mathcal{L}$ with respect to p gives the variational formulation of the state equation for u.
- The partial derivative of $\mathcal{L}$ with respect to u gives the variational formulation of the adjoint equation for p.
- The partial derivative of $\mathcal{L}$ with respect to h, evaluated at u and p, gives the formula of the differential $J'(h)$.
- This method is simple but does not prove that one can differentiate $J(h)$.

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

More can be said ! We use the dual or complementary energy

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

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.

Lemma. The function $\phi(a,\sigma) = a^{-1}|\sigma|^2$, defined from $\mathbb{R}^+ \times \mathbb{R}^N$ into $\mathbb{R}$, is convex and satisfies

$$\phi(a,\sigma) = \phi(a_0,\sigma_0) + \phi'(a_0,\sigma_0)\cdot(a-a_0,\sigma-\sigma_0) + \phi(a,\sigma - \frac{a}{a_0}\sigma_0),$$

where the derivative is given by

$$\phi'(a_0,\sigma_0)\cdot(b,\tau) = -\frac{b}{a_0^2}|\sigma_0|^2 + \frac{2}{a_0}\sigma_0\cdot\tau.$$

Theorem. There exists a minimizer to the compliance minimization problem.

Proof. Use the direct method fo the calculus of variations and the convexity property of $\phi(a,\sigma)$.

Lemma. Take $\tau \in L^2(\Omega)^N$. 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

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

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

This is at the root of a numerical algorithm called "optimality criteria" or "alternate minimization".

Projected gradient

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

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

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).

Projection operator

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

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

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 **dichotomy** algorithm based on the monotonicity of

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

which is strictly increasing on an interval $[\ell^-, \ell^+]$ and constant outside.

Numerical results for an elastic plate

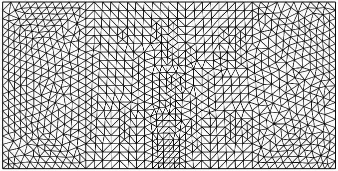
Replace the membrane model by the 2-d elasticity equations

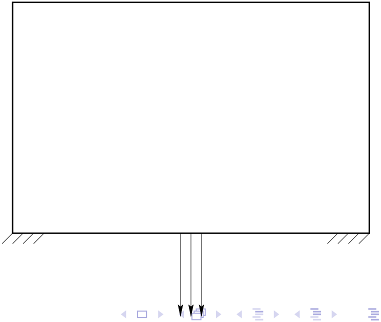
$$\begin{cases} -\operatorname{div}\sigma = f & \text{in } \Omega \\ \sigma = 2\mu h\, e(u) + \lambda h \operatorname{tr}(e(u))\, \mathrm{Id} & \text{in } \Omega \\ u = 0 & \text{on } \Gamma_D \\ \sigma n = g & \text{on } \Gamma_N \end{cases}$$

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

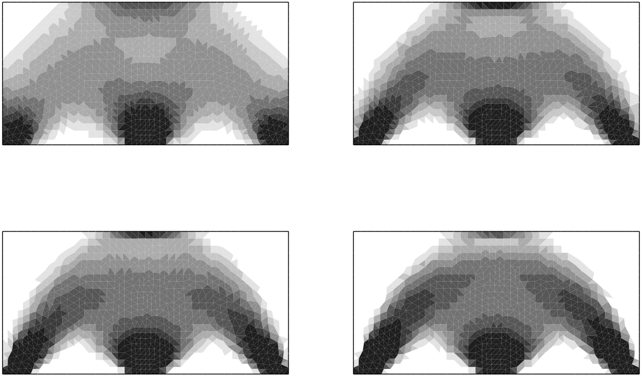
FreeFem++ computations ; scripts available on the web page
`http://www.cmap.polytechnique.fr/~allaire/cours_X_annee3.html`

Mesh and boundary conditions:

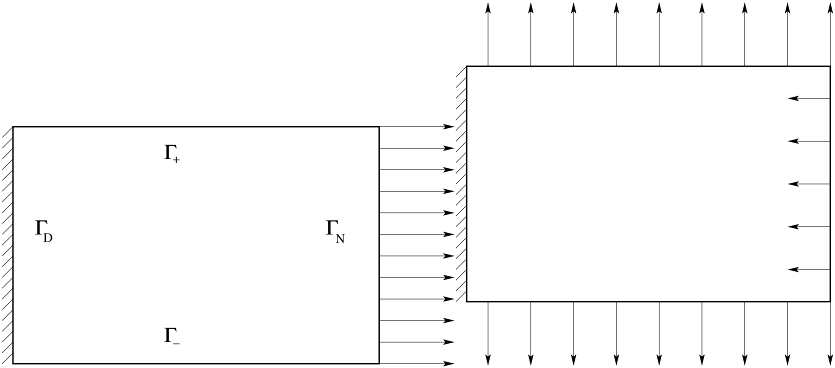




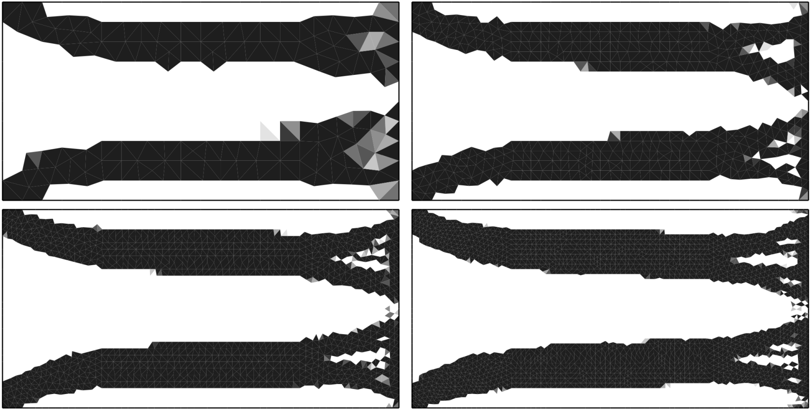
Compliance minimization: iterations 1, 5, 10 and 30



Boundary conditions and target displacement u_0:



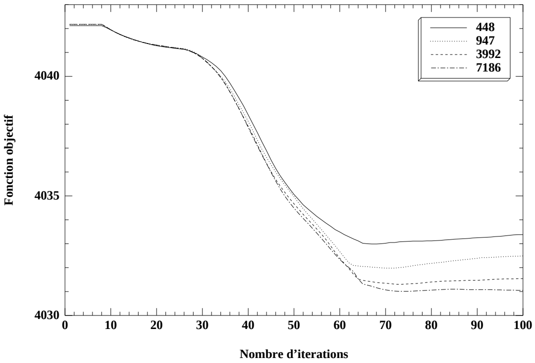
Optimal shapes for meshes with 448, 947, 3992, 7186 triangles



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.



Exercises (just in case !)

If you want to practice the adjoint method, find the adjoint and the objective differential for the following problems.

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

where $\partial\Omega = \Gamma_D \cup \Gamma_N$.

1. $J_1(h) = \int_\Omega |\nabla u|^2 dx$
2. $J_2(h) = \int_\Omega |h\nabla u|^2 dx$
3. $J_3(h) = \int_{\Gamma_N} |u - u_0|^2 ds$