OPTIMAL DESIGN OF STRUCTURES (MAP 562)

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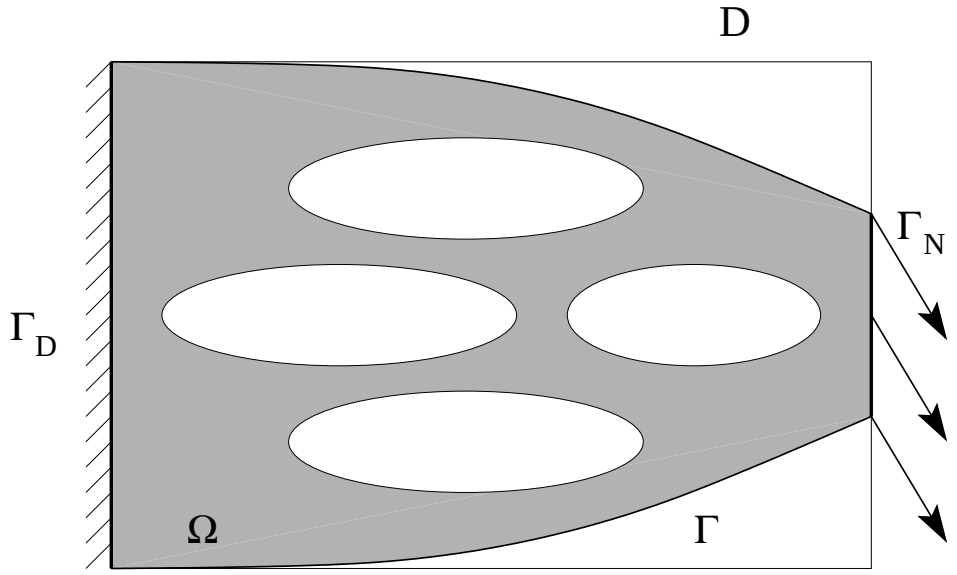
CHAPTER VII (the end)

TOPOLOGY OPTIMIZATION

BY THE HOMOGENIZATION METHOD

7.5 Shape optimization in the elasticity setting



Bounded working domain $D \in \mathbb{R}^N$ $(N = 2, 3)$.

Linear isotropic elastic material, with Hooke's law A

$$A = (\kappa - \frac{2\mu}{N}) I_2 \otimes I_2 + 2\mu I_4, \quad 0 < \kappa, \mu < +\infty$$

Homogenized formulation of shape optimization

We introduce composite structures characterized by a local volume fraction $\theta(x)$ of the phase A (taking any values in the range $[0,1]$) and an homogenized tensor $A^*(x)$, corresponding to its microstructure.

The set of admissible homogenized designs is

$$\mathcal{U}_{ad}^* = \left\{ (\theta, A^*) \in L^\infty \left(D; [0,1] \times \mathbb{R}^{N^4} \right), A^*(x) \in G_{\theta(x)} \text{ in } D \right\}.$$

The homogenized state equation is

$$\begin{cases} \sigma = A^* e(u) & \text{with } e(u) = \frac{1}{2} \left(\nabla u + (\nabla u)^t \right), \\ \text{div}\sigma = 0 & \text{in } D, \\ u = 0 & \text{on } \Gamma_D \\ \sigma n = g & \text{on } \Gamma_N \\ \sigma n = 0 & \text{on } \partial D \setminus (\Gamma_D \cup \Gamma_N). \end{cases}$$

The homogenized compliance is defined by

$$c(\theta, A^*) = \int_{\Gamma_N} g \cdot u \, ds.$$

The relaxed or homogenized optimization problem is

$$\min_{(\theta, A^*) \in \mathcal{U}_{ad}^*} \left\{ J(\theta, A^*) = c(\theta, A^*) + \ell \int_D \theta(x) \, dx \right\}.$$

Bad news: in the elasticity setting an explicit characterization of G_θ is still lacking !

Good news: for compliance one can replace G_θ by its explicit subset L_θ of laminated composites.

Furthermore, an optimal composite is a rank-N sequential laminate with lamination directions given locally by the eigendirections of the stress σ.

7.5.2 Sequential laminates in elasticity

$$A\xi = 2\mu_A\xi + \lambda_A(tr\xi)I, \quad B\xi = 2\mu_B\xi + \lambda_B(tr\xi)I,$$

with the identity matrix I_2, and $\kappa_{A,B} = \lambda_{A,B} + 2\mu_{A,B}/N$. We assume B to be weaker than A

$$0 \leq \mu_B < \mu_A, \quad 0 \leq \kappa_B < \kappa_A.$$

We work with stresses rather than strains, thus we use inverse elasticity tensors.

Lemma 7.24. The Hooke's law of a simple laminate of A and B in proportions θ and $(1-\theta)$, respectively, in the direction e, is

$$(1-\theta)\left(A^{*-1} - A^{-1}\right)^{-1} = \left(B^{-1} - A^{-1}\right)^{-1} + \theta f_A^c(e)$$

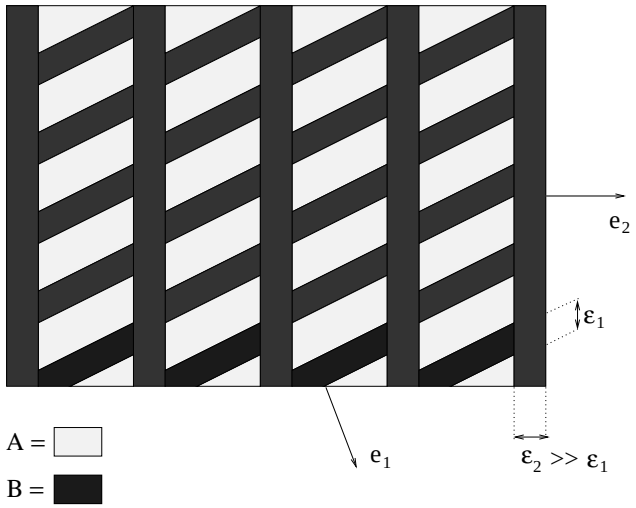
with $f_A^c(e)$ the tensor defined, for any symmetric matrix ξ, by

$$f_A^c(e_i)\xi\cdot\xi = A\xi\cdot\xi - \frac{1}{\mu_A}|A\xi e_i|^2 + \frac{\mu_A+\lambda_A}{\mu_A(2\mu_A+\lambda_A)}((A\xi)e_i\cdot e_i)^2.$$

Reiterated lamination formula

Proposition 7.25. A rank-p sequential laminate with matrix A and inclusions B, in proportions θ and $(1-\theta)$, respectively, in the directions $(e_i)_{1\le i\le p}$ with parameters $(m_i)_{1\le i\le p}$ such that $0 \le m_i \le 1$ and $\sum_{i=1}^{p} m_i = 1$, is given by

$$(1-\theta)\left(A^{*-1} - A^{-1}\right)^{-1} = \left(B^{-1} - A^{-1}\right)^{-1} + \theta \sum_{i=1}^{p} m_i f_A^c(e_i)$$



7.5.3 Hashin-Shtrikman bounds in elasticity

Theorem 7.26. Let A^* be a homogenized elasticity tensor in G_θ which is assumed to be isotropic

$$A^* = 2\mu_* I_4 + \left(\kappa_* - \frac{2\mu_*}{N}\right) I_2 \otimes I_2.$$

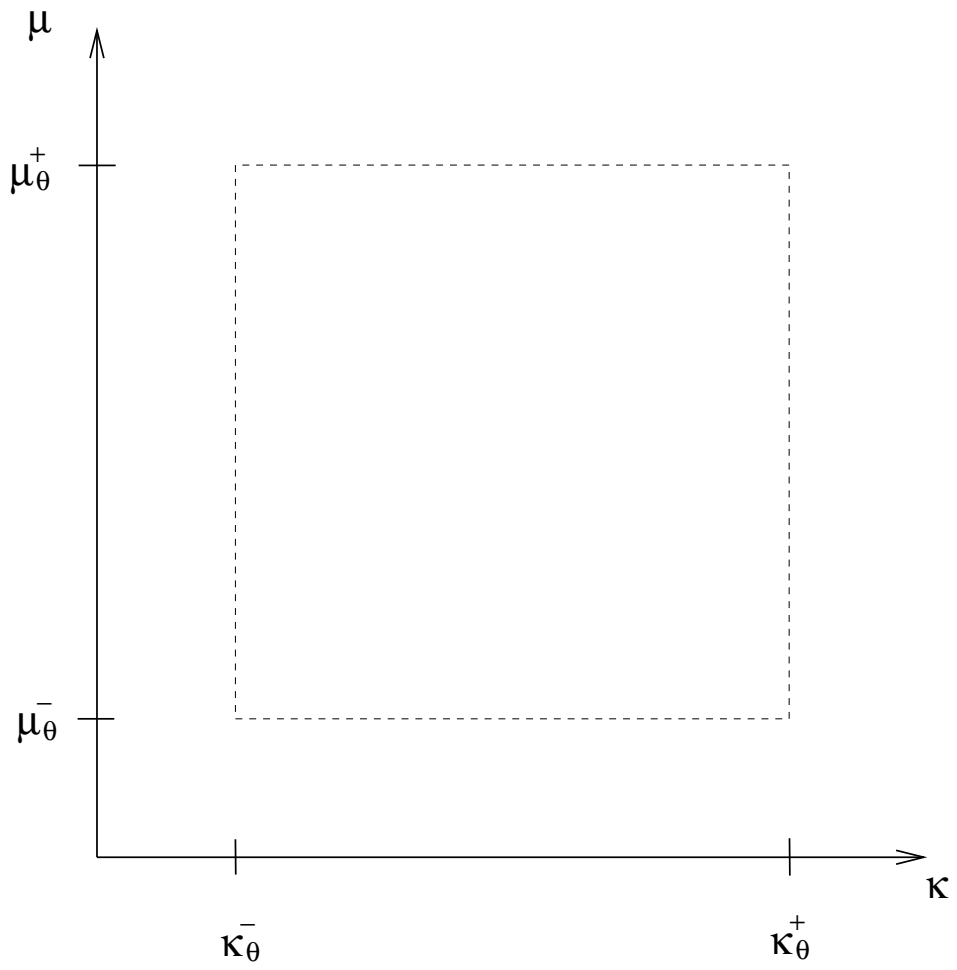
Then, there exist explicit bounds such that its bulk κ_* and shear μ_* moduli satisfy

$$\kappa_\theta^- \leq \kappa_* \leq \kappa_\theta^+ \quad \text{and} \quad \mu_\theta^- \leq \kappa_* \leq \mu_\theta^+$$

They are called Hashin-Shtrikman bounds.

Furthermore, the two lower bounds, as well as the two upper bounds are simultaneously attained by a rank-p sequential laminate with $p = 3$ if $N = 2$, and $p = 6$ if $N = 3$.

Hashin-Shtrikman bounds in elasticity



Back to compliance minimization

The key argument to avoid the knowledge of G_θ is that, thanks to the complementary energy minimization, compliance can be rewritten as

$$c(\theta, A^*) = \int_{\Gamma_N} g \cdot u \, ds = \min_{\substack{div\sigma = 0 \text{ in } D \\ \sigma n = g \text{ on } \Gamma_N \\ \sigma n = 0 \text{ on } \partial D \setminus \Gamma_N \cup \Gamma_D}} \int_D A^{*-1}\sigma \cdot \sigma \, dx.$$

The shape optimization problem thus becomes a double minimization and the orders of minimization can be exchanged (we already used this argument in chapter 5).

Energy bounds and laminates

$$\min_{\substack{div\sigma=0 \text{ in } D \\ \sigma n=g \text{ on } \Gamma_N \\ \sigma n=0 \text{ on } \partial D\setminus\Gamma_N\cup\Gamma_D}} \int_D \min_{\substack{0\le\theta\le 1 \\ A^*\in G_\theta}} \left(A^{*-1}\sigma\cdot\sigma+\ell\theta\right)dx.$$

Optimality condition. If (θ, A^*, σ) is a minimizer, then A^* is a rank-N sequential laminate aligned with σ and with explicit proportions

$$A^{*-1} = A^{-1} + \frac{1-\theta}{\theta}\left(\sum_{i=1}^{N} m_i f_A^c(e_i)\right)^{-1},$$

and θ is given in 2-D (similar formula in 3-D)

$$\theta_{opt} = \min\left(1, \sqrt{\frac{\kappa+\mu}{4\mu\kappa\ell}}\left(|\sigma_1|+|\sigma_2|\right)\right),$$

where σ is the solution of the homogenized equation.

7.5.5 Numerical algorithm for compliance minimization

Double "alternating" minimization in σ and in (θ, A^*).

- intialization of the shape (θ_0, A_0^*)
- iterations $n \geq 1$ until convergence
  - given a shape $(\theta_{n-1}, A_{n-1}^*)$, we compute the stress σ_n by solving a linear elasticity problem (by a finite element method)
  - given a stress field σ_n, we update the new design parameters (θ_n, A_n^*) with the explicit optimality formula in terms of σ_n.

Remarks.

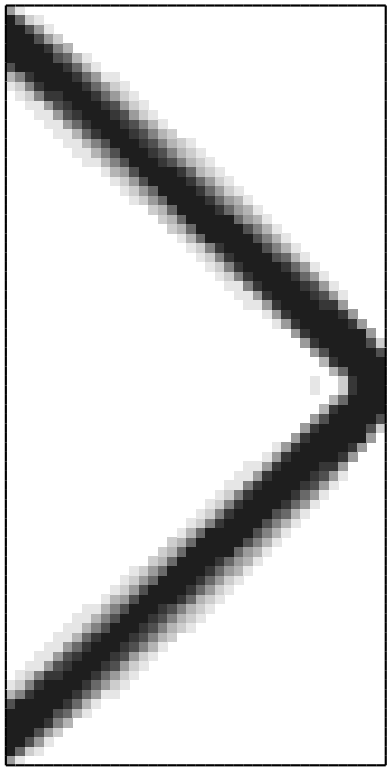
☞ For compliance, the problem is self-adjoint.

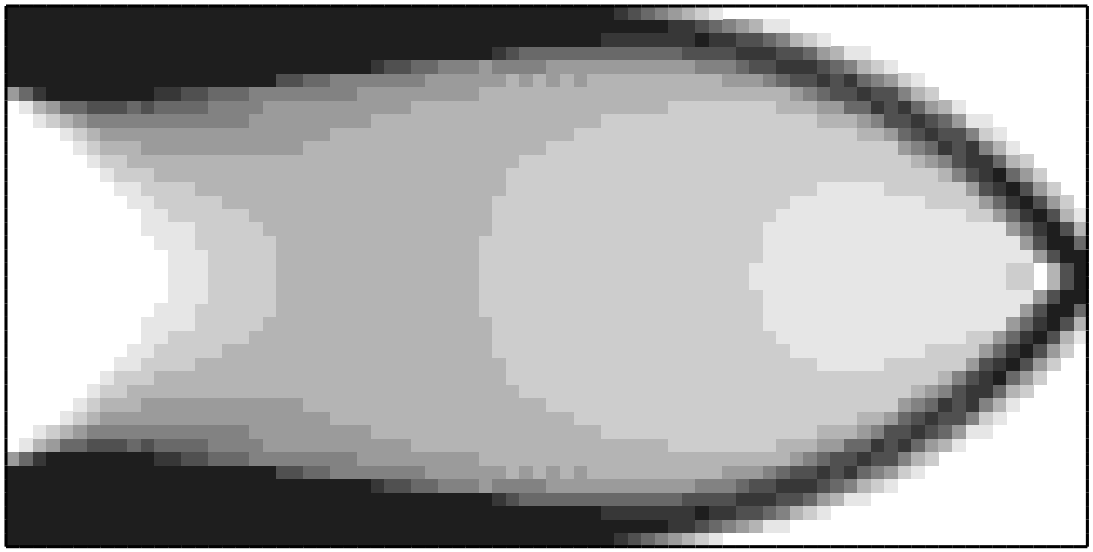
☞ Micro-macro method (local microstructure / global density).

Remarks

- The objective function always decreases.
- Algorithm of the type "optimality criteria".
- Algorithme of "shape capturing" on a fixed mesh of Ω.
- We replace void by a weak "ersatz" material, or we impose $\theta \geq 10^{-3}$ to get an invertible rigidity matrix.
- A few tens of iterations are sufficient to converge.

Example: optimal cantilever





Penalization

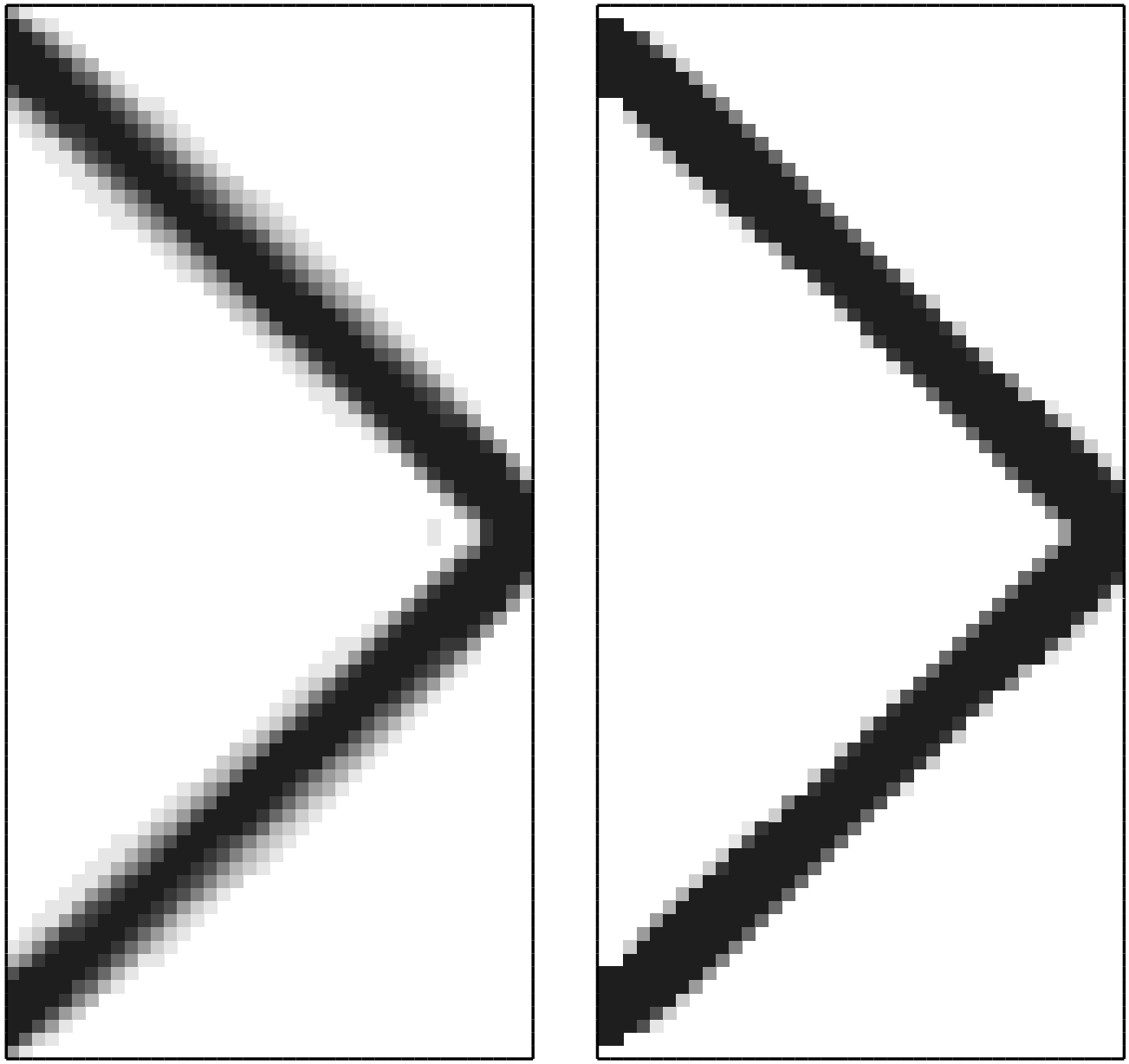
The previous algorithm compute **composite** shapes instead of **classical** shapes.

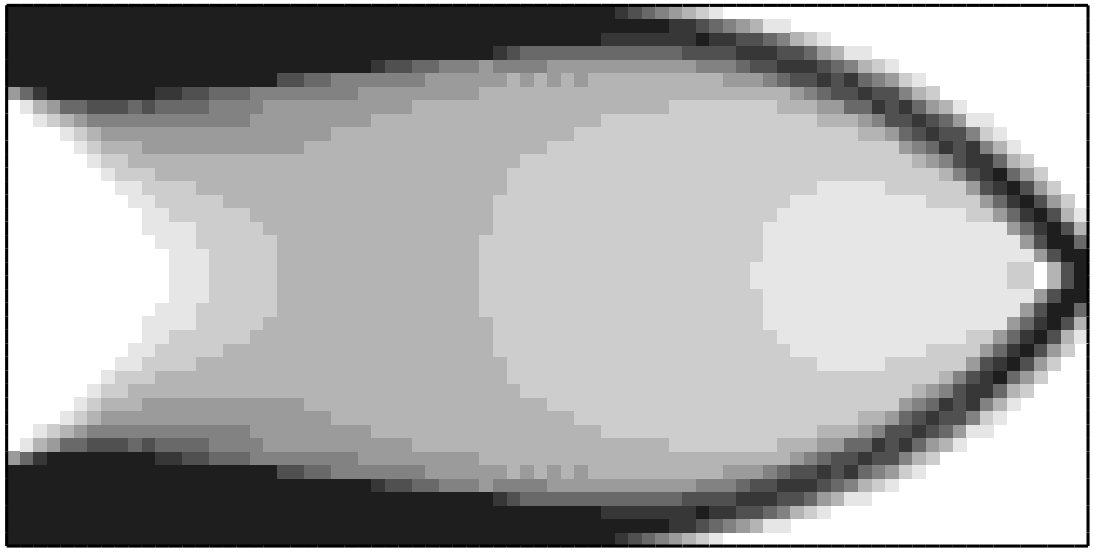
Thus we use a penalization technique to force the density in taking values close to 0 or 1.

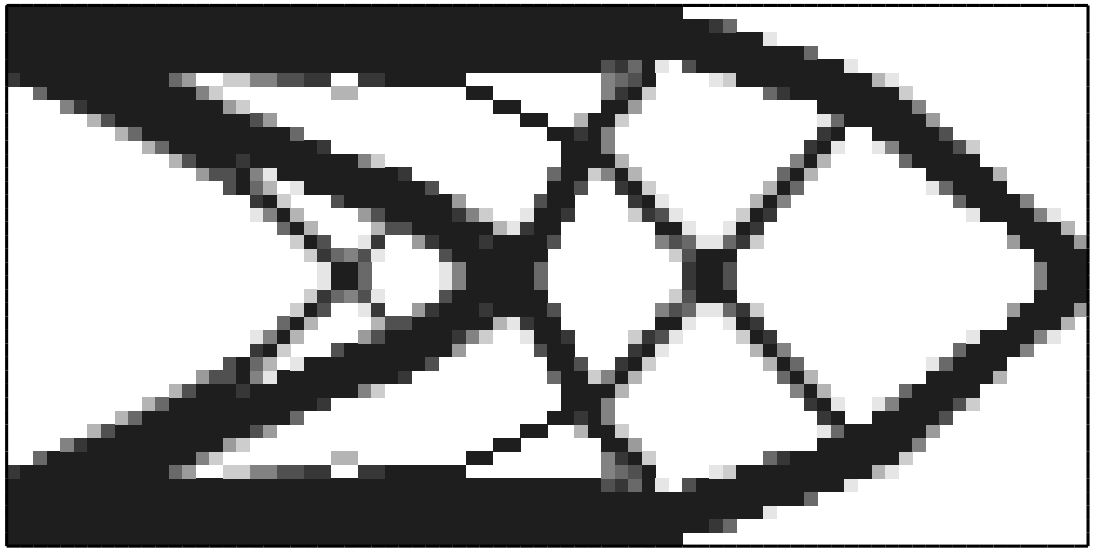
Algorithm: after convergence to a composite shape, we perform a few more iterations with a penalized density

$$\theta_{pen} = \frac{1 - \cos(\pi\theta_{opt})}{2}.$$

If $0 < \theta_{opt} < 1/2$, then $\theta_{pen} < \theta_{opt}$, while, if $1/2 < \theta_{opt} < 1$, then $\theta_{pen} > \theta_{opt}$.

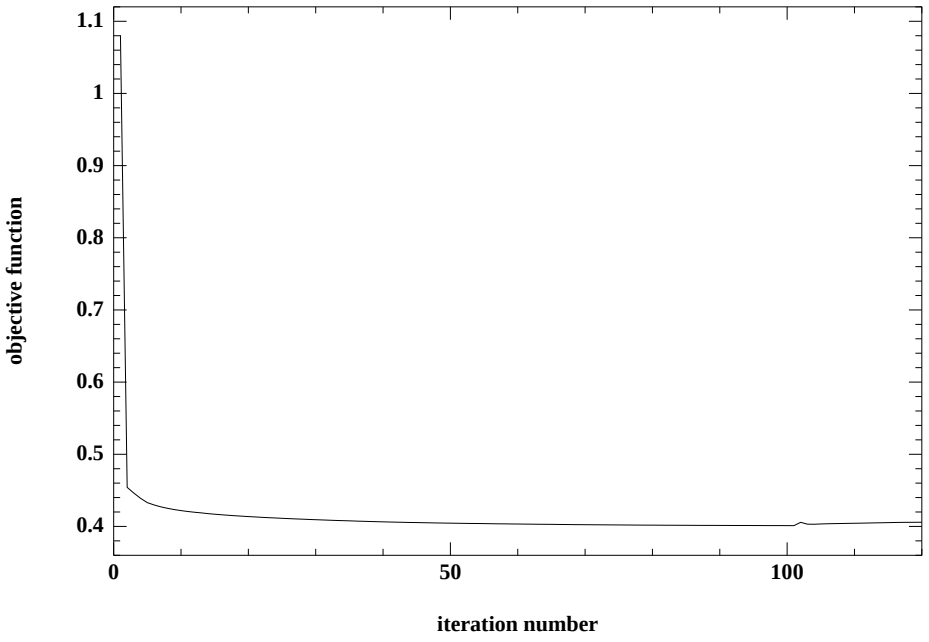


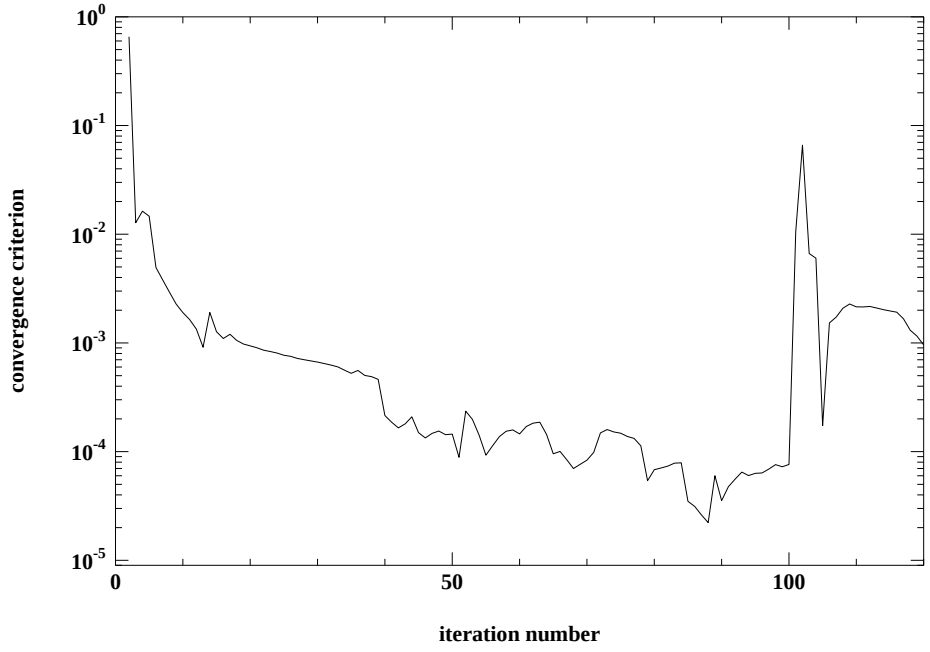




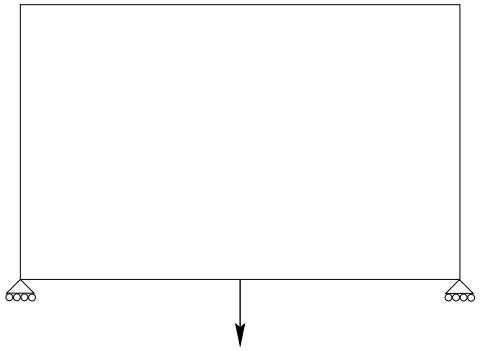
Convergence history:

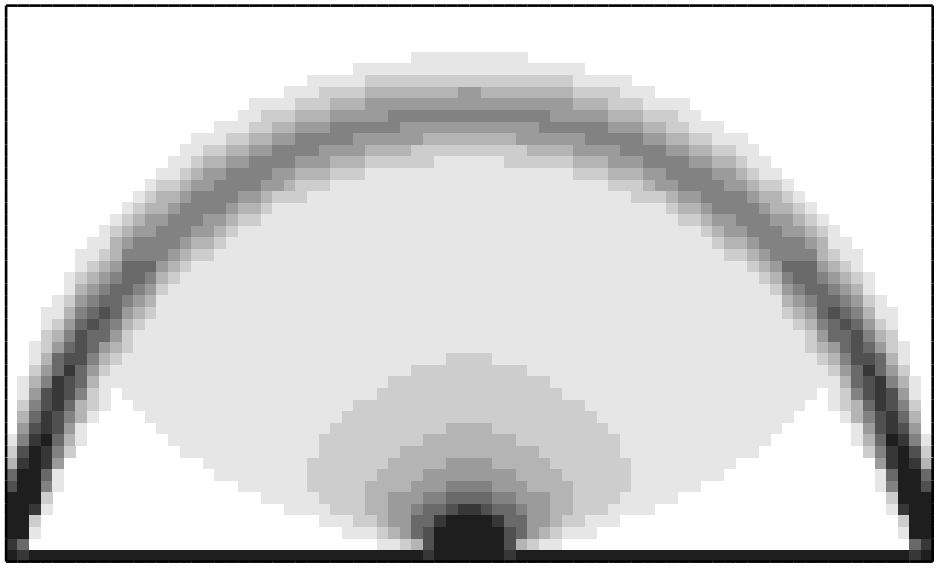
objective function (left), and residual (right),
in terms of the iteration number.

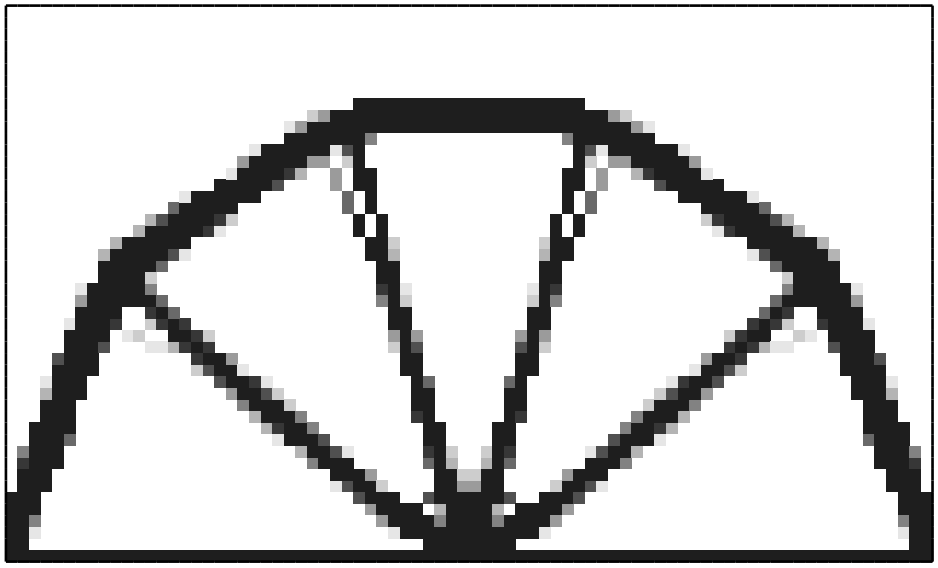




Example: optimal bridge







7.5.6. Convexification and "fictitious materials"

Idea. In the homogenization method composite materials are introduced but discarded at the end by penalization. Can we simplify the approach by introducing merely a density θ ?

A classical shape is parametrized by $\chi(x) \in \{0, 1\}$.

If we **convexify** this admissible set, we obtain $\theta(x) \in [0, 1]$.

The Hooke's law, which was $\chi(x)A$, becomes $\theta(x)A$. We also call this **fictitious materials** because one can not realize them by a true homogenization process (in general). Combined with a penalization scheme, this methode is called **SIMP** (Solid Isotropic Material with Penalization).

Convexified formulation with $0 \leq \theta(x) \leq 1$

$$\begin{cases} \sigma = \theta(x) A e(u) & \text{with } e(u) = \frac{1}{2}\left(\nabla u + (\nabla u)^t\right), \\ \text{div}\sigma = 0 & \text{in } D, \\ u = 0 & \text{on } \Gamma_D \\ \sigma n = g & \text{on } \Gamma_N \\ \sigma n = 0 & \text{on } \partial D \setminus (\Gamma_D \cup \Gamma_N). \end{cases}$$

Compliance minimization

$$\min_{0 \leq \theta(x) \leq 1} \left(c(\theta) + \ell \int_D \theta(x) \right).$$

with

$$c(\theta) = \int_{\Gamma_N} g \cdot u = \int_D (\theta(x)A)^{-1}\sigma \cdot \sigma = \min_{\substack{div\tau = 0 \text{ in } D \\ \tau n = g \text{ on } \Gamma_N \\ \tau n = 0 \text{ on } \partial D \setminus \Gamma_N \cup \Gamma_D}} \int_D (\theta(x)A)^{-1}\tau \cdot \tau \, dx.$$

Now, there is **only one single** design parameter: the material density θ (the microstructure A^* has disappeared).

Existence of solutions

Theorem 7.33. The convexified formulation

$$\min_{0\le\theta(x)\le 1} \quad \min_{\substack{div\tau=0 \text{ in } D \\ \tau n=g \text{ on } \Gamma_N \\ \tau n=0 \text{ on } \partial D\setminus\Gamma_N\cup\Gamma_D}} \int_D (\theta(x)A)^{-1}\tau\cdot\tau\,dx + \ell\int_D \theta\,dx$$

admits at least one solution.

Proof. The function, defined on $\mathbb{R}^+\times\mathcal{M}_n^s$,

$$\phi(a,\sigma) = a^{-1}A^{-1}\sigma\cdot\sigma,$$

is convex because

$$\phi(a,\sigma) = \phi(a_0,\sigma_0) + D\phi(a_0,\sigma_0)\cdot(a-a_0,\sigma-\sigma_0) + \phi(a,\sigma-aa_0^{-1}\sigma_0),$$

where the derivative $D\phi$ is given by

$$D\phi(a_0,\sigma_0)\cdot(b,\tau) = -\frac{b}{a_0^2}A^{-1}\sigma_0\cdot\sigma_0 + 2a_0^{-1}A^{-1}\sigma_0\cdot\tau.$$

Optimality condition

If we exchange the minimizations in τ and in θ, we can compute the optimal θ which is

$$\theta(x) = \begin{cases} 1 & \text{if } A^{-1}\tau \cdot \tau \geq \ell \\ \sqrt{\ell^{-1} A^{-1}\tau \cdot \tau} & \text{if } A^{-1}\tau \cdot \tau \leq \ell \end{cases}$$

Again we can use an "alternating" double minimization algorithm.

Numerical algorithm

- intialization of the shape θ_0
- iterations $k \geq 1$ until convergence
  - given a shape θ_{k-1}, we compute the stress σ_k by solving an elasticity problem (by a finite element method)
  - given a stress field σ_k, we update the new material density θ_k with the explicit optimality formula in terms of σ_k.

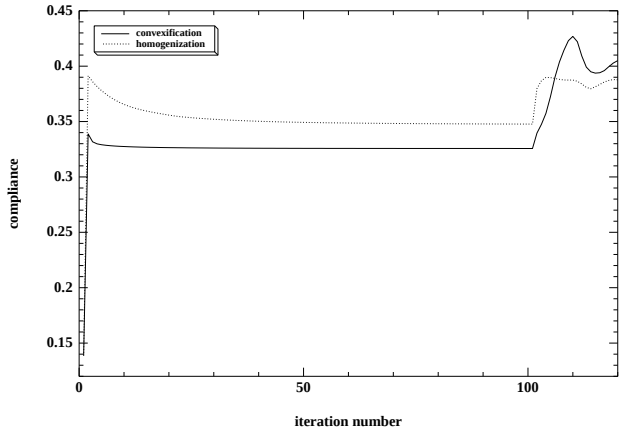
Penalization: we use a penalized density

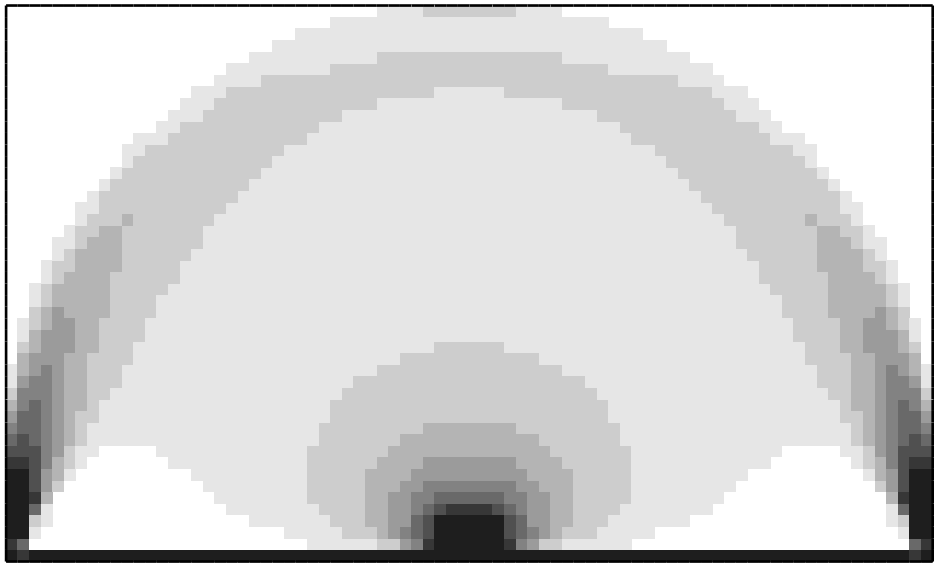
$$\theta_{pen} = \frac{1 - \cos(\pi\theta_{opt})}{2} \quad \text{or (SIMP)} \quad \theta_{pen} = \theta^p \quad p > 1.$$

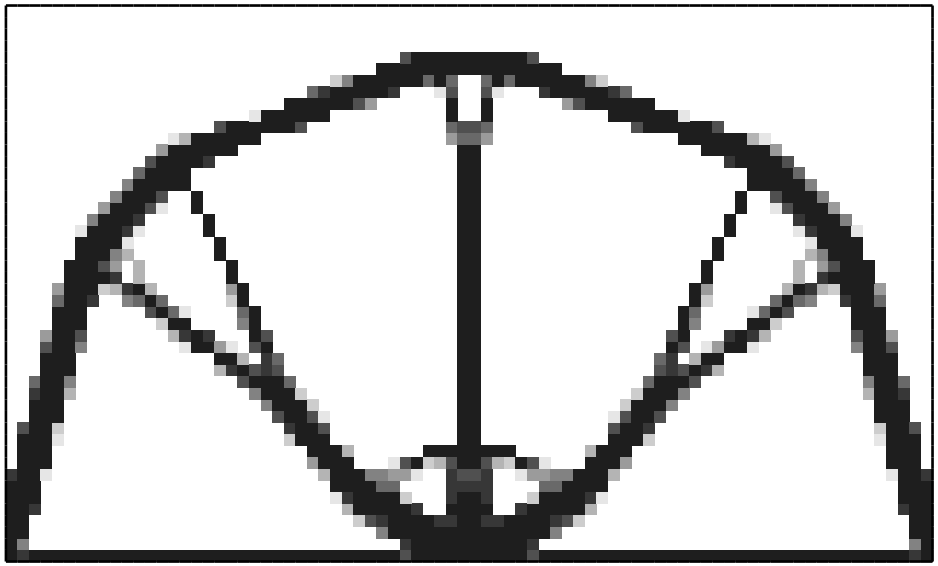
In practice: it is extremely simple ! But the numerical results are not as good ! An explanation is the lack of a relaxation theorem.

Be careful: very delicate monitoring of the penalization...

Optimal bridge by the convexification method







Conclusion

- SIMP (or convexification, or "fictitious materials") is very simple and **very popular** (many commercial codes are using it).
- SIMP uses very few informations on composites ! In particular, it is isotropic.
- On the contrary to the homogenization method, SIMP **is not a relaxation method**: it changes the problem !
- There is a gap between the true minimal value of the objective function and that of SIMP.
- SIMP can be delicate to monitor: how to increase the penalization parameter ?

Generalizations of the homogenization method

- multiple loads
- vibration eigenfrequency
- general criterion of the least square type

The two first cases are self-adjoint and we have a complete understanding and justification of the relaxation process. However, the third case is not self-adjoint and only a partial relaxation is known.

Multiple loads

Optimal composites are still sequential laminates.

For n loads $(f_i)_{1\leq i\leq n}$, the homogenized formulation is

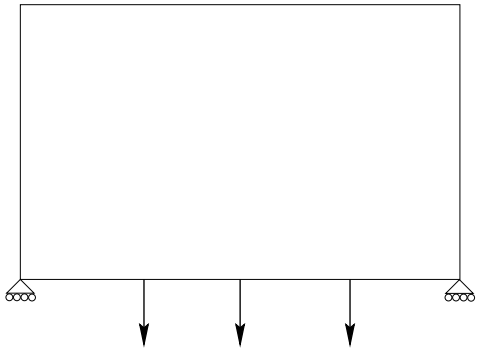
$$\min_{\substack{\mathrm{div}\sigma_i=0 \text{ in } D\\ \sigma_i n=g_i \text{ on } \Gamma_N}} \int_D \min_{0\leq\theta\leq 1} \min_{A^*\in L_\theta} \left(\sum_{i=1}^n A^{*-1}\sigma_i\cdot\sigma_i + \ell\theta\right) dx$$

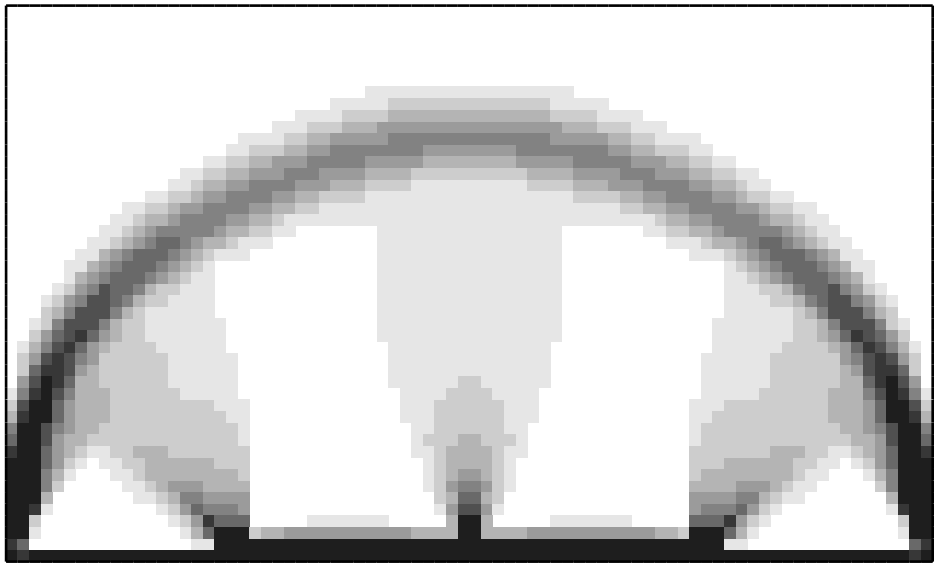
with $A^* \in L_\theta$ and

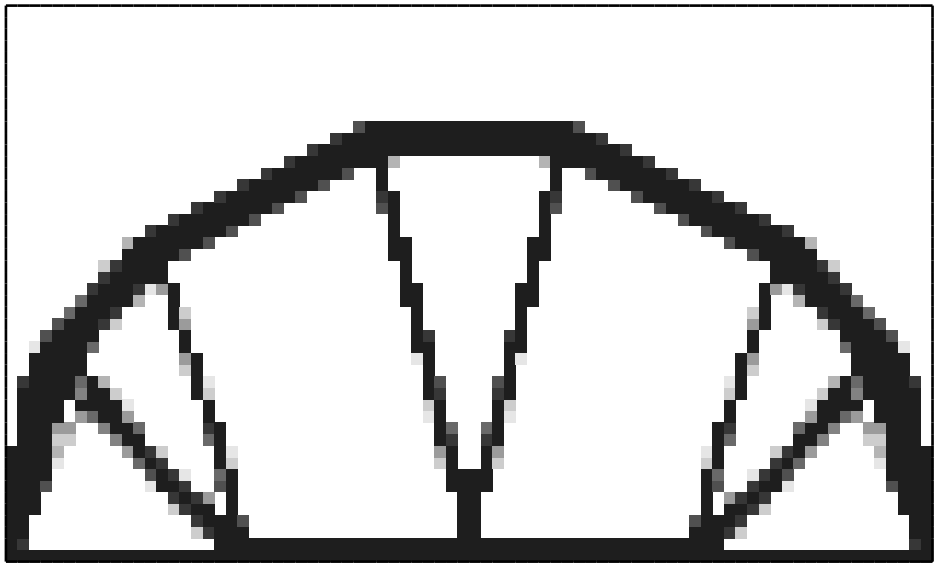
$$(1-\theta)\left(A^{*-1}-A^{-1}\right)^{-1} = \left(B^{-1}-A^{-1}\right)^{-1} + \theta\sum_{i=1}^p m_i f_A^c(e_i)$$

The optimal laminate is no more of rank N. The m_i's optimization is now done numerically (with numerous enough lamination directions).

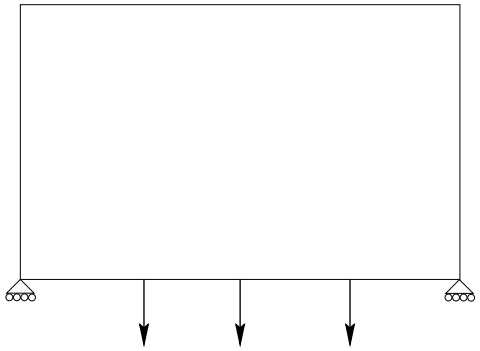
Optimal bridge for 3 simultaneously applied loads

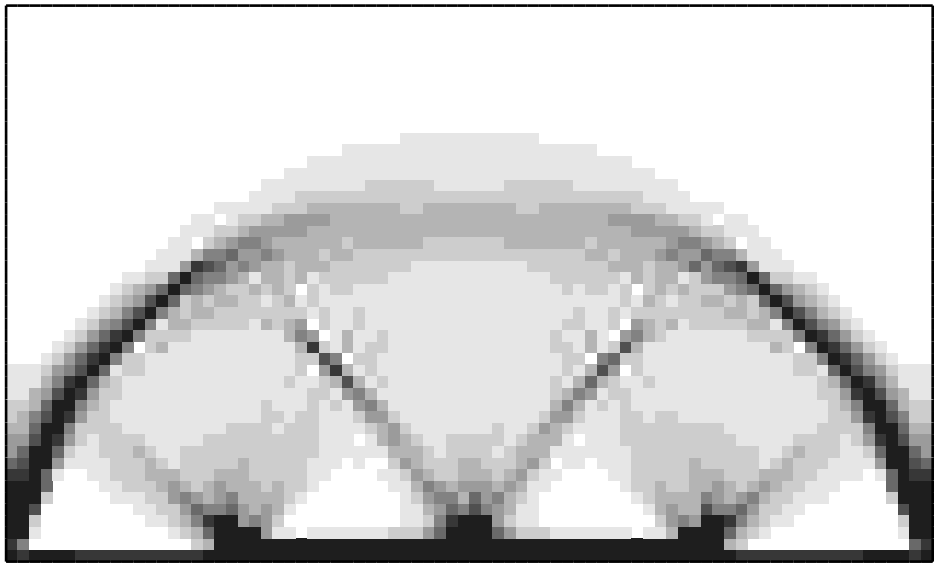


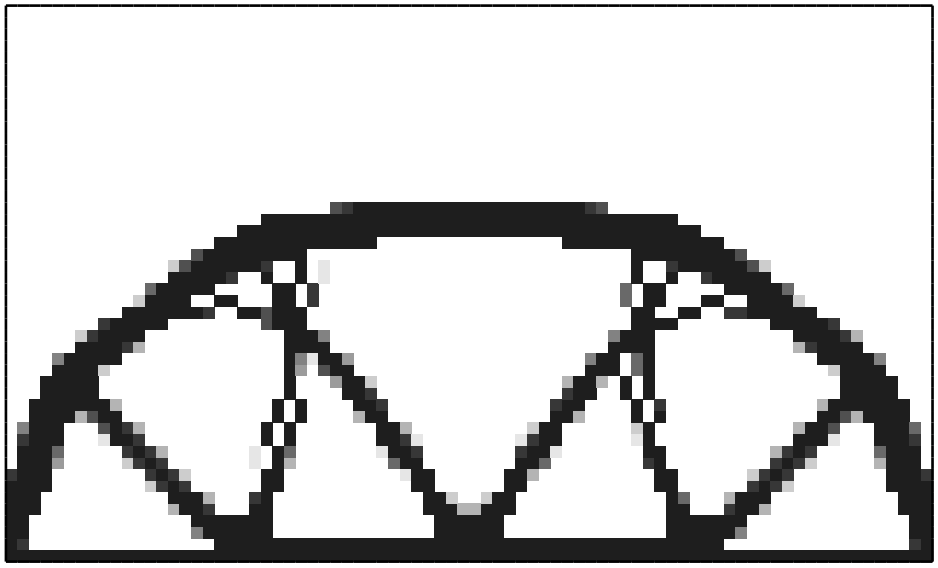




Optimal bridge for 3 independently applied loads







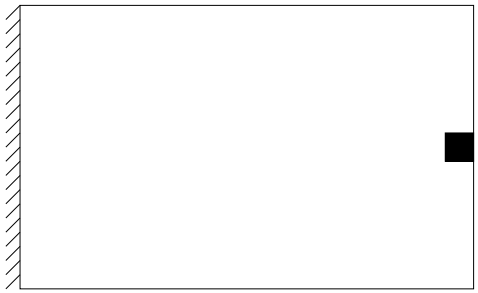
Vibration eigenfrequencies

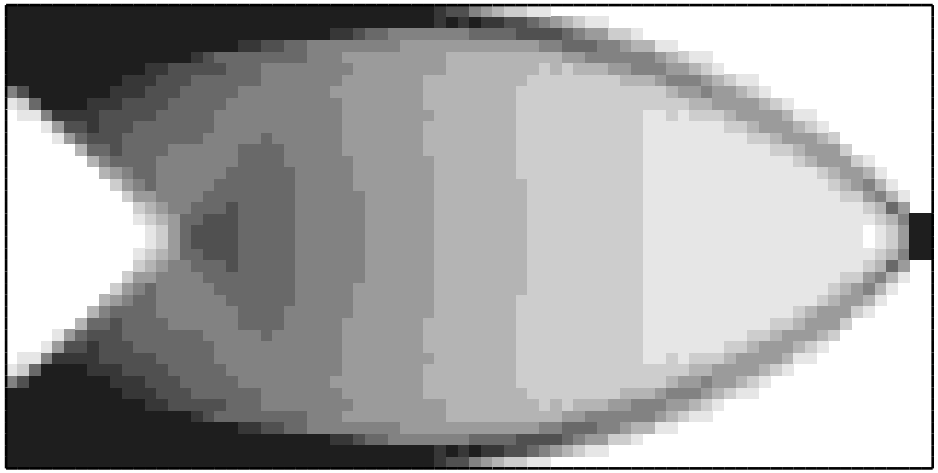
Optimal composites are still sequential laminates.

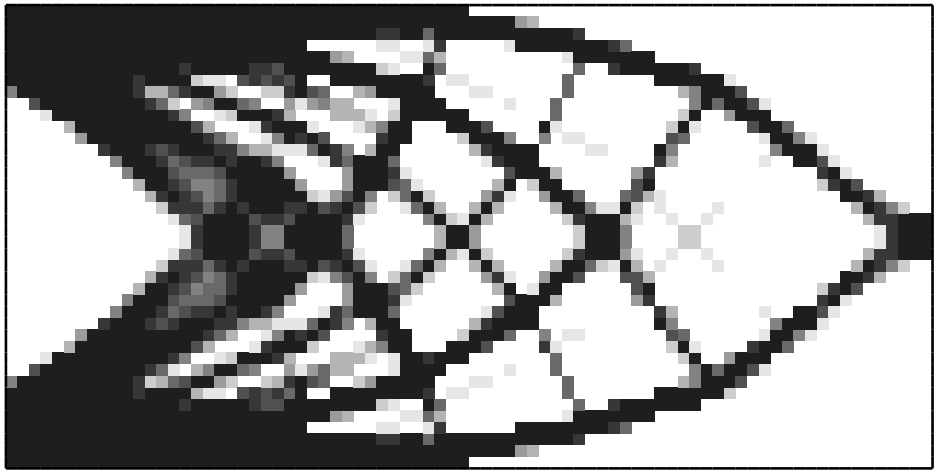
We maximize the first vibration eigenfrequency

$$\min_{0\le\theta\le 1,\ A^*\in L_\theta} \left\{ \omega_1^2(\theta, A^*) = \min_{u\in\mathcal{H}} \frac{\displaystyle\int_D A^* e(u)\cdot e(u) dx}{\displaystyle\int_D \overline{\rho}|u|^2 dx} \right\}$$

with the density $\overline{\rho} = \theta\rho_A + (1-\theta)\rho_B$, and the space of admissible displacements $\mathcal{H} = \left\{ u \in H^1(D)^N \text{ such that } u = 0 \text{ on } \Gamma_D \right\}$.







Least square objective functions

Homogenized formulation:

$$\min_{0\le\theta\le 1,\ A^*\in G_\theta} J^*(\theta, A^*) = \int_\Omega \Big(k|u-u_0|^2 + \ell\theta \Big) dx$$

with u solution of

$$\begin{cases} -\operatorname{div}\left(A^* e(u)\right) = f & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega, \end{cases}$$

Difficulty: we don't know G_θ and we cannot replace it by L_θ. In other words, we don't know which microstructures are optimal...

Partial relaxation: we nevertheless replace G_θ by L_θ. We thus loose the existence of an optimal solution but we keep the link with the original problem.

Partial relaxation

We restrict ourselves to sequential laminates A^* with matrix A and inclusions B. The number of laminations and their directions are fixed. We merely optimize with respect to θ and the proportions $(m_i)_{1\le i\le p}$

$$(1-\theta)\,(A-A^*)^{-1} \;=\; (A-B)^{-1} - \theta\sum_{i=1}^{q} m_i f_A(e_i),$$

with $\forall e\in\mathbb{R}^N,\ |e|=1,\ \forall\xi$ symmetric matrix

$$f_A(e)\xi\cdot\xi = \frac{1}{\mu_A}\left(|\xi e|^2-(\xi e\cdot e)^2\right)+\frac{1}{\lambda_A+2\mu_A}(\xi e\cdot e)^2.$$

Thus, the objective function is

$$J^*(\theta,A^*)\equiv J^*(\theta,m_i)$$

with the constraints $0\le\theta\le 1$, $m_i\ge 0$, $\sum_{i=1}^p m_i = 1$.

We compute its gradient with the help of an adjoint state.

Numerical algorithm of gradient type

Projected gradient with a variable step:

1. Initialization of the design parameters $\theta_0, m_{i,0}$ (for example, constants satisfying the constraints).

2. Iterations until convergence, for $k \geq 0$:

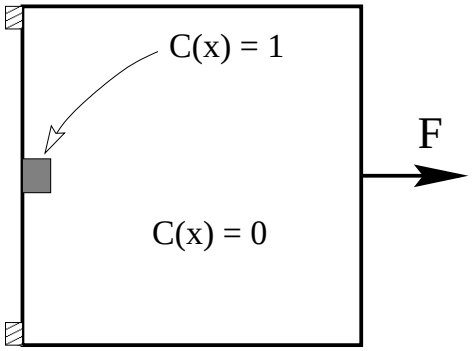
   (a) Computation of the state u_k and the adjoint p_k, with the previous design parameters $\theta_k, m_{i,k}$.

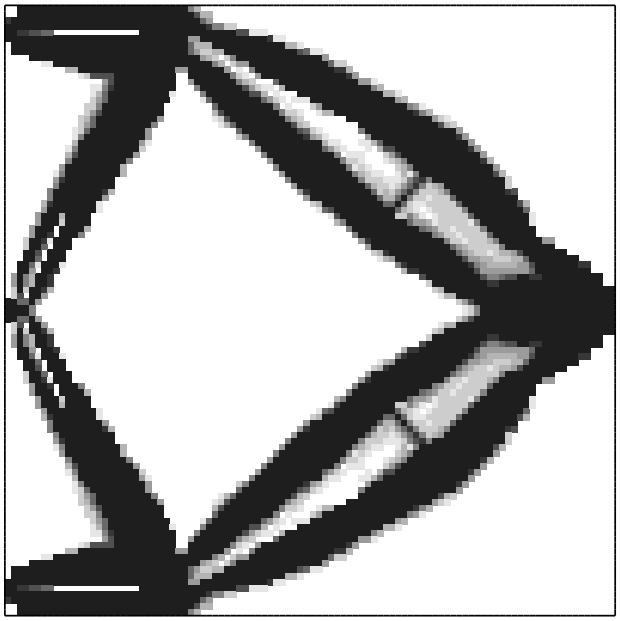
   (b) Update of the design parameters :

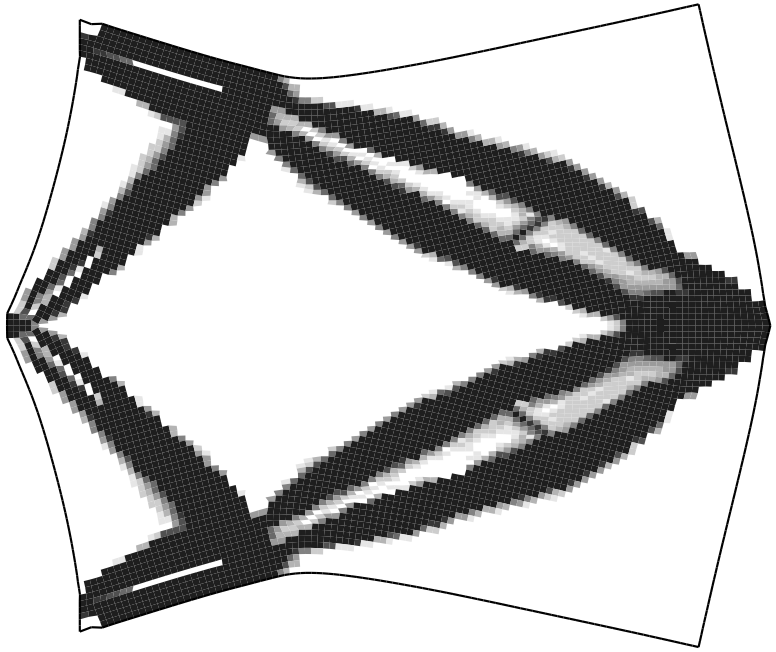
$$\begin{aligned} \theta_{k+1} &= \max\left(0, \min\left(1, \theta_k - t_k \nabla_\theta J_k^*\right)\right), \\ m_{i,k+1} &= \max\left(0, m_{i,k} - t_k \nabla_{m_i} J_k^* + \ell_k\right), \end{aligned}$$

where ℓ_k is a Lagrange multiplier for the constraint $\sum_{i=1}^q m_{i,k} = 1$, iteratively updated, and $t_k > 0$ is a descent step such that $J^*(\theta_{k+1}, m_{k+1}) < J^*(\theta_k, m_k)$.

Example: force inverter







Other methods of topology optimization

- Discrete 0/1 optimization (no gradients): genetic algorithms.
- Level set methods based on geometric optimization.
- Topological derivative: sensitivity to the nucleation of a small hole.
- Phase-field methods.

A few words about the levet set method for shape optimization

It is a combination of:

- Hadamard shape derivative in geometric optimization,
- the level set method of Osher and Sethian for front propagation (JCP, 1988).

Level set methods have many applications !

- Multi-phase fluid mechanics.
- Combustion, dendritic or crystal growth.
- Crack propagation.
- Image processing.
- Geometry.

FRONT PROPAGATION BY LEVEL SET

More general problem: how to move a hypersurface $x(t)$ according to a given velocity $\vec{v}(t,x)$.

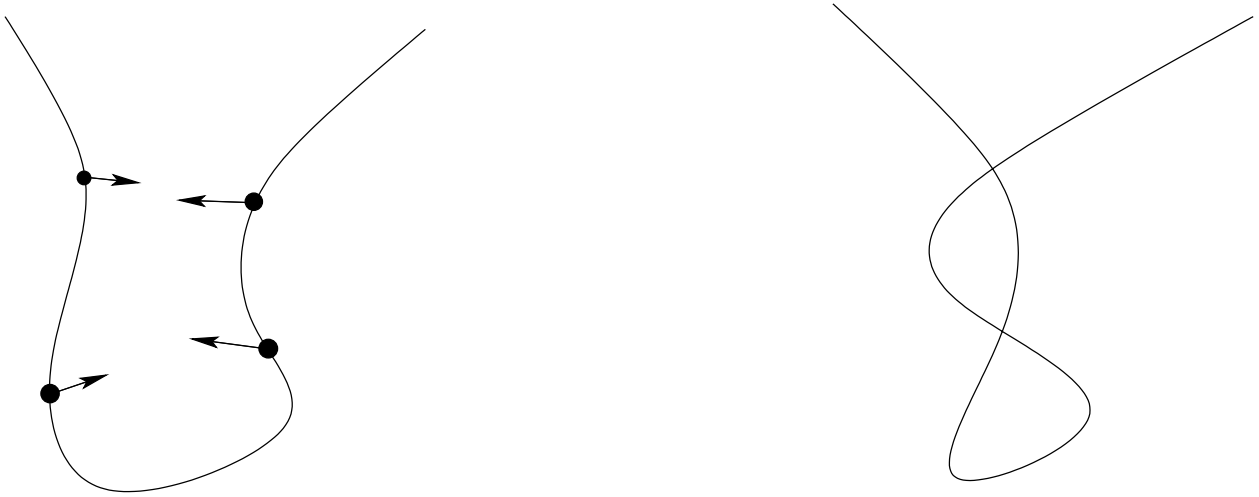
Lagrangian approach: let us solve o.d.e.'s

$$\begin{cases} \dfrac{dx}{dt} = \vec{v}(t,x(t)) \\ \\ x(0) = x_0 \end{cases}$$

$$\Gamma(0) = \{x_0\} \quad \Rightarrow \quad \Gamma(t) = \{x(t)\}$$

☞ Reversible method: to go back in time, change the velocity sign !

☞ **Shape tracking method**.



- Problems with self-intersection and singularity !
- How to handle a velocity $\vec{v}$ which depends on the surface through its normal, mean curvature, etc. ?
- How to devise **an Eulerian approach** ?
- Idea: make the evolution irreversible.

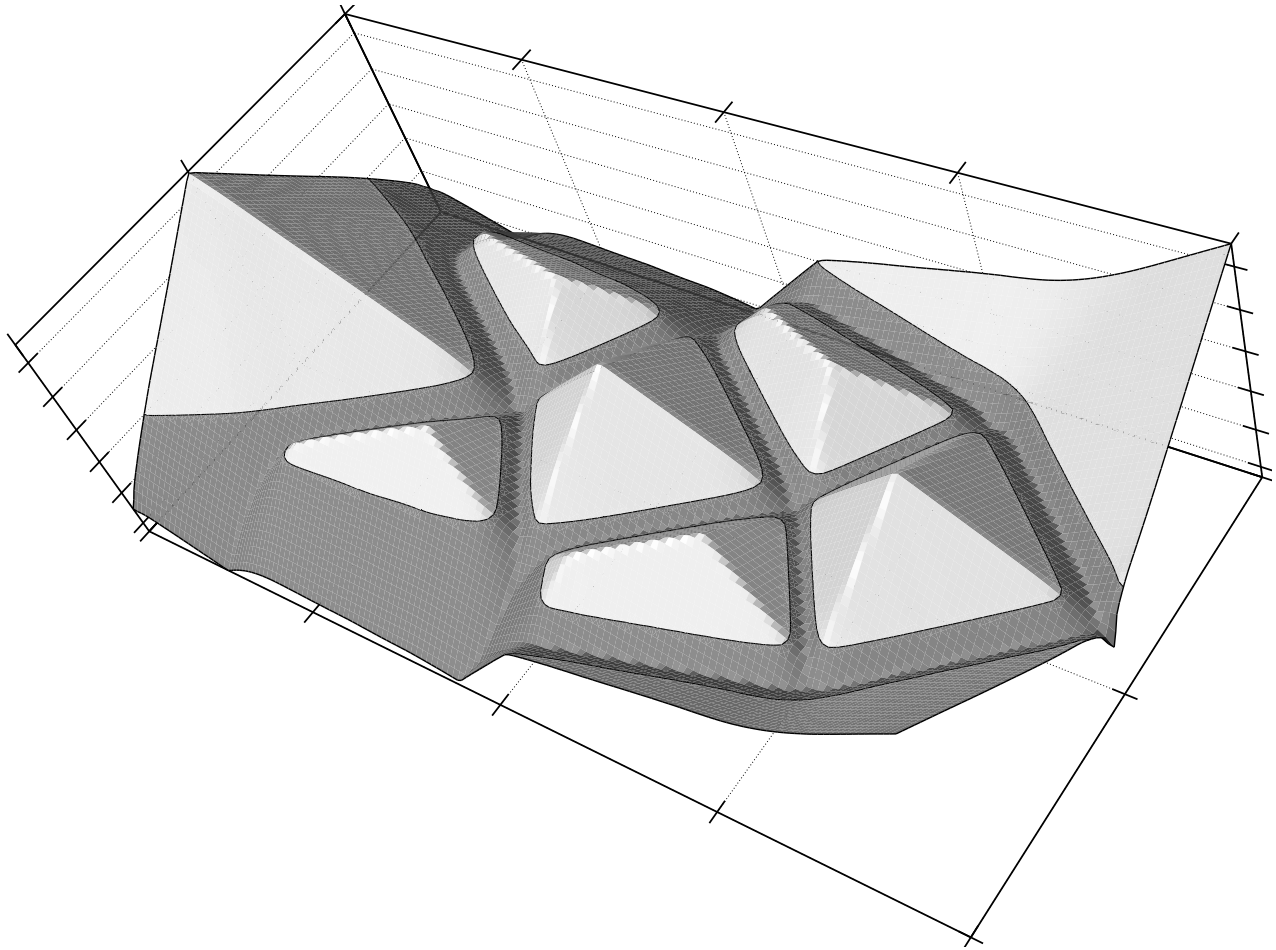
The level set method of Osher and Sethian

Shape capturing method on a fixed mesh of a "large" box D.

A shape Ω is parametrized by a level set function

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

The normal n to Ω is given by $\nabla\psi/|\nabla\psi|$ and the mean curvature H is the divergence of n. These formulas make sense everywhere in D on not only on the boundary $\partial\Omega$.



Hamilton Jacobi equation

Assume that the shape $\Omega(t)$ evolves with a normal velocity $V(t,x)$. Then

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

Deriving in t yields

$$\frac{\partial \psi}{\partial t} + \dot{x}(t) \cdot \nabla_x \psi = \frac{\partial \psi}{\partial t} + V n \cdot \nabla_x \psi = 0.$$

(The same is true for any level set $\psi\Big(t, x(t)\Big) = C$.)

Since $n = \nabla_x \psi / |\nabla_x \psi|$ we obtain

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

This Hamilton Jacobi equation is posed in the whole box D, and not only on the boundary $\partial\Omega$, if the velocity V is known everywhere.

Example

Choice of the velocity: $\vec{v} = \alpha \vec{n}$ with $\vec{n}$ =normal vector

$$V = \alpha.$$

(This is the typical case for shape optimization and Hadamard derivative.)

We deduce

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

This Hamilton-Jacobi equation admits a unique viscosity solution global in time (Crandall-Lions).

Invariance with respect to the extension out of the surface

The only meaningfull information is the level set $\psi(t) = 0$. It should not depend on the choice of extended initial data ψ_0 such that $\Gamma(0) = \{\psi_0 = 0\}$.

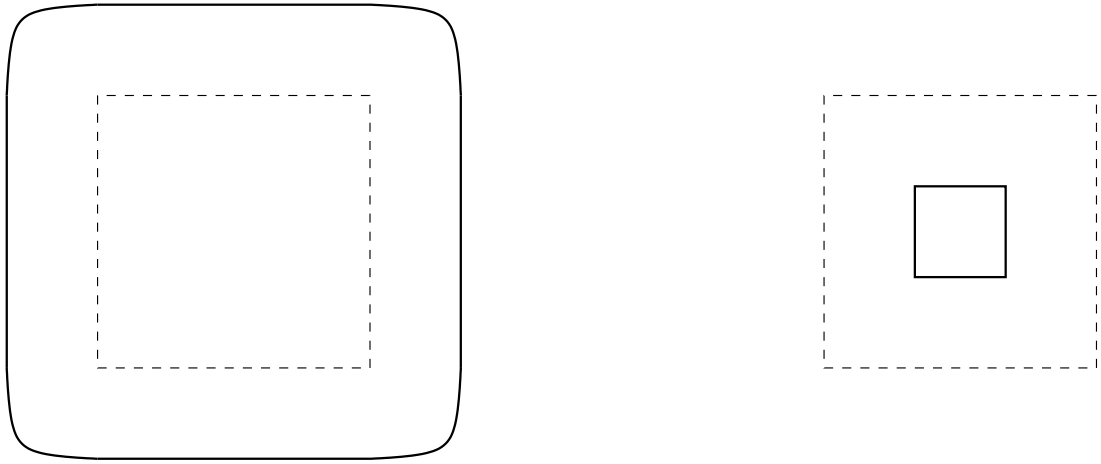
Lemma. Let $z \to h(z)$ be an increasing function such that $h(0) = 0$. If ψ is a H-J solution for the initial data ψ_0, then $h(\psi)$ is a solution for $h(\psi_0)$ too.

Formal proof. Multiply the H-J equation by $h'(\psi) \geq 0$ which can be put inside the absolute values.

Consequence: the level set $h(\psi)(t) = 0$ is the same whatever the choice of the function h.

Cf. works of Barles, Chen-Giga-Goto, Evans-Spruck.

Example of an explicit solution



c=1 c=-1

Take $\alpha = c$, $\beta = 0$ $\Rightarrow$ $\dfrac{\partial \psi}{\partial t} + c|\nabla \psi| = 0.$

A viscosity solution is $\boxed{\psi(t,x) = d(x,\Gamma_0) - c\,t}$ with $d(x,\Gamma_0)$ the signed distance to the initial surface. Irreversible solution !

Conclusion: some corners remain corners, others get rounded !

We must have numerical schemes preserving this property.

Upwind scheme for Hamilton-Jacobi

To solve the eikonal transport equation $\dfrac{\partial \psi}{\partial t} + c|\nabla \psi| = 0$ in D we must use an upwind scheme to make a difference between sharp corners and rounding corners.