Shape Optimization by the level-set method

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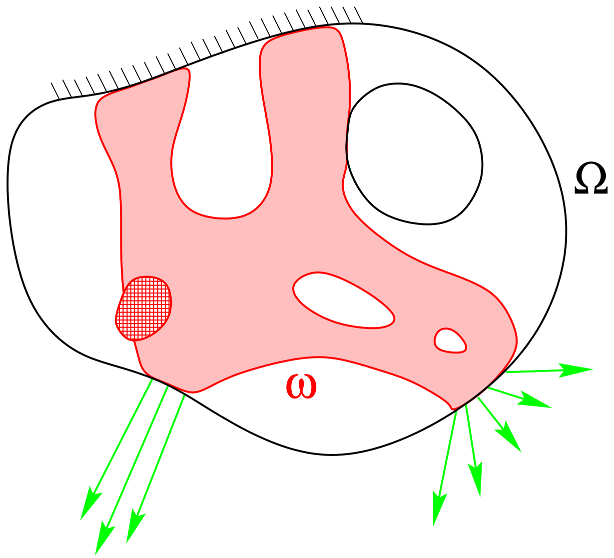
Model problem



Find the *most rigid* structure ω, of prescribed volume, contained into a given domain Ω, when given external forces are applied.

$$\inf_{\omega\subset\Omega, |\omega|=V} J(\omega)$$

where $J(\omega)$ is the *objective-function*.

1) Shape sensitivity optimization

- Hadamard method, revisited by many authors (Murat-Simon, Pironneau, Nice's school, etc.).

- Ill posed problem: many local minima, no convergence under mesh refinement.

- En practice, topology changes very difficult to handle.

- Very costly because of remeshing (3d).

- Very general: any model or objective function.

- Widely used method.

2) Topology optimization

• Homogenization method (Murat-Tartar, Lurie-Cherkaev, Kohn-Strang, Bendsoe-Kikuchi, Allaire-Bonnetier-Francfort-FJ, etc.).

$\longrightarrow$ simple objective functions, linear models but well posed problem.

• Evolutionary algorithms (Schoenauer, etc.).

• Topological asymptotics, topological gradient (Sokolowski, Masmoudi, etc.).

• Very cheap because it captures shapes on a fixed mesh.

Combine the advantages of the two approaches

- Fixed mesh $\longrightarrow$ low computational cost.
  $\longrightarrow$ less instabilities.

- General method based on shape derivative.

Main tools:
1. shape derivative (Murat-Simon),
2. level-set method (Osher-Sethian).

• Some previous works: Sethian and Wiegmann (JCP 2000), Osher and Santosa (JCP 2001), Wang, Wang and Guo (CMAME 2003). Similar (but different) from the phase field approach of Bourdin and Chambolle (COCV 2003).

• Remaining drawbacks:
1. reduction of topology (rather than variation) in 2d,
2. local minima.

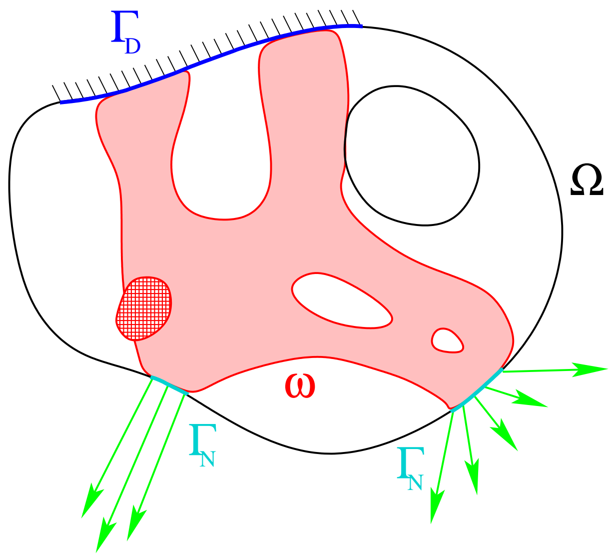
Hint: topological gradient

Setting of the problem

Linearly elastic material. Isotropic Hooke's law A (nonlinear will take place at the end of the talk).
u displacement field, $e(u) = \frac{1}{2}\left(\nabla u + \nabla u^T\right)$ deformation tensor.

Linearized elasticity system posed on ω:

$$\begin{cases} -\mathrm{div}\big(Ae(u)\big) & = & 0 & \text{in } \omega \\ u & = & 0 & \text{on } \partial\omega \cap \Gamma_D \\ \big(Ae(u)\big)\cdot n & = & g & \text{on } \partial\omega \cup \Gamma_N \end{cases}$$



It admits a unique solution.

Various objective functions

* **Compliance :**

$$J(\omega) = \int_\omega Ae(u) : e(u)dx = \int_\omega A^{-1}\sigma : \sigma dx = \int_{\partial\omega} f \cdot u\, ds = c(\omega)$$

Global measurement of rigidity.
The most widely used in structural topology optimization. Good theory and very efficient numerical methods.

* **Least square criteria :** for example

$$J(\omega) = \left\{ \int_\omega k(x)|u(x) - u_0(x)|^\alpha dx \right\}^{1/\alpha}$$

where u_0 is a given *target-displacement*, $\alpha \geq 2$ and k a given multiplier.
$\longrightarrow$ *Micromechanical systems optimization (MEMS)*

* **Stress-dependent objective function :** for example $J(\omega) = \int_\omega |\sigma|^2$

Existence theory

Minimal set of admissible shapes

$$\mathcal{U}_{ad} = \left\{ \omega \subset \Omega, \ \ \text{vol}(\omega) = V_0, \ \Gamma_D \cup \Gamma_N \subset \partial\omega \right\}$$

where Ω is open and bounded in $\mathbb{R}^N$.

Usually, the minimization problem has no solutions in $\mathcal{U}_{ad}$.

Existence under additional conditions:

- *Uniform cone condition* (D.Chenais)
- *Perimeter constraint* (L.Ambrosio, G.Buttazzo)
- In 2d, *a uniformly bounded number of connected components of* $\Omega \setminus \omega$ (A.Chambolle)

Numerical method strategy

1) Computation of the shape derivatives of the objectives functions (in a continuous framework). $\longrightarrow$ Murat-Simon method.

2) The derivatives are discretized. The shapes are modeled by a level-set function on a fixed mesh. The shape is varied by advecting the level-set function following the flow of the shape gradient.
$\longrightarrow$ transport equation of Hamilton-Jacobi type.

3) After convergence (to a local minimum), additional computation of the topological gradient to guess where it may be advantageous to dig new holes (and back to point 1)).

Shape derivative (Murat-Simon)

Let ω_0 be a reference domain. Consider domains of the type

$$\omega = \big(Id + \theta\big)\omega_0 \quad \text{with} \quad \theta \in W^{1,\infty}(\mathbb{R}^N; \mathbb{R}^N).$$

Lemma: For any $\theta \in W^{1,\infty}(\mathbb{R}^N; \mathbb{R}^N)$ such that $\|\theta\|_{W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)} < 1$, $(Id + \theta)$ is a diffeomorphism in $\mathbb{R}^N$.

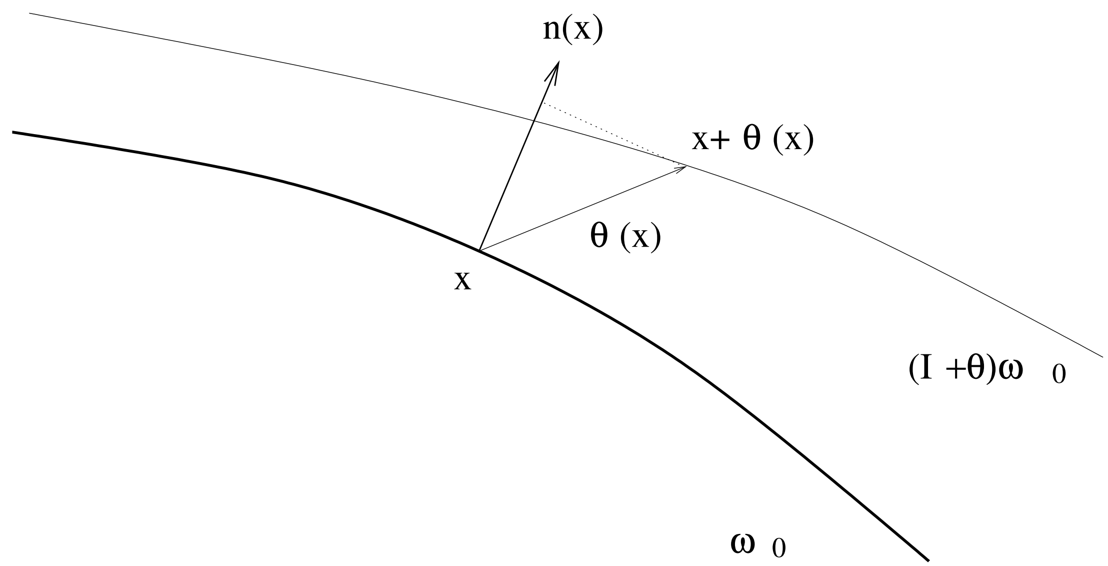
Definition: the shape derivative of $J(\omega)$ at ω_0 is the Fréchet differential of $\theta \to J\big((Id + \theta)\omega_0\big)$ at 0.

The set $\omega = (Id + \theta)(\omega_0)$ is defined by

$$\omega = \{x + \theta(x) \mid x \in \omega_0\}.$$

$\theta(x)$ can be understood as a vector field *advecting* the reference domain ω_0.

The shape derivative $J'(\omega_0)(\theta)$ depends only of $\theta \cdot n$ on the boundary $\partial\omega_0$.



Lemma: Let ω_0 be a smooth bounded open set and $J(\omega)$ at differentiable function at ω_0. Its derivative satisfies

$$J'(\omega_0)(\theta_1) = J'(\omega_0)(\theta_2)$$

if $\theta_1, \theta_2 \in W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$ are such that

$$\begin{cases} \theta_2 - \theta_1 \in \mathcal{C}^1(\mathbb{R}^N;\mathbb{R}^N) \\ \theta_1 \cdot n = \theta_2 \cdot n \quad \text{on } \partial\omega_0. \end{cases}$$

Examples of shape derivatives (I)

Objective-function defined in the domain: Let ω_0 be a smooth bounded open set of class $\mathcal{C}^1$ of $\mathbb{R}^N$. Let $f(x) \in W^{1,1}(\mathbb{R}^N)$ and J defined by

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

Then J is differentiable at ω_0 and

$$J'(\omega_0)(\theta) = \int_{\omega_0} \mathrm{div}\,\big(\theta(x)\,f(x)\big)\,dx = \int_{\partial\omega_0} \theta(x)\cdot n(x)\,f(x)\,ds$$

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

Examples of shape derivatives (II)

Objective-function defined on the boundary: Let ω_0 be a smooth bounded open set of class $\mathcal{C}^1$ of $\mathbb{R}^N$. Let $f(x) \in W^{2,1}(\mathbb{R}^N)$ and J defined by

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

Then J is differentiable at ω_0 and

$$J'(\omega_0)(\theta) = \int_{\partial\omega_0} \big(\nabla f \cdot \theta + f\big(\mathrm{div}\,\theta - \nabla\theta n \cdot n\big)\big)\, ds$$

for all $\theta \in W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$. Moreover if ω_0 is smooth of class $\mathcal{C}^2$, then

$$J'(\omega_0)(\theta) = \int_{\partial\omega_0} \theta \cdot n \left(\frac{\partial f}{\partial n} + Hf\right) ds,$$

where H is the mean curvature of $\partial\omega_0$ defined by $H = \mathrm{div}\, n$.

Shape derivative of the compliance

$$J(\omega) = \int_{\Gamma \cup \Gamma_N} g \cdot u \, ds = \int_\omega A\, e(u) \cdot e(u) \, dx,$$

$$J'(\omega_0)(\theta) = \int_{\Gamma_0} \left(2 \left[\frac{\partial (g \cdot u)}{\partial n} + H g \cdot u \right] - A e(u) \cdot e(u) \right) \theta \cdot n \, ds,$$

where u is the state (displacement field) in ω_0, and H the mean curvature of Γ_0.

No adjoint state involved. The compliance problem is self-adjoint.

Shape derivative of the least-square criteria

$$J(\omega) = \left(\int_\omega k(x) |u - u_0|^\alpha dx \right)^{1/\alpha},$$

$$J'(\omega_0)(\theta) = \int_{\Gamma_0} \left(\frac{\partial (g \cdot p)}{\partial n} + H g \cdot p - Ae(p) \cdot e(u) + \frac{C_0}{\alpha} k |u - u_0|^\alpha \right) \theta \cdot n \, ds,$$

where the state u is solution of the elasticity system and the adjoint state p is solution of

$$\begin{cases} -\mathrm{div}\ (A\, e(p)) = C_0 k(x) |u - u_0|^{\alpha-2} (u - u_0) & \text{in } \omega_0 \\ p = 0 & \text{on } \Gamma_D \\ \big(Ae(p)\big) \cdot n = 0 & \text{on } \Gamma_N \cup \Gamma_0, \end{cases}$$

with $C_0 = \left(\int_{\omega_0} k(x) |u(x) - u_0(x)|^\alpha dx \right)^{1/\alpha - 1}.$

“Classical” numerical method

- Parameterization of the boundary by control points.
- Evaluation of the state and the adjoint to compute the shape derivative.
- Displacement of the control points in the gradient direction.

$\longrightarrow$ Convergence to a local minimum.
$\longrightarrow$ Strong influence of the initial choice and the mesh size.
$\longrightarrow$ Topology (number of holes) cannot vary.
$\longrightarrow$ Very complex and costly remeshing. Almost impossible in 3d.

Front propagation by level-set

Shapes are not meshed, but captured on a fixed mesh of a large box Ω.

Parameterization of the shape ω by a level-set function:

$$\begin{cases} \psi(x) = 0 & \Leftrightarrow x \in \partial\omega \cap \Omega \\ \psi(x) < 0 & \Leftrightarrow x \in \omega \\ \psi(x) > 0 & \Leftrightarrow x \in (\Omega \setminus \omega) \end{cases}$$

- Exterior normal to ω : $n = \nabla\psi / |\nabla\psi|$.
- Mean curvature : $H = \mathrm{div}\ n$.
- These formula make sense everywhere in Ω, not only on the boundary $\partial\omega$.

Hamilton-Jacobi equation

If the shape $\omega(t)$ evolves in pseudo-time t with a normal speed $V(t,x)$, then ψ satisfies a Hamilton-Jacobi equation:

$$\psi\Big(t, x(t)\Big) = 0 \quad \text{for all } x(t) \in \partial\omega(t).$$

deriving in t yields

$$\frac{\partial\psi}{\partial t} + \dot{x}(t)\cdot\nabla\psi = \frac{\partial\psi}{\partial t} + Vn\cdot\nabla\psi = 0.$$

As $n = \nabla\psi/|\nabla\psi|$ we obtain

$$\frac{\partial\psi}{\partial t} + V|\nabla\psi| = 0.$$

This equation is valid on the whole domain Ω, not only on the boundary $\partial\omega$, assuming that the velocity is known everywhere.

Application to shape optimization

Shape derivative:

$$J'(\omega_0)(\theta) = \int_{\Gamma_0} j(u,p,n)\,\theta\cdot n\,ds.$$

Gradient method on the shape

$$\omega_{k+1} = \Big(Id - j(u_k,p_k,n_k)n_k\Big)\omega_k$$

because the normal n_k is naturally extended to the whole Ω. The boundary of the shape is advected with the normal speed $-j$.

$\longrightarrow$ Introducing a "pseudo-time" (descent parameter) we solve

$$\frac{\partial\psi}{\partial t} - j|\nabla\psi| = 0 \quad \text{in } \Omega$$

Numerical algorithm

1. Initialization of the level-set function ψ_0 (e.g. a product of de sinus).

2. Iterations until convergence for $k \geq 1$:

   (a) Computation of u_k and eventually p_k by solving a linearized elasticity problem on the shape ψ_k. Computation of the shape gradient $\rightarrow$ normal velocity V_k

   (b) Transport of the shape by the speed V_k (Hamilton-Jacobi equation) to obtain a new shape ψ_{k+1}. (Several successive time steps can be applied for a same velocity field). The descent step is controlled by the CFL condition on the transport equation and by the decreasing of the objective function.

   (c) Possible reinitialization of the level-set function such that ψ_{k+1} is the signed distance to the interface.

3. *Optionally: computation of the topological gradient to guess where holes may be dig, and return to loop 2.*

Topological Gradient (Sokolovki et al., Masmoudi et al.)

A scalar criterion used to guess where it may be useful to dig additional holes in a converged solution that could be a local minimum.

Examples of topological gradients (2d elasticity, plane strains, Neuman boundary conditions for the holes):

- Example 1 (Compliance optimization):

$$TG = \frac{\pi(\lambda + 2\mu)}{2\mu(\lambda + \mu)} \{4\mu\sigma(u) : e(u) + (\lambda - \mu)\mathrm{tr}\sigma(u)\mathrm{tr}e(u)\}$$

- Example 2 (Minimization of $\int k(x)|u - u_0|^\alpha$):

$$TG = \frac{\pi}{\alpha} C_0 k(x)|u(x) - u_0(x)|^\alpha + \frac{\pi(\lambda + 2\mu)}{2\mu(\lambda + \mu)} \{4\mu\sigma(u) : e(p) + (\lambda - \mu)\mathrm{tr}\sigma(u)\mathrm{tr}e(p)\}$$

Some technical points

• Q1 quadangular structured meshes (2d-3d) $\longrightarrow$ classical upwind transport schemes.

• Possibilities of unstructured meshes $\longrightarrow$ more complicated schemes for Hamilton-Jacobi equation (Abgrall).

• ψ discretized at mesh nodes.

• Resolution of elasticity systems by finite elements:

$$\left\{ \begin{array}{c} -\mathrm{div}\big(\theta(x)Ae(u)\big) = 0 \quad \text{in } \Omega \\ +\text{B.C.} \end{array} \right.$$

with $\theta(x)$ a piecewise constant field defined by

$$\left\{ \begin{array}{lll} \theta & = & \varepsilon \ (\approx 10^{-3}) & \text{if } \psi > 0 \text{ for all the nodes of the element} \\ \theta & = & \text{ad-hoc proportion} & \text{if the 0 level-set goes through the element} \\ \theta & = & 1 & \text{si } \psi < 0 \text{ for all the nodes of the element} \end{array} \right.$$

Transport (structured mesh)

Resolution of

$$\frac{\partial \psi}{\partial t} - j|\nabla \psi| = 0 \quad \text{in } \Omega$$

by an explicit upwind scheme of 1st or 2nd order

$$\frac{\psi_i^{n+1} - \psi_i^n}{\Delta t} - \max(j_i^n, 0)\, g^+(D_x^+ \psi_i^n, D_x^- \psi_i^n) - \min(j_i^n, 0)\, g^-(D_x^+ \psi_i^n, D_x^- \psi_i^n) = 0$$

with $D_x^+ \psi_i^n = \dfrac{\psi_{i+1}^n - \psi_i^n}{\Delta x}, \quad D_x^- \psi_i^n = \dfrac{\psi_i^n - \psi_{i-1}^n}{\Delta x}$, and

$$g^-(d^+, d^-) = \sqrt{\min(d^+, 0)^2 + \max(d^-, 0)^2},$$

$$g^+(d^+, d^-) = \sqrt{\max(d^+, 0)^2 + \min(d^-, 0)^2}.$$

Reinitialization

To regularize the level-set function and avoid it to be *too flat* ($\longrightarrow$ poor precision on ψ) or *too steep* ($\longrightarrow$ poor precision on $\nabla\psi$ i.e. the normal) after some transport steps, a reinitialization is done *from time to time*.

We solve

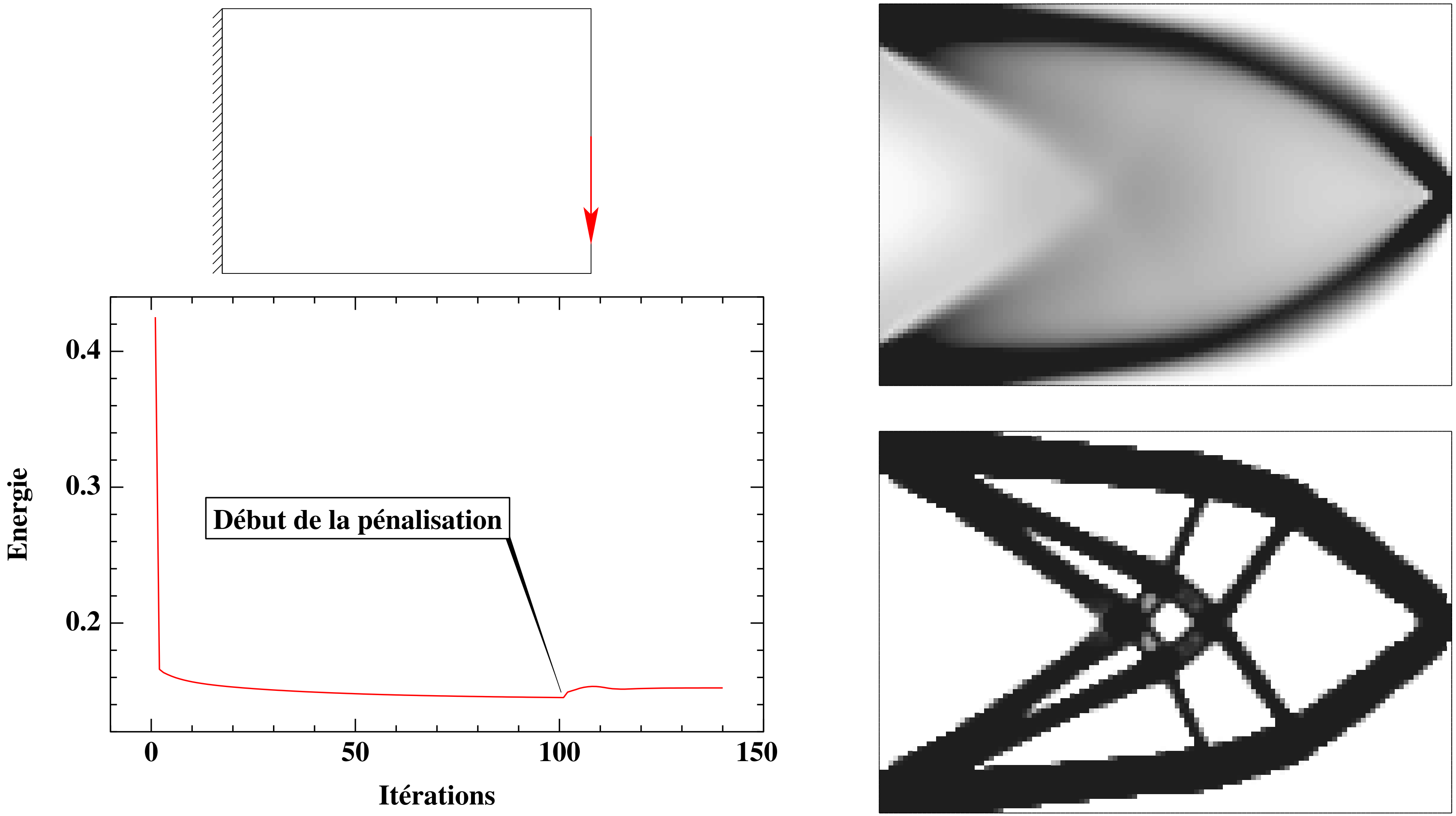
$$\frac{\partial \psi}{\partial t} + \text{sign}(\psi)\Big(|\nabla\psi| - 1\Big) = 0 \quad \text{in } \Omega,$$

whose stationary solution is the function signed distance to the interface:

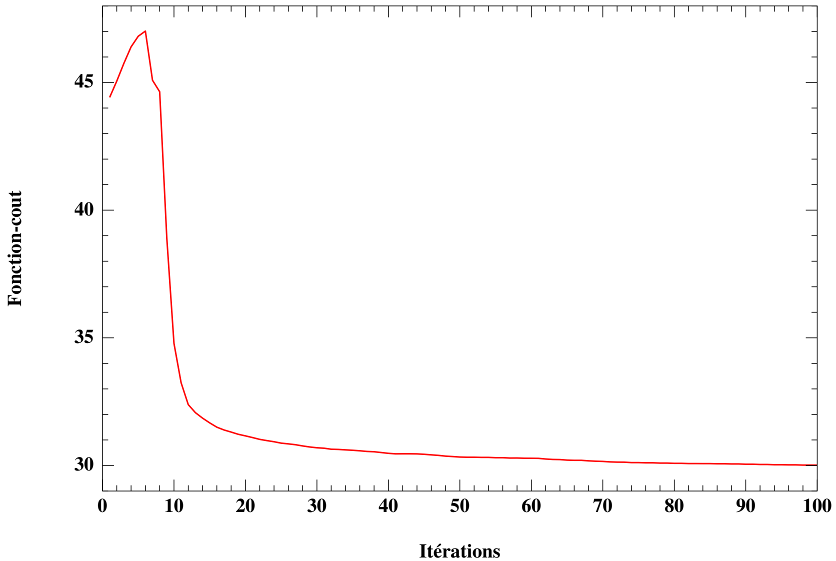
$$\Big\{\psi(t=0,x) = 0\Big\}.$$

- Classical idea in fluid mechanics applications.
- Tricky to pilot...
- Reinitialization is very efficient on some problems.
- Not very well understood...

A numerical result with the homogenization method



Definition of the problem, composite solution, penalized solution, convergence of the objective-function.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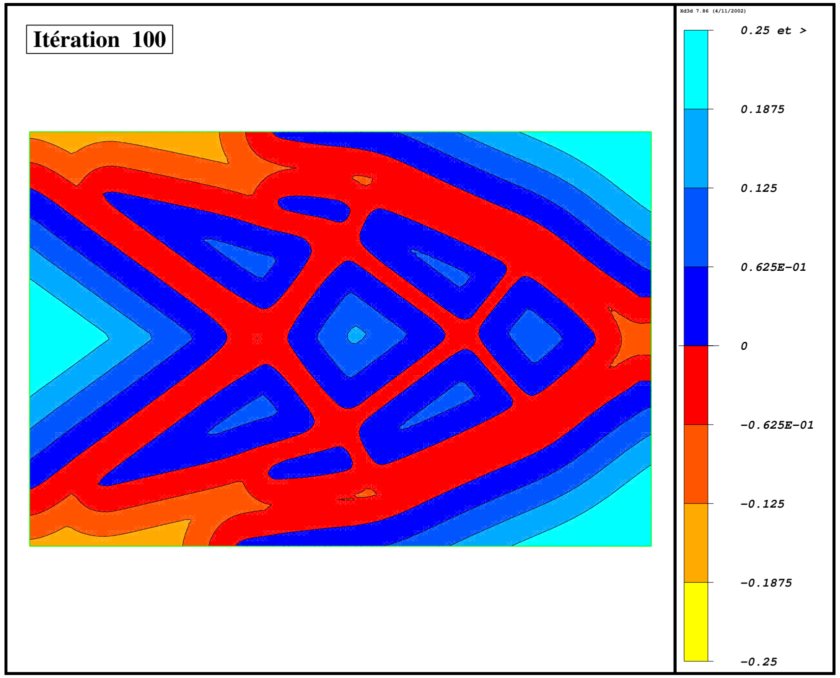
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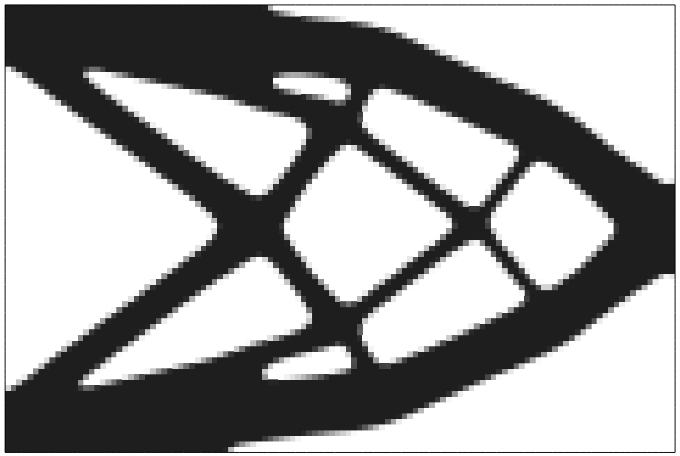

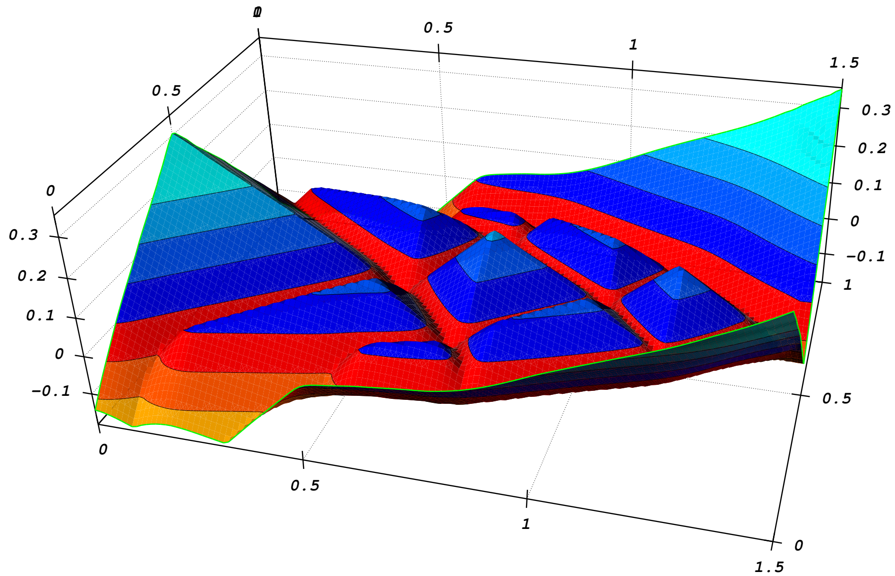
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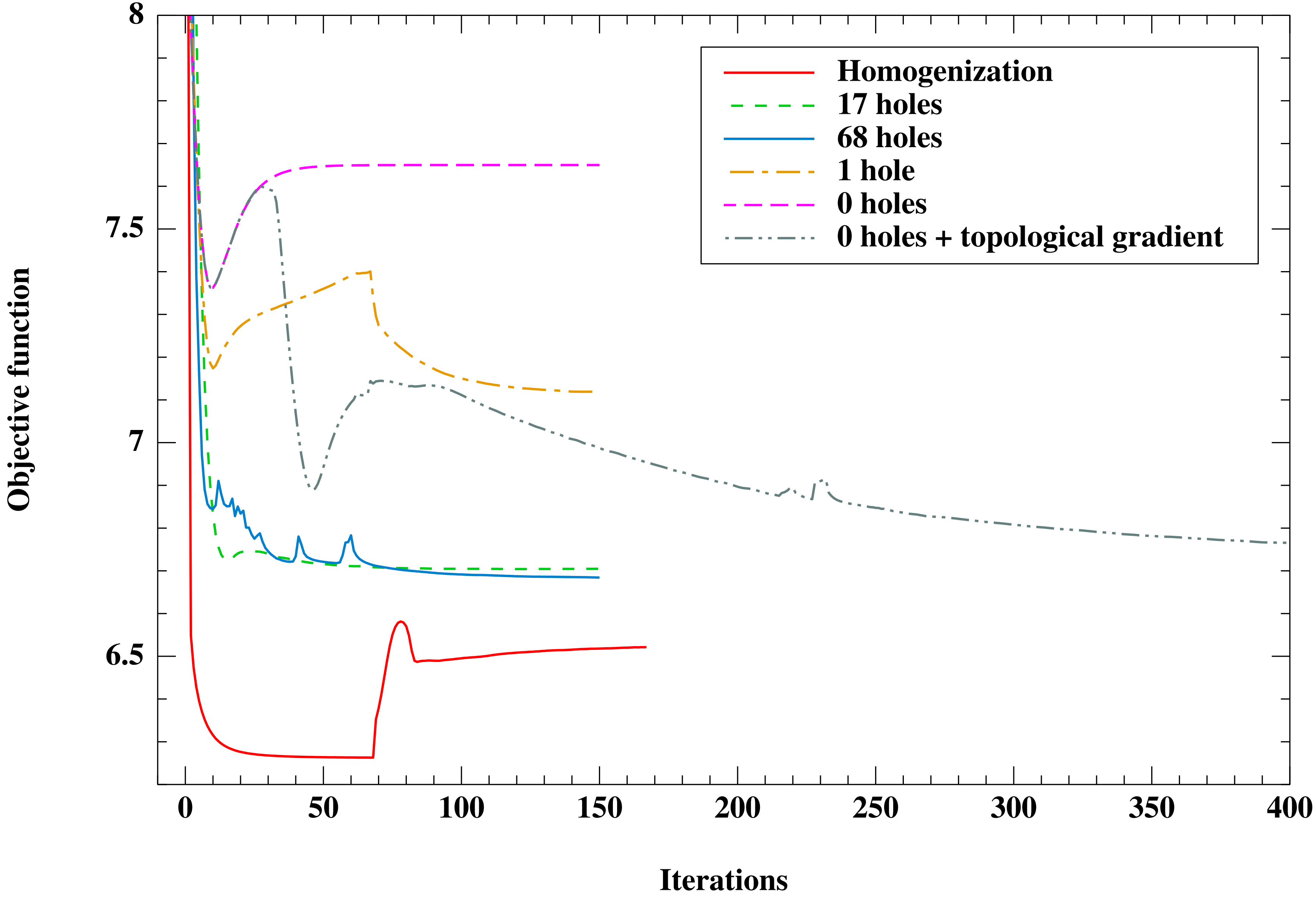
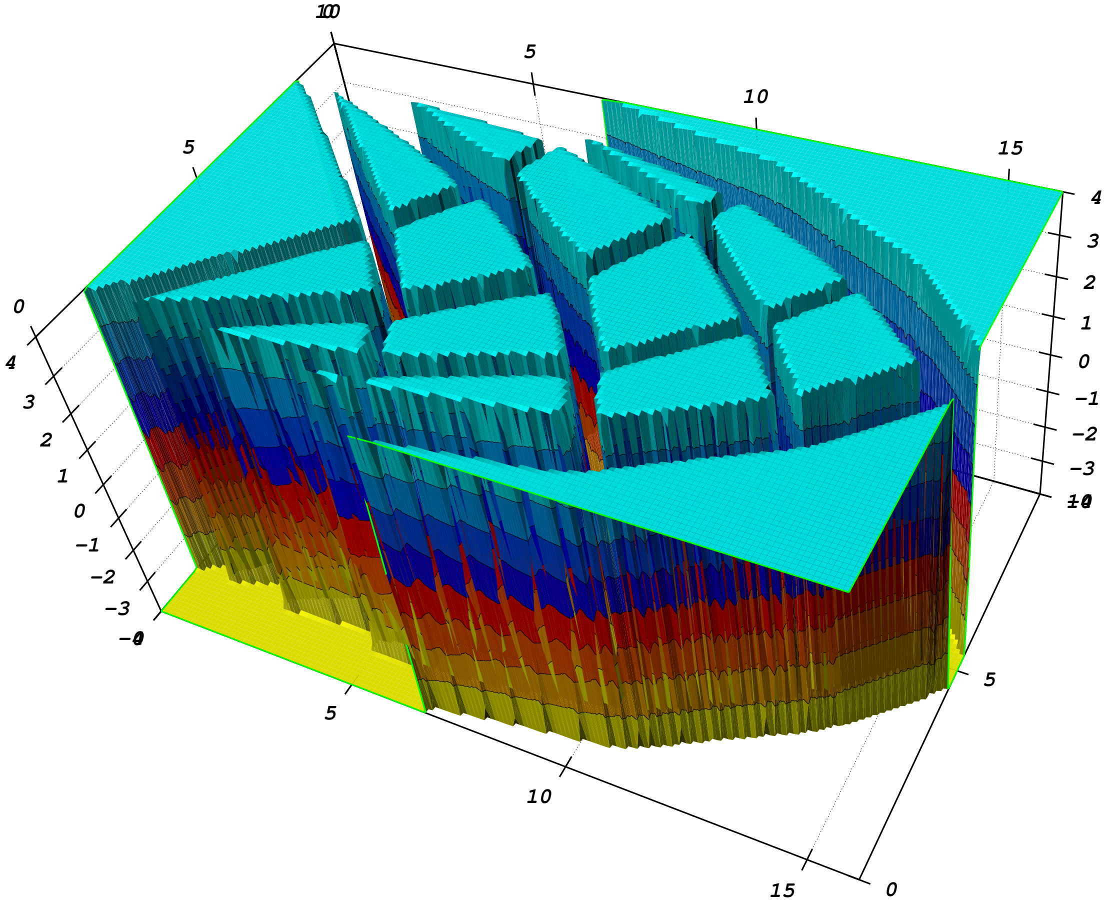
1
1.5

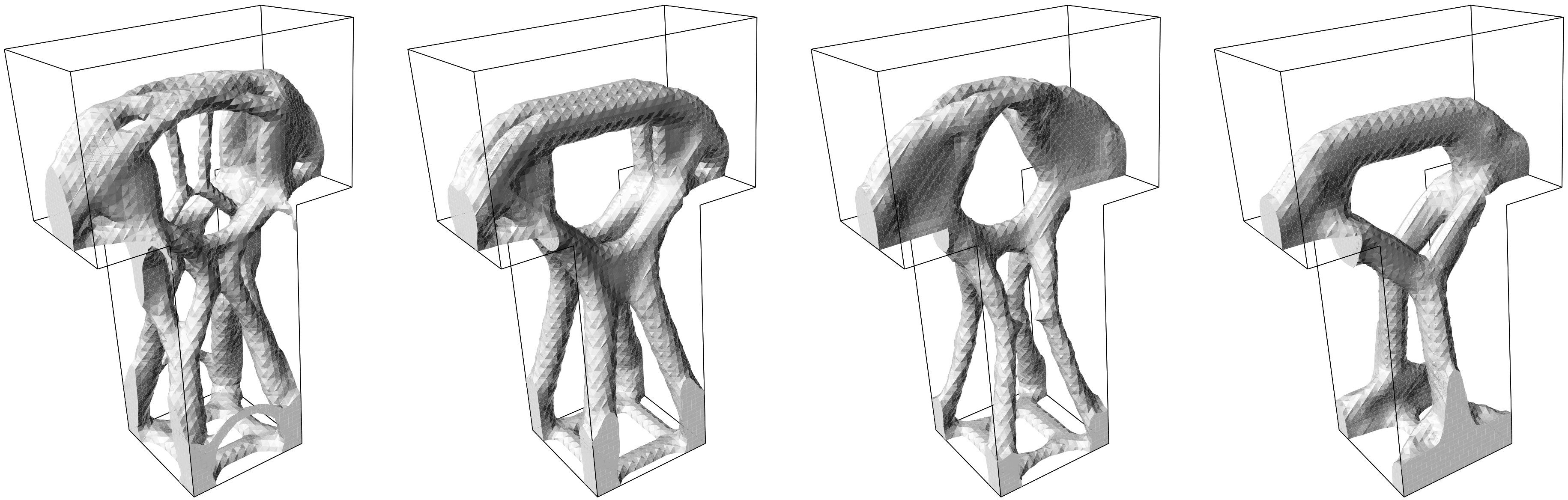


Homogenization
17 holes
68 holes
1 hole
0 holes
0 holes + topological gradient
Objective function
Iterations
8
7.5
7
6.5
0
50
100
150
200
250
300
350
400

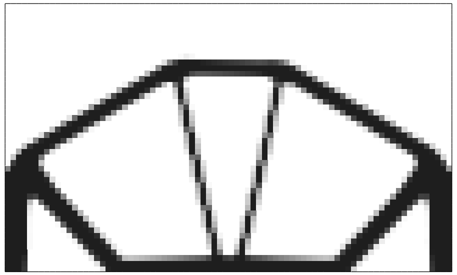
No reinitialization !

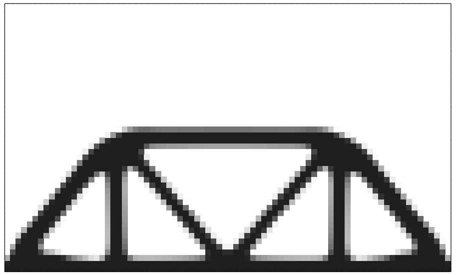


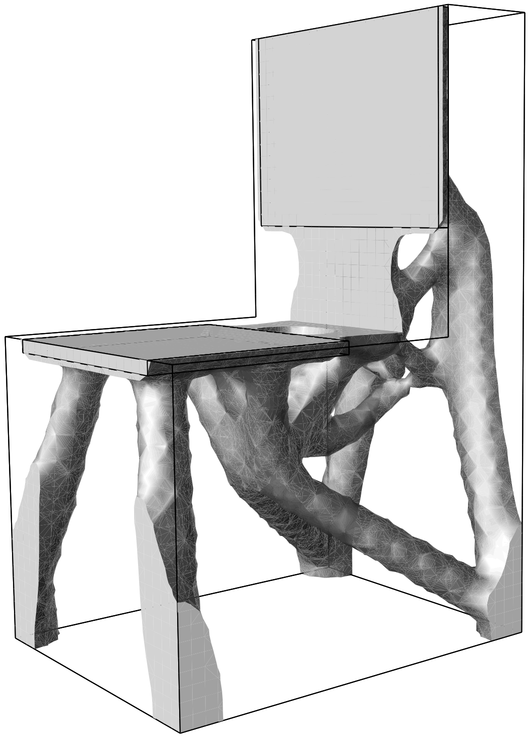
3d

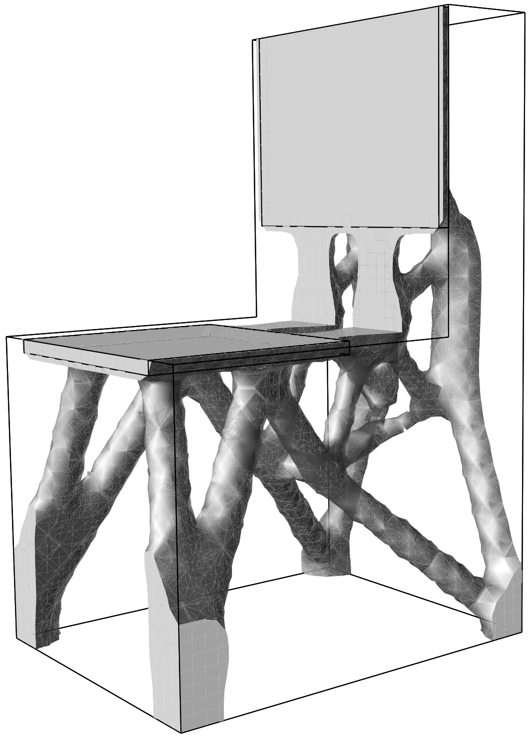


Multi loads

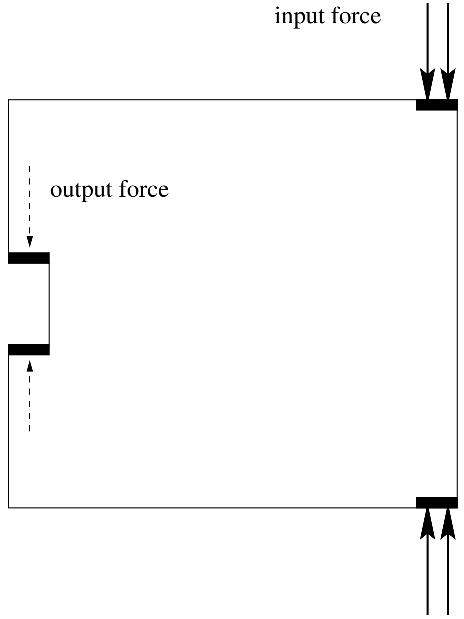


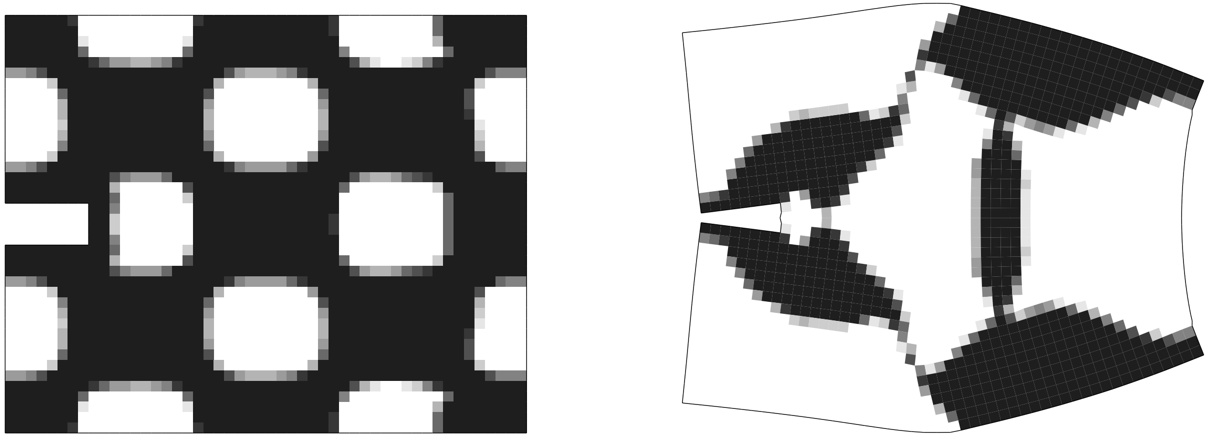




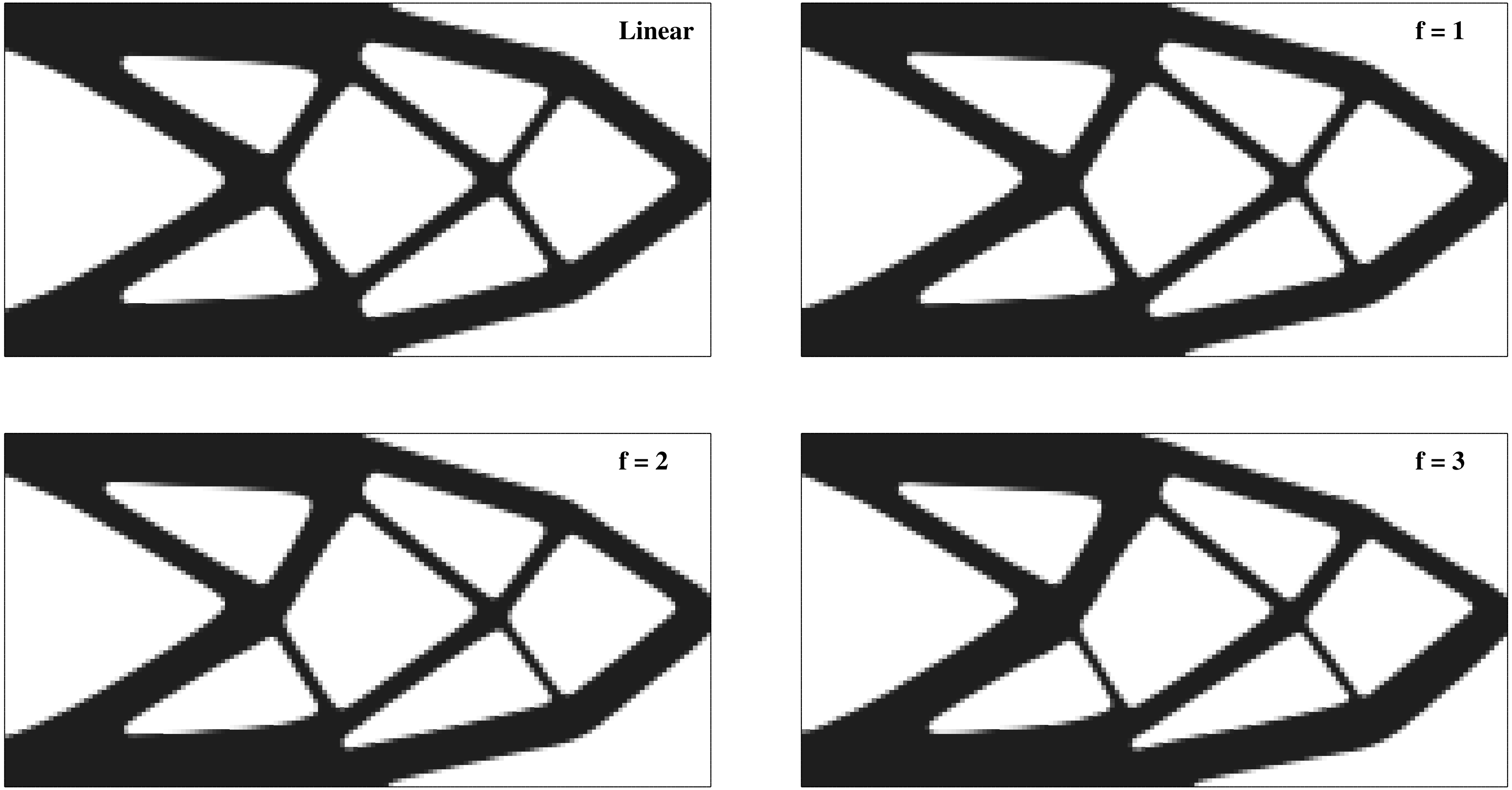


Other objective-function: micro-mechanism optimization

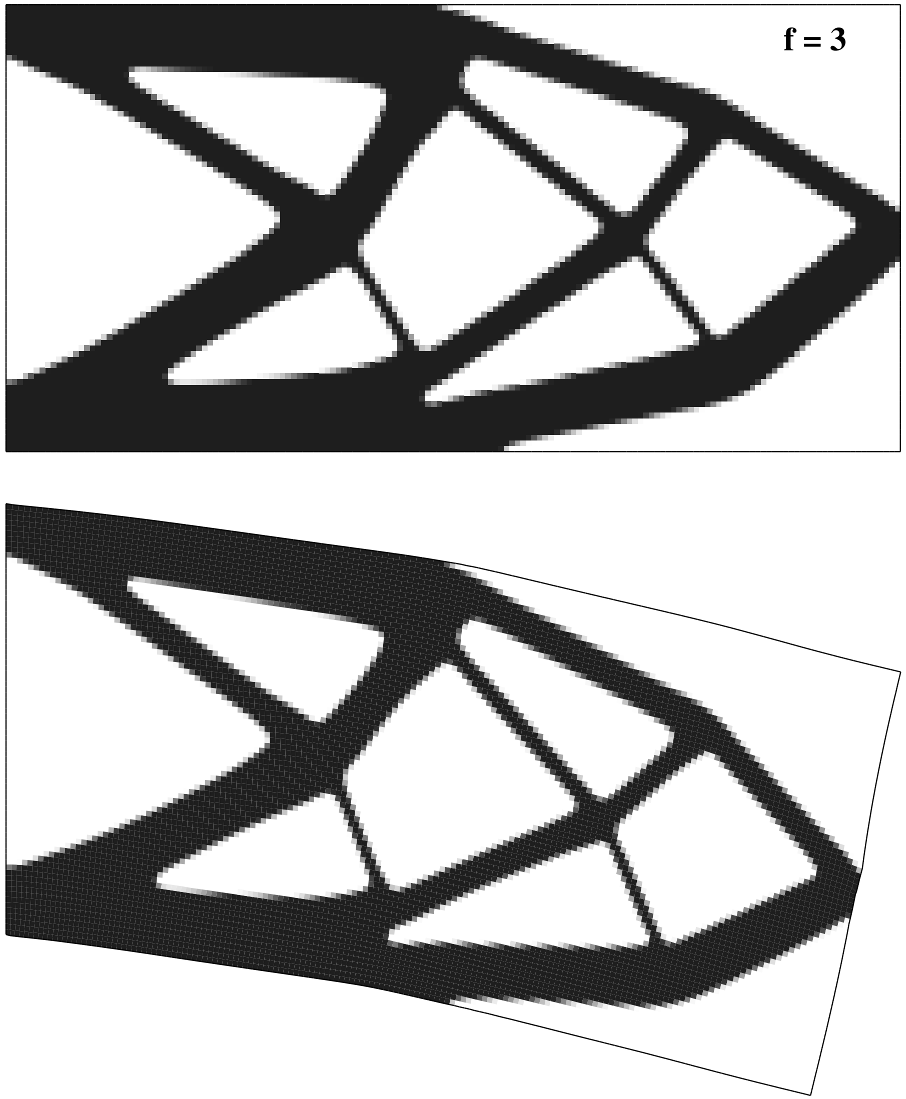




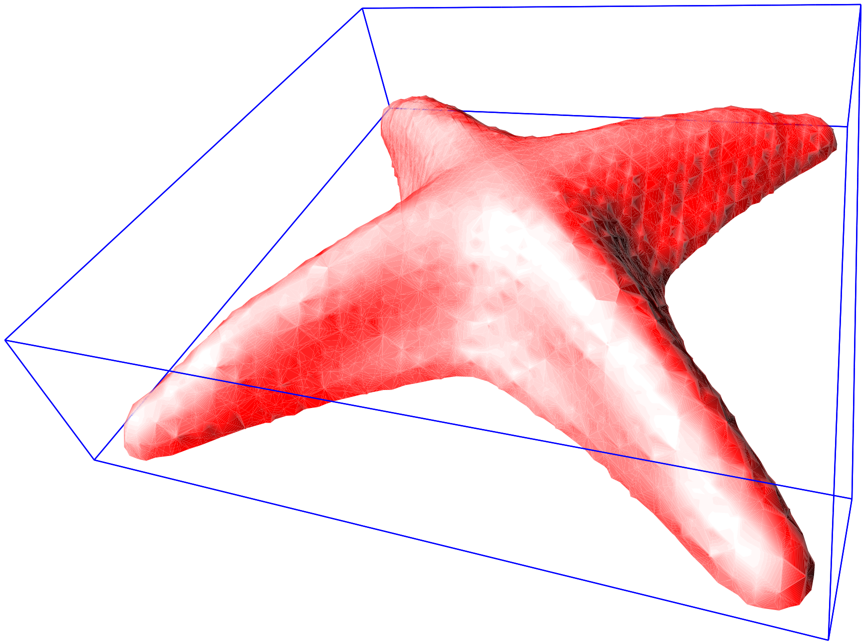
It also works for nonlinear elasticity

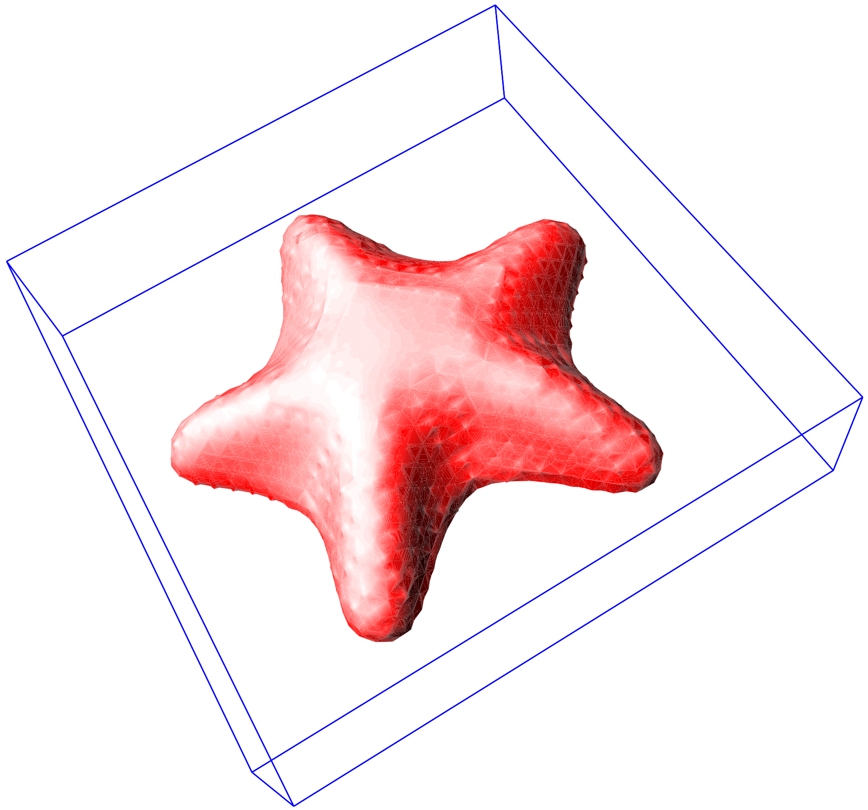


No trick. You can see the large displacements



And also with pressure applied on the (variable) boundary





Advertising

- Various results of the Shape Optimization Group at CMAP:

`www.cmap.polytechnique.fr/~optopo`

- `xd3d` : visualization software used in this talk:

`www.cmap.polytechnique.fr/~jouve/xd3d`