OPTIMAL DESIGN OF STRUCTURES (MAP 562)

CHAPTER VII

Topology optimization by the homogenization method (first part)

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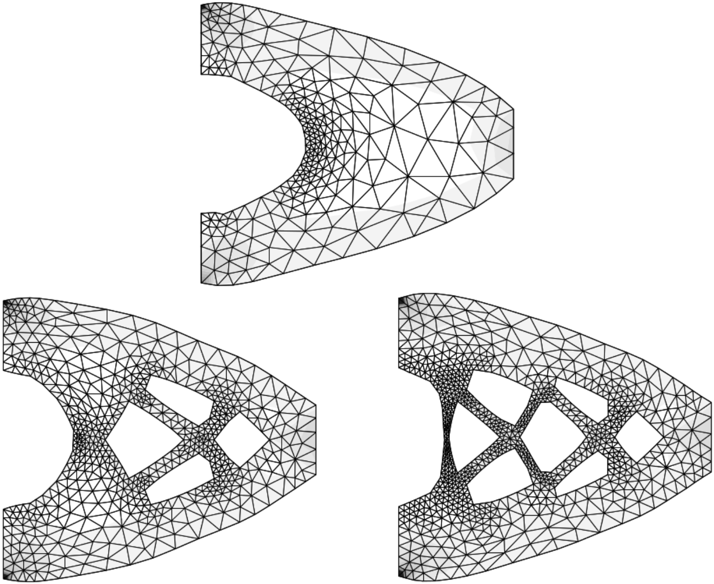
Why topology optimization ?

Drawbacks of geometric optimization:

- no variation of the topology (number of holes in 2-d),
- many local minima,
- CPU cost of remeshing (mostly in 3-d),
- ill-posed problem: non-existence of optimal solutions (in the absence of constraints). It shows up in numerics !

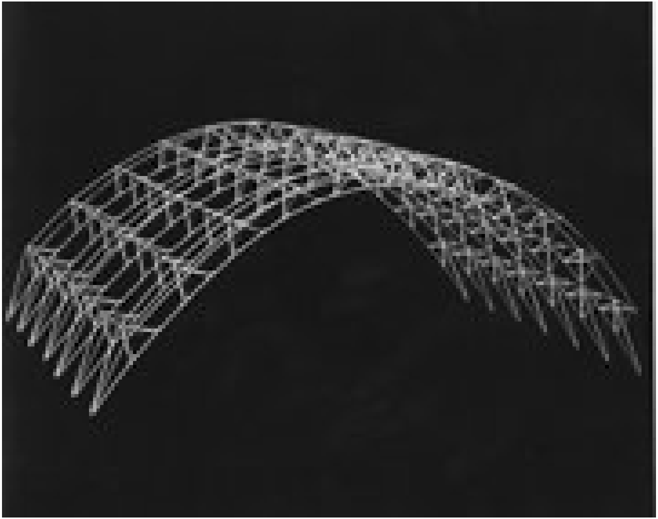
Topology optimization: we improve not only the boundary location but also its topology (i.e., its number of connected components in 2-d).



Minimal compliance for different topologies

The art of structure is where to put the holes.

Robert Le Ricolais, architect and engineer, 1894-1977



Methods for topology optimization

- **Level-set methods**:
$$\Omega = \{x \in D, \psi(x) < 0\},$$
with ψ updated according to the shape derivative.
$\rightsquigarrow$ fixed mesh, possibility to merge holes
- **topological derivative**
$$J(\Omega \backslash B(x,\rho)) = J(\Omega) = f(\rho)g(x) + o(f(\rho)), \qquad \lim_{\rho \to 0} f(\rho) = 0.$$
$\rightsquigarrow$ specifically dedicated to nucleate holes
- **Homogenization**: enlarge the admissible set to microstructures $\rightsquigarrow$ multiscale analysis, ends up with a parametric optimization problem
- Simplified homogenization (**SIMP**)
$\rightsquigarrow$ restricted to isotropic microstructures, very popular in the industry
- Combinations of these tools

This is an ongoing field of research.

In this course **we focus on the homogenization approach.**

Principles of the homogenization method

The homogenization method is based on the concept of "relaxation": it makes ill-posed problems well-posed by enlarging the space of admissible shapes.
We introduce "generalized" shapes but not too generalized... We require the generalized shapes to be "limits" of minimizing sequences of classical shapes.

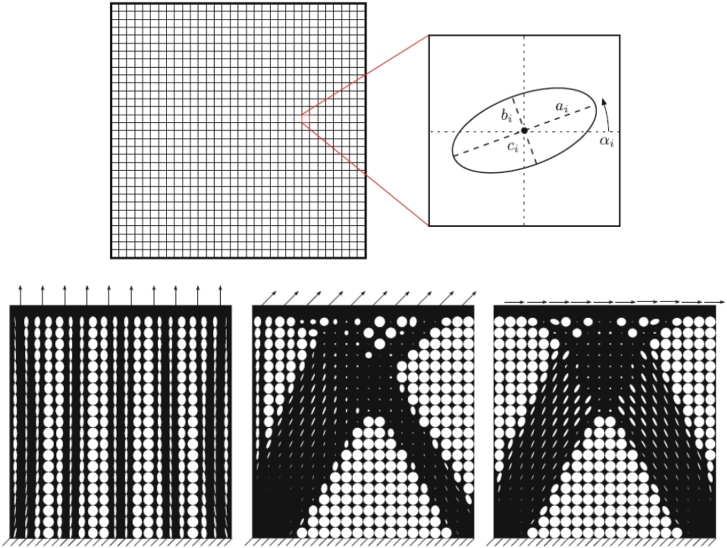
Remember the counter-example of existence: the minimizing sequences of shapes had a tendency to build fine mixtures of material and void.
Homogenization allows as admissible shapes **composite materials** obtained by microperforation of the original material.

Notations

- A classical shape is parametrized by a characteristic function

$$\chi(x) = \begin{cases} 1 \text{ inside the shape,} \\ 0 \text{ in the rest of the computational domain.} \end{cases}$$

- From now on, the holes can be microscopic as well as macroscopic $\Rightarrow$ porous composite materials !
- We parametrize a generalized shape by a material density $\theta(x) \in [0,1]$, and a microstructure (microperforations).
- The shape of the microperforations is very important ! It induces a new optimization variable which is the effective behavior $A^*(x)$ of the composite material (defined by homogenization theory).
- (θ, A^*) are the two new optimization variables.



b_i
a_i
c_i
α_i

Model problem

Simplifying assumption: the "holes" with a free boundary condition (Neumann) are actually filled with a weak ("ersatz") material $\alpha << \beta$.

For $f \in L^2(\Omega)$ is the applied load, the displacement satisfies

$$\begin{cases} -\operatorname{div}\left((\chi\beta + (1-\chi)\alpha)\nabla u_\chi\right) = f & \text{in } \Omega \\ u_\chi = 0 & \text{on } \partial\Omega. \end{cases}$$

Optimizing the membrane's shape amounts to solve

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

with

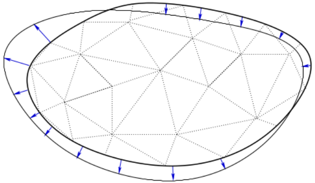
$$J(\chi) = \int_\Omega f u_\chi \, dx, \quad \text{or} \quad J(\chi) = \int_\Omega |u_\chi - u_0|^2 dx,$$

$$\mathcal{U}_{ad} = \left\{ \chi \in L^\infty(\Omega; \{0,1\}), \ \int_\Omega \chi(x)\, dx = V \right\}.$$

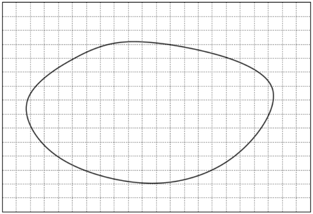
Goals of the homogenization method

- To introduce the notion of generalized shapes made of composite material.
- To show that those generalized shapes are limits of sequences of classical shapes (in a sense to be made precise).
- To compute the generalized objective function and its gradient.
- To prove an existence theorem of optimal generalized shapes (it is not the goal of the present course).
- To derive new numerical algorithms for topology optimization (it is the main goal of this chapter).

While geometric optimization was producing **shape tracking** algorithms, homogenization yields **shape capturing** algorithms.



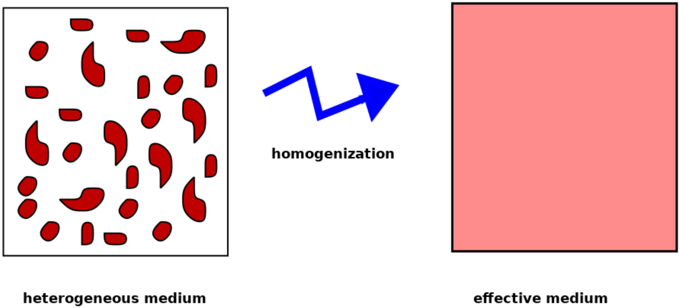
Shape tracking



Shape capturing

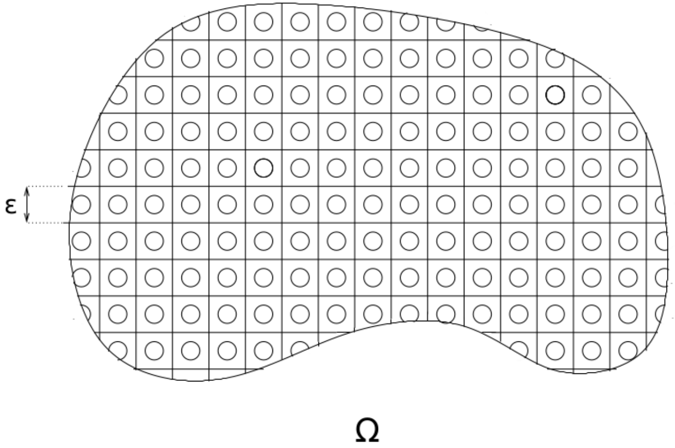
Shape capturing vs shape tracking: the mesh is fixed.

Homogenization



- Averaging method for partial differential equations.
- Determination of averaged parameters (or effective, or homogenized, or equivalent, or macroscopic) for an heterogeneous medium.

Periodic homogenization



Different approaches are possible: we describe the simplest one, i.e., periodic homogenization.

Assumption: we consider periodic heterogeneous media.

Periodic homogenization (Ctd.)

- Ratio of the period with the characteristic size of the structure $= \epsilon$.
- Although, for the "true" problem under consideration, there is only one physical value ϵ_0 of the parameter ϵ, we consider a sequence of problems with smaller and smaller ϵ.
- We perform an asymptotic analysis as ϵ goes to 0.
- We shall approximate the "true" problem ($\epsilon = \epsilon_0$) by the limit problem obtained as $\epsilon \to 0$.

Model problem: elastic membrane made of composite material

For example: periodically distributed fibers in an epoxy resin.
Variable Hooke's law: $A(y)$ is an Y-periodic function with $Y = (0,1)^N$ the Representative Volume Element, i.e.

$$A(y + e_i) = A(y) \quad \forall e_i \text{ } i\text{-th vector of the canonical basis.}$$

We replace y by $\frac{x}{\epsilon}$:

$$x \to A(\frac{x}{\epsilon}) \text{ periodic of period } \epsilon \text{ in all axis directions.}$$

Bounded domain Ω, load $f(x)$, displacement $u_\epsilon(x)$ solution of

$$\begin{cases} -\operatorname{div}\left(A(\frac{x}{\epsilon})\nabla u_\epsilon\right) = f & \text{in } \Omega \\ u_\epsilon = 0 & \text{on } \partial\Omega. \end{cases}$$

A direct computation of u_ϵ can be very expensive (since the mesh size h should satisfy $h < \epsilon$), thus we seek only the locally averaged values of u_ϵ.

Two-scale asymptotic expansions

2 scales $\rightsquigarrow$ 2 space variables: slow variable x (macro), fast variable y (micro, position within the RVE, re-scaled). We assume (**a priori formal**) that

$$u_\epsilon(x) = \hat{u}_\epsilon(x, \frac{x}{\epsilon}), \qquad \hat{u}_\epsilon(x, y) = \sum_{i=0}^{+\infty} \epsilon^i u_i(x, y)$$

$$\Rightarrow \qquad u_\epsilon(x) = \sum_{i=0}^{+\infty} \epsilon^i u_i(x, \frac{x}{\epsilon}),$$

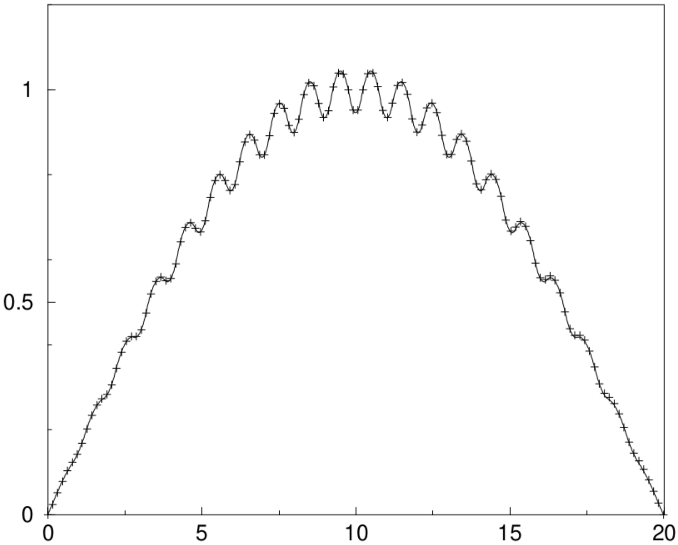
with $u_i(x, y)$ function of the two variables x and y, periodic in y of period $Y = (0, 1)^N$. Plugging this series in the equation, we use the derivation rule

$$\nabla \left(u_i(x, \frac{x}{\epsilon}) \right) = \left(\epsilon^{-1} \nabla_y u_i + \nabla_x u_i \right) (x, \frac{x}{\epsilon}).$$

Thus

$$\nabla u_\epsilon(x) = \epsilon^{-1} \nabla_y u_0(x, \frac{x}{\epsilon}) + \sum_{i=0}^{+\infty} \epsilon^i \left(\nabla_y u_{i+1} + \nabla_x u_i \right) (x, \frac{x}{\epsilon}).$$

Typical oscillating behavior of $x \to u_i(x, \frac{x}{\epsilon})$



The equation becomes a series in ϵ

$$-\epsilon^{-2}\left[\operatorname{div}_y\big(A\nabla_y u_0\big)\right](x,\frac{x}{\epsilon})$$

$$-\epsilon^{-1}\left[\operatorname{div}_y\big(A(\nabla_x u_0+\nabla_y u_1)\big)+\operatorname{div}_x\big(A\nabla_y u_0\big)\right](x,\frac{x}{\epsilon})$$

$$-\sum_{i=0}^{+\infty}\epsilon^i\left[\operatorname{div}_x\big(A(\nabla_x u_i+\nabla_y u_{i+1})\big)+\operatorname{div}_y\big(A(\nabla_x u_{i+1}+\nabla_y u_{i+2})\big)\right]$$

$$(x,\tfrac{x}{\epsilon})=f(x).$$

- We identify each power of ϵ.
- We notice that $\phi(x,\frac{x}{\epsilon})=0\ \forall x,\epsilon \quad\Leftrightarrow\quad \phi(x,y)\equiv 0\ \forall x,y$.
- Only the first three terms of the series really matter.

We start by a technical lemma.

Lemma. Take $g \in L^2(Y)$. The equation

$$\begin{cases} -\operatorname{div}_y \left(A(y)\nabla_y v(y)\right) = g(y) \text{ in } Y \\ y \to v(y) \;\; Y\text{-periodic} \end{cases}$$

admits a unique solution $v \in H^1_\#(Y)/\mathbb{R}$ if and only if

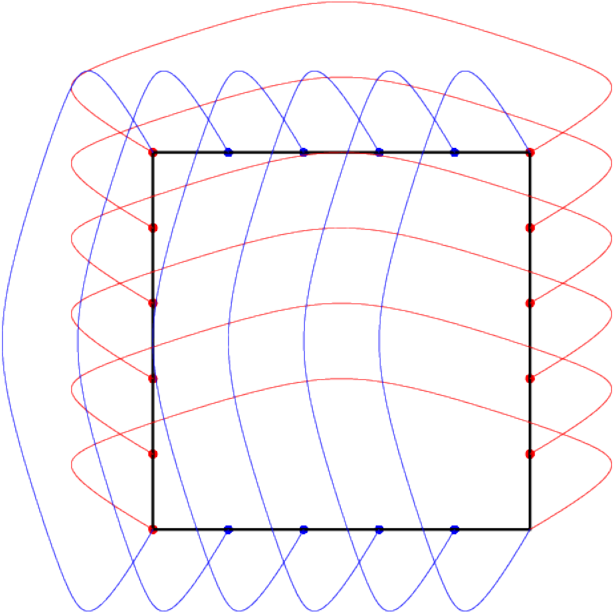
$$\int_Y g(y)\, dy = 0.$$

Proof. Let us check that it is a necessary condition for existence. Integrating the equation on Y

$$\int_Y \operatorname{div}_y \Big(A(y)\nabla_y v(y)\Big)\, dy = \int_{\partial Y} A(y)\nabla_y v(y) \cdot n\, ds = 0$$

because of the periodic boundary conditions: $A(y)\nabla_y v(y)$ is periodic but the normal n changes its sign on opposite faces of Y. The sufficient condition is obtained by applying the Lax-Milgram theorem in $H^1_\#(Y)/\mathbb{R}$.

Periodic boundary conditions in $H^1_{\#}(Y)$



Equation of order ϵ^{-2}:

$$\begin{cases} -\operatorname{div}_y \left(A(y)\nabla_y u_0(x,y)\right) = 0 \text{ in } Y \\ y \to u_0(x,y) \; Y\text{-periodic} \end{cases}$$

It is a p.d.e. with respect to y (x is just a parameter).
By uniqueness of the solution (up to an additive constant), we deduce

$$\boxed{u_0(x,y) \equiv u(x).}$$

Equation of order ϵ^{-1}:

$$\begin{cases} -\operatorname{div}_y\left(A(y)\nabla_y u_1(x,y)\right) = \operatorname{div}_y\left(A(y)\nabla_x u(x)\right) \text{ in } Y \\ y \to u_1(x,y) \ Y\text{-periodic} \end{cases}$$

The necessary and sufficient condition of existence is satisfied.
Thus u_1 depends linearly on $\nabla_x u(x)$.
We introduce the cell problems

$$\begin{cases} -\operatorname{div}_y\left(A(y)\left(e_i + \nabla_y w_i(y)\right)\right) = 0 & \text{in } Y \\ y \to w_i(y) & Y\text{-periodic,} \end{cases}$$

with $\left(e_i\right)_{1\leq i\leq N}$, the canonical basis of $\mathbb{R}^N$. Then

$$\boxed{u_1(x,y) = \sum_{i=1}^{N} \frac{\partial u}{\partial x_i}(x) w_i(y).}$$

Equation of order ϵ^0:

$$\begin{cases} -\operatorname{div}_y \left(A(y)\nabla_y u_2(x,y)\right) = \operatorname{div}_y \left(A(y)\nabla_x u_1\right) \\ \qquad\qquad\qquad\qquad\qquad + \operatorname{div}_x \left(A(y)(\nabla_y u_1 + \nabla_x u)\right) + f(x) \text{ in } Y \\ y \to u_2(x,y) \; Y\text{-periodic} \end{cases}$$

The necessary and sufficient condition of existence of the solution u_2 is:

$$\int_Y \Big(\operatorname{div}_y \big(A(y)\nabla_x u_1\big) + \operatorname{div}_x \big(A(y)(\nabla_y u_1 + \nabla_x u)\big) + f(x) \Big) dy = 0$$

We replace u_1 by its value in terms of $\nabla_x u(x)$

$$\operatorname{div}_x \int_Y A(y) \left(\sum_{i=1}^N \frac{\partial u}{\partial x_i}(x) \nabla_y w_i(y) + \nabla_x u(x) \right) dy + f(x) = 0$$

and we find the homogenized problem

$$\begin{cases} -\operatorname{div}_x \left(A^* \nabla_x u(x)\right) = f(x) \text{ in } \Omega \\ u = 0 \text{ on } \partial\Omega. \end{cases}$$

Homogenized tensor:

$$A^*_{ji} = \int_Y A(y)(e_i + \nabla_y w_i) \cdot e_j \, dy,$$

or, integrating by parts

$$A^*_{ji} = \int_Y A(y) \left(e_i + \nabla_y w_i(y)\right) \cdot \left(e_j + \nabla_y w_j(y)\right) dy.$$

Indeed, the cell problem yields

$$\int_Y A(y) \left(e_i + \nabla_y w_i(y)\right) \cdot \nabla_y w_j(y) \, dy = 0.$$

- The formula for A^* is not fully explicit because cell problems must be solved.
- A^* does not depend on Ω, nor f, nor the boundary conditions.
- **The tensor A^* characterizes the microstructure.**
- Later, we shall compute explicitly some examples of A^*.

Two-phase mixtures

We mix two isotropic constituents $A(y) = \alpha\chi(y) + \beta(1 - \chi(y))$ with a characteristic function $\chi(y) = 0$ or 1.
Let $\theta = \int_Y \chi(y)\, dy$ be the volume fraction of phase α and $(1 - \theta)$ that of phase β.

Definition. We define the set G_θ of all homogenized tensors A^* obtained by homogenization of the two phases α and β in proportions θ and $(1 - \theta)$.

Of course, we have $G_0 = \{\beta\}$ and $G_1 = \{\alpha\}$.
But usually, G_θ is a (very) large set of tensors (corresponding to different choices of $\chi(y)$).

Non-periodic case

Homogenization works for non-periodic media too.
The full (and **rigorous**) theory involves a special concept of convergence: H-convergence. In the periodic case the equations derived from the first 3 terms of the two-scale asymptotic expansion are retrieved.

For two-phase mixtures, the density $\theta(x)$, as well as the homogenized tensor $A^*(x)$ depend on the position x.

Application to shape optimization

Let χ_ϵ be a sequence (minimizing or not) of characteristic functions. By homogenization theory (compactness of H-convergence), as $\epsilon \to 0$, it holds for a subsequence

$$\chi_\epsilon(x) \rightharpoonup \theta(x), \quad u_\epsilon(x) \to u(x), \quad \left(A_\epsilon(x) \xrightarrow{\mathrm{H}} A^*(x)\right)$$

$$J(\chi_\epsilon) = \int_\Omega j(u_\epsilon)\,dx \to \int_\Omega j(u)\,dx = J(\theta, A^*),$$

with u, solution of the homogenized state equation

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

In particular, the objective function is unchanged when:

$$J(\theta, A^*) = \int_\Omega fu\,dx, \quad \text{or} \quad J(\theta, A^*) = \int_\Omega |u - u_0|^2 dx.$$

Homogenized formulation of shape optimization

We define the set of admissible homogenized shapes

$$\mathcal{U}_{ad}^* = \Big\{ (\theta, A^*) \in L^\infty \left(\Omega; [0,1] \times \mathbb{R}^{N^2} \right),$$
$$A^*(x) \in G_{\theta(x)} \text{ in } \Omega, \int_\Omega \theta(x)\, dx = V \Big\}.$$

The relaxed or homogenized optimization problem is

$$\inf_{(\theta, A^*) \in \mathcal{U}_{ad}^*} J(\theta, A^*).$$

Remarks

- $\mathcal{U}_{ad} \subset \mathcal{U}^*_{ad}$: we have enlarged the set of admissible shapes.
- One can prove that the relaxed problem always admit an optimal solution.
- We shall exhibit very efficient numerical algorithms for computing homogenized optimal shapes.
- Homogenization does not change the problem: homogenized shapes are just the characterization of limits of sequences of classical shapes

$$\lim_{\epsilon \to 0} J\left(\chi_\epsilon\right) = J(\theta, A^*).$$

- We need to find an explicit characterization of the set G_θ.

Strategy of the course

The goal is to find the set G_θ of all composite materials obtained by mixing α and β in proportions θ and $(1-\theta)$.

- One could do numerical optimization with respect to the geometry of the mixture $\chi(y)$ in the unit cell.
- We follow a different (and analytical) path.
- **First,** we build a class of explicit composites (so-called sequential laminates) which cover an apriori subset G_θ.
- **Second,** we prove "bounds" on A^* which prove that no composite can be outside our previous guess of G_θ.

Composite materials

Theoretical study of composite materials:

- In dimension $N = 1$: explicit formula for A^*, the so-called harmonic mean.
- In dimension $N \geq 2$, for two-phase mixtures: explicit characterization of G_θ thanks to the variational principle of Hashin and Shtrikman.

Underlying assumptions:

- Linear model of conduction or membrane stiffness (it is more delicate for linearized elasticity and very few results are known in the non-linear case).
- Perfect interfaces between the phases (continuity of both displacement and normal stress): no possible effects of delamination or debonding.

Dimension $N = 1$

Cell problem: $\begin{cases} -\Big(A(y)\,(1+w'(y))\Big)' = 0 & \text{in } [0,1] \\ y \to w(y) & \text{1-periodic} \end{cases}$

We explicitly compute the solution

$$w(y) = -y + \int_0^y \frac{C_1}{A(t)}dt + C_2 \quad \text{with} \quad C_1 = \left(\int_0^1 \frac{1}{A(y)}dy\right)^{-1}.$$

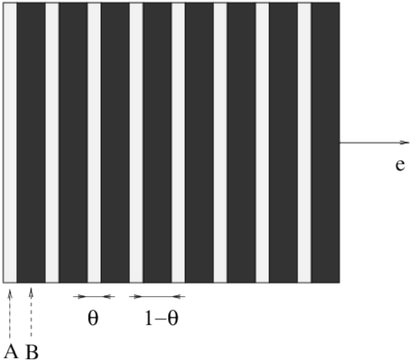
The formula for A^* is $A^* = \displaystyle\int_0^1 A(y)\,\big(1+w'(y)\big)^2\,dy$, which yields the harmonic mean of $A(y)$

$$A^* = \left(\int_0^1 \frac{1}{A(y)}dy\right)^{-1}.$$

Two-phase case:

$$A(y) = \alpha\chi(y) + \beta\,(1-\chi(y)) \quad \Rightarrow \quad A^* = \left(\frac{\theta}{\alpha} + \frac{1-\theta}{\beta}\right)^{-1}$$

Simple laminated composites



In dimension $N \geq 2$ we consider parallel layers of two isotropic phases α and β, orthogonal to the direction e_1

$$\chi(y_1) = \begin{cases} 1 & \text{if } 0 < y_1 < \theta \\ 0 & \text{if } \theta < y_1 < 1, \end{cases} \qquad \text{with} \quad \theta = \int_Y \chi \, dy.$$

We denote by A^* the homogenized tensor of $A(y) = \alpha\chi(y_1) + \beta\,(1 - \chi(y_1))$.

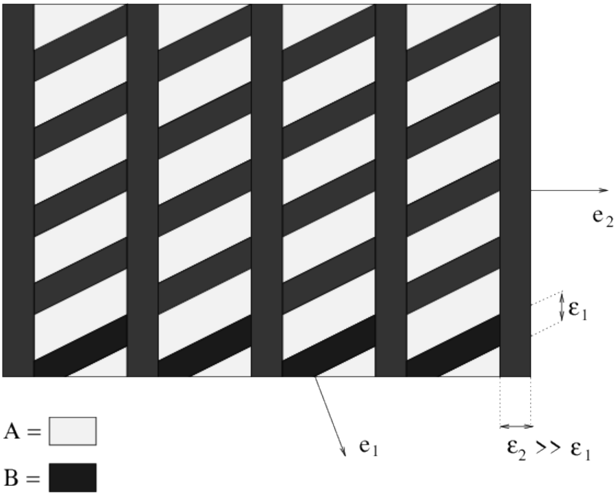
Lemma. Define $\lambda_\theta^- = \left(\frac{\theta}{\alpha} + \frac{1-\theta}{\beta}\right)^{-1}$ and $\lambda_\theta^+ = \theta\alpha + (1-\theta)\beta$.

We have

$$A^* = \begin{pmatrix} \lambda_\theta^- & & & 0 \\ & \lambda_\theta^+ & & \\ & & \ddots & \\ 0 & & & \lambda_\theta^+ \end{pmatrix}.$$

Interpretation (resistance = inverse of conductivity). Resistances, placed in series (in the direction e_1), average arithmetically, while resistances, placed in parallel (in directions orthogonal to e_1) average harmonically.

Sequential laminated composites



We laminate again a laminated composite with one of the pure phases.

Simple laminate of two non-isotropic phases

Lemma. The homogenized tensor A^* of a simple laminate made of A and B in proportions θ and $(1-\theta)$ in the direction e_1 is

$$A^* = \theta A + (1-\theta)B - \frac{\theta(1-\theta)\,(A-B)e_1 \otimes (A-B)^t e_1}{(1-\theta)Ae_1\cdot e_1 + \theta Be_1\cdot e_1}.$$

If we assume that $(A-B)$ is invertible, then this formula is equivalent to

$$\boxed{\theta\,(A^*-B)^{-1} = (A-B)^{-1} + \frac{(1-\theta)}{Be_1\cdot e_1} e_1 \otimes e_1.}$$

Sequential lamination

We laminate again the preceding composite with always the same phase B.

Recall that the homogenized tensor A_1^* of a simple laminate is

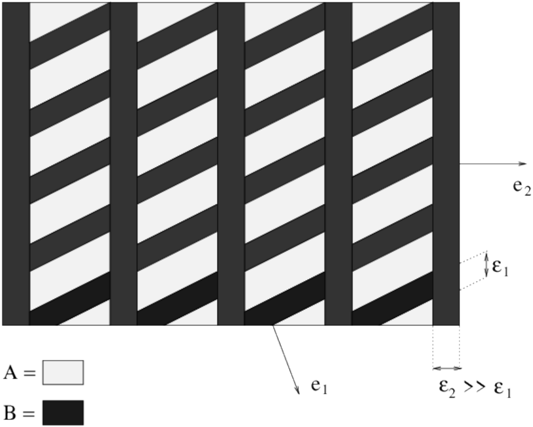
$$\theta \left(A_1^* - B\right)^{-1} = (A - B)^{-1} + (1 - \theta) \frac{e_1 \otimes e_1}{Be_1 \cdot e_1}.$$

Lemma. If we laminate p times with B, we obtain a rank-p sequential laminate with matrix B and inclusion A, in proportions $(1 - \theta)$ and θ

$$\theta \left(A_p^* - B\right)^{-1} = (A - B)^{-1} + (1 - \theta) \sum_{i=1}^{p} m_i \frac{e_i \otimes e_i}{Be_i \cdot e_i}.$$

with

$$\sum_{i=1}^{p} m_i = 1 \text{ and } m_i \geq 0,\ 1 \leq i \leq p.$$



- A appears only at the first lamination: it is thus surrounded by B. In other words, A =inclusion and B = matrix.
- The thickness scales of the layers are very different between two lamination steps.
- Lamination parameters (m_i, e_i).

Proof. By induction we obtain A_p^* by laminating A_{p-1}^* and B in the direction e_p and in proportions θ_p, $(1-\theta_p)$, respectively

$$\theta_p \left(A_p^* - B\right)^{-1} = \left(A_{p-1}^* - B\right)^{-1} + (1-\theta_p)\frac{e_p \otimes e_p}{Be_p \cdot e_p}.$$

Replacing $(A_{p-1}^* - B)^{-1}$ in this formula by the similar formula defining $(A_{p-2}^* - B)^{-1}$, and so on, we obtain

$$\left(\prod_{j=1}^{p}\theta_j\right)\left(A_p^* - B\right)^{-1} = (A-B)^{-1} + \sum_{i=1}^{p}\left((1-\theta_i)\prod_{j=1}^{i-1}\theta_j\right)\frac{e_i \otimes e_i}{Be_i \cdot e_i}.$$

We make the change of variables

$$(1-\theta)m_i = (1-\theta_i)\prod_{j=1}^{i-1}\theta_j \quad 1 \leq i \leq p$$

which is indeed one-to-one with the constraints on the m_i's and the θ_i's ($\theta = \prod_{i=1}^{p}\theta_i$).

The same can be done when exchanging the roles of A and B.

Lemma. A rank-p sequential laminate with matrix A and inclusion B, in proportions θ and $(1-\theta)$, is defined by

$$(1-\theta)\left(A_p^* - A\right)^{-1} = (B-A)^{-1} + \theta \sum_{i=1}^{p} m_i \frac{e_i \otimes e_i}{Ae_i \cdot e_i}.$$

with

$$\sum_{i=1}^{p} m_i = 1 \text{ and } m_i \geq 0,\ 1 \leq i \leq p.$$

Remark. Sequential laminates form a very rich and explicit class of composite materials which, as we shall see, describe completely the boundaries of the set G_θ.

Variational characterization of homogenized tensors

From now on, we assume that the microscopic tensor $A(y)$ is symmetric. Then A^* is symmetric too.

Furthermore, A^* is characterized by the variational principle

$$A^*\xi\cdot\xi = \min_{w\in H^1_\#(Y)/\mathbb{R}} \int_Y A(y)\,(\xi+\nabla w)\cdot(\xi+\nabla w)\,dy.$$

Indeed, if w_ξ is the minimizer, then it satisfies the Euler optimality condition

$$\begin{cases} -\mathrm{div}\Big(A(y)\,(\xi+\nabla w_\xi(y))\Big) = 0 & \text{in } Y \\ y \to w_\xi(y) & Y\text{-periodic.} \end{cases}$$

By linearity, we have $w_\xi = \sum_{i=1}^N \xi_i w_i$ and thus

$$\int_Y A(y)\,(\xi+\nabla w_\xi)\cdot(\xi+\nabla w_\xi)\,dy = \sum_{i,j=1}^N \xi_i\xi_j A^*_{ij} = A^*\xi\cdot\xi.$$

Arithmetic and harmonic mean bounds

Taking $w = 0$ in the variational principle, we deduce the arithmetic mean bound

$$A^*\xi \cdot \xi \leq \left(\int_Y A(y)\, dy \right) \xi \cdot \xi$$

Enlarging the minimization space, we obtain the harmonic mean bound

$$A^*\xi \cdot \xi \geq \left(\int_Y A^{-1}(y)\, dy \right)^{-1} \xi \cdot \xi.$$

These bounds can be improved for two-phase composites !

Indeed, since $\int_Y \nabla w \, dy = 0$, we enlarge the minimization space by replacing ∇w with any vector field $\zeta(y)$ with zero-average on Y

$$A^*\xi \cdot \xi \geq \min_{\zeta \in L^2_\#(Y)^N, \ \int_Y \zeta \, dy = 0} \int_Y A(y) \left(\xi + \zeta(y)\right) \cdot \left(\xi + \zeta(y)\right) dy.$$

The Euler-Lagrange equation for the minimizer $\zeta_\xi(y)$ of this convex problem is

$$A(y) \left(\xi + \zeta_\xi(y)\right) = \lambda$$

where $\lambda \in \mathbb{R}^N$ is the Lagrange multiplier for the constraint $\int_Y \zeta \, dy = 0$. We deduce

$$\xi + \zeta_\xi(y) = A(y)^{-1}\lambda \ \Rightarrow \xi = \left(\int_Y A(y)^{-1} \, dy \right) \lambda$$

and thus

$$\int_Y A(y)\Big(\xi + \zeta_\xi(y)\Big) \cdot \Big(\xi + \zeta_\xi(y)\Big) dy = \left(\int_Y A(y)^{-1} \, dy \right)^{-1} \xi \cdot \xi.$$

Characterization of G_θ

We consider two isotropic phases $A = \alpha\,\mathrm{Id}$ and $B = \beta\,\mathrm{Id}$ with $0 < \alpha < \beta$.

Theorem. The set G_θ of all homogenized tensors obtained by mixing α and β in proportions θ and $(1-\theta)$ is the set of all symmetric matrices A^* with eigenvalues $\lambda_1, ..., \lambda_N$ such that

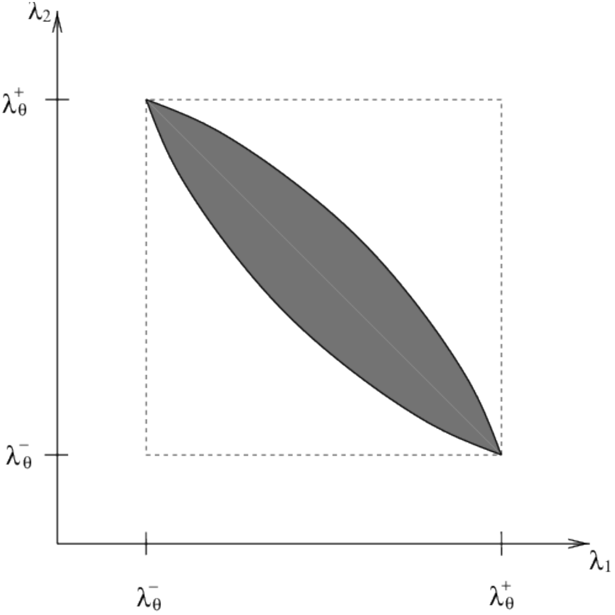
$$\left(\frac{\theta}{\alpha} + \frac{1-\theta}{\beta}\right)^{-1} = \lambda_\theta^- \le \lambda_i \le \lambda_\theta^+ = \theta\alpha + (1-\theta)\beta \quad 1 \le i \le N$$

$$\sum_{i=1}^{N} \frac{1}{\lambda_i - \alpha} \le \frac{1}{\lambda_\theta^- - \alpha} + \frac{N-1}{\lambda_\theta^+ - \alpha}$$

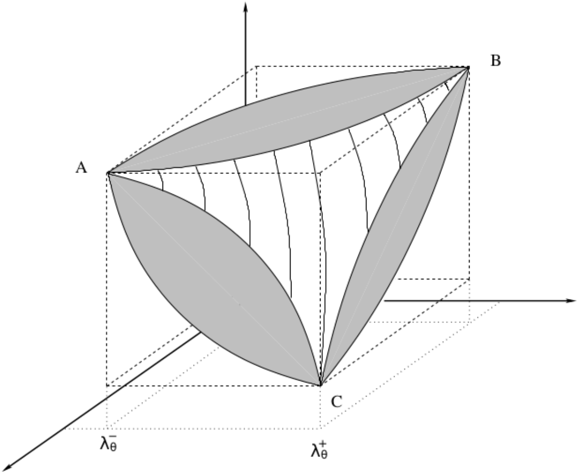
$$\sum_{i=1}^{N} \frac{1}{\beta - \lambda_i} \le \frac{1}{\beta - \lambda_\theta^-} + \frac{N-1}{\beta - \lambda_\theta^+}.$$

Furthermore, these so-called Hashin and Shtrikman bounds are optimal and attained by rank-N sequential laminates.

Set G_θ in dimension $N = 2$



Set G_θ in dimension $N = 3$



Homogenized formulation of shape optimization

The relaxed or homogenized optimization problem is

$$\min_{(\theta, A^*)\in \mathcal{U}^*_{ad}} J(\theta, A^*),$$

with an objective function

$$J(\theta, A^*) = \int_\Omega f u \, dx, \quad \text{or} \quad J(\theta, A^*) = \int_\Omega |u - u_0|^2 dx,$$

and an homogenized admissible set given by

$$\mathcal{U}^*_{ad} = \Big\{ (\theta, A^*) \in L^\infty\left(\Omega; [0,1] \times \mathbb{R}^{N^2}\right), \\ A^*(x) \in G_{\theta(x)} \text{ in } \Omega, \int_\Omega \theta(x)\, dx = V \Big\},$$

where G_θ is explicitly characterized.
The homogenized state equation is

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

Theorem (admitted). The homogenized formulation is actually a **relaxation** of the original shape optimization problem in the sense that:

- there exists, at least, one optimal composite shape (θ, A^*),
- any minimizing sequence of classical shapes χ converges, in the sense of homogenization, to a composite optimal solution (θ, A^*),
- any composite optimal solution (θ, A^*) is the limit of a minimizing sequence of classical shapes.

The minima of the original and homogenized objective functions coincide

$$\inf_{\chi \in \mathcal{U}_{ad}} J(\chi) = \min_{(\theta, A^*) \in \mathcal{U}^*_{ad}} J(\theta, A^*).$$

Remark.

- The shape optimization problem is thus not changed by relaxation.
- Close to any optimal composite shape, we are sure to find a quasi-optimal classical shape.
- This theorem is at the root of new numerical algorithms.

Optimality conditions

We now compute the gradient of the following objective function

$$J(\theta, A^*) = \int_\Omega |u - u_0|^2 dx,$$

where $u_0 \in L^2(\Omega)$. We introduce the adjoint state p, unique solution in $H_0^1(\Omega)$ of

$$\begin{cases} -\operatorname{div}(A^* \nabla p) = -2(u - u_0) & \text{in } \Omega \\ p = 0 & \text{on } \partial\Omega. \end{cases}$$

Proposition. Let $\alpha > 0$ and $\mathcal{M}_\alpha$ be the set of symmetric positive definite matrices M such that $M \geq \alpha \, \mathrm{Id}$. The functional J is differentiable with respect to A^* in $L^\infty(\Omega; \mathcal{M}_\alpha)$, and its derivative is

$$\nabla_{A^*} J(\theta, A^*) = \nabla u \otimes \nabla p \, .$$

Remark. The partial derivative with respect to θ vanishes because θ appears only in the constraint $A^* \in G_\theta$.

Proof.

It is standard ! It became a parametric (sizing) shape optimization problem where A^* plays the role of a thickness.

We introduce the Lagrangian

$$\mathcal{L}(A^*, v, q) = \int_\Omega |v - u_0|^2 dx + \int_\Omega A^* \nabla v \cdot \nabla q \, dx - \int_\Omega fq \, dx$$

Its partial derivative with respect to q yields the state.
Its partial derivative with respect to v yields the adjoint.
Its partial derivative with respect to A^* yields the gradient

$$\nabla_{A^*} J(\theta, A^*) = \frac{\partial \mathcal{L}}{\partial A^*}(A^*, u, p) = \nabla u \otimes \nabla p \, .$$

Essential consequence

Theorem. Let (θ, A^*) be a global minimizer of J in $\mathcal{U}^*_{ad}$ which admits u and p as state and adjoint. There exists $(\tilde{\theta}, \tilde{A}^*)$, another global minimizer of J in $\mathcal{U}^*_{ad}$, which admits the same state and adjoint u and p, and such that $\tilde{A}^*$ is a rank-1 simple laminate.

Simplification: in the definition of $\mathcal{U}^*_{ad}$ the set G_θ can be replaced by its simpler subset of rank-1 simple laminates.

Remark.

- Optimality condition $\Rightarrow$ simplification of the problem.
- We actually use this simplification in the numerical algorithms.
- Simplification which holds true for other objective functions, but not for multiple loads optimization.

Proof. We fix θ and make variations of A^* only. Remarking that G_θ is convex (not obvious), the optimality condition is an Euler inequality which is

$$\int_\Omega (A^0 - A^*)\nabla u \cdot \nabla p \, dx \geq 0$$

for any $A^0 \in G_\theta$, which is equivalent to

$$A^*\nabla u \cdot \nabla p = \min_{A^0 \in G_\theta} \left(A^0 \nabla u \cdot \nabla p \right) \quad \forall\, x \in \Omega.$$

If ∇u or ∇p vanishes, then any A^* is optimal. Otherwise, we define

$$e = \frac{\nabla u}{|\nabla u|} \quad \text{and} \quad e' = \frac{\nabla p}{|\nabla p|},$$

and we look for minimizers A^* of

$$\min_{A^0 \in G_\theta} 4A^0 e \cdot e' = A^0(e + e') \cdot (e + e') - A^0(e - e') \cdot (e - e').$$

A lower bound is easily obtained

$$\min_{A^0 \in G_\theta} 4A^0 e \cdot e' \geq \min_{A^0 \in G_\theta} A^0(e+e') \cdot (e+e') - \max_{A^0 \in G_\theta} A^0(e-e') \cdot (e-e') = \lambda_\theta^- |e+e'|^2 - \lambda_\theta^+ |e-e'|^2.$$

This lower bound is actually the precise minimal value.
Indeed, choosing $A^0 = A^1$ which is a rank-1 simple laminate in the direction $e+e'$, orthogonal to $e-e'$, we get

$$A^1(e+e') = \lambda_\theta^-(e+e') \quad \text{and} \quad A^1(e-e') = \lambda_\theta^+(e-e')$$

and an easy computation shows that

$$4A^1 e \cdot e' = \lambda_\theta^- |e+e'|^2 - \lambda_\theta^+ |e-e'|^2.$$

Thus

$$\min_{A^0 \in G_\theta} 4A^0 e \cdot e' = \lambda_\theta^- |e+e'|^2 - \lambda_\theta^+ |e-e'|^2.$$

If now A^* is any optimal tensor, then, like a rank-1 laminate, it satisfies

$$A^*(e+e') = \lambda_\theta^-(e+e') \quad \text{and} \quad A^*(e-e') = \lambda_\theta^+(e-e'). \quad (1)$$

Indeed, if (1) does not hold true, one of the arithmetic and harmonic bounds would give a strict inequality

$$4A^*e\cdot e' = A^*(e+e')\cdot(e+e') - A^*(e-e')\cdot(e-e') > \lambda_\theta^-|e+e'|^2 - \lambda_\theta^+|e-e'|^2$$

which is a contradiction with the optimal character of A^*.

We deduce that any optimal A^* satisfies, like the rank-1 simple laminate A^1,

$$
\begin{aligned}
2A^*\nabla u = \; & 2A^1\nabla u = & \left(\lambda_\theta^+ + \lambda_\theta^-\right)\nabla u - \left(\lambda_\theta^+ - \lambda_\theta^-\right)\frac{|\nabla u|}{|\nabla p|}\nabla p \\
2A^*\nabla p = \; & 2A^1\nabla p = & \left(\lambda_\theta^+ + \lambda_\theta^-\right)\nabla p - \left(\lambda_\theta^+ - \lambda_\theta^-\right)\frac{|\nabla p|}{|\nabla u|}\nabla u.
\end{aligned}
$$

Therefore any optimal tensor A^* can be replaced by this rank-1 simple laminate A^1 without changing u and p:

$$
-\operatorname{div}\Big(A^*\nabla u\Big) = -\operatorname{div}\Big(A^1\nabla u\Big) = f
$$

$$
-\operatorname{div}\Big(A^*\nabla p\Big) = -\operatorname{div}\Big(A^1\nabla p\Big) = -2(u - u_0).
$$

Parametrization of rank-1 simple laminates

In space dimension $N = 2$ (to simplify) a rank-1 laminate is defined by

$$A^*(\theta, \phi) = \begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix} \begin{pmatrix} \lambda_\theta^+ & 0 \\ 0 & \lambda_\theta^- \end{pmatrix} \begin{pmatrix} \cos\phi & -\sin\phi \\ \sin\phi & \cos\phi \end{pmatrix},$$

$\phi \in [0, \pi]$. The admissible set is thus simply

$$\mathcal{U}_{ad}^L = \Big\{ (\theta, \phi) \in L^\infty\left(\Omega; [0,1] \times [0, \pi]\right), \int_\Omega \theta(x)\, dx = V \Big\}.$$

Proposition. The objective function $J(\theta, \phi)$ is differentiable with respect to (θ, ϕ) in $\mathcal{U}_{ad}^L$, and its derivative is

$$\nabla_\phi J(\theta, \phi) = \frac{\partial A^*}{\partial \phi} \nabla u \cdot \nabla p \quad \text{and} \quad \nabla_\theta J(\theta, \phi) = \frac{\partial A^*}{\partial \theta} \nabla u \cdot \nabla p.$$

Numerical algorithm

Projected gradient algorithm for the minimization of $J(\theta, \phi)$.

1. We initialize the design parameters θ_0 and ϕ_0 (for example, equal to constants).
2. Until convergence, for $k \geq 0$ we iterate by computing the state u_k and adjoint p_k, solutions with the previous design parameters (θ_k, ϕ_k), then we update these parameters by

$$\theta_{k+1} = \max\left(0, \min\left(1, \theta_k - t_k\left(\ell_k + \frac{\partial A^*}{\partial \theta}(\theta_k, \phi_k)\nabla u_k \cdot \nabla p_k\right)\right)\right)$$

$$\phi_{k+1} = \phi_k - t_k \frac{\partial A^*}{\partial \phi}(\theta_k, \phi_k)\nabla u_k \cdot \nabla p_k$$

with ℓ_k a Lagrange multiplier for the volume constraint (iteratively enforced), and $t_k > 0$ a descent step such that $J(\theta_{k+1}, \phi_{k+1}) < J(\theta_k, \phi_k)$.

The self-adjoint case

A first example: maximization of torsional rigidity (maximization of compliance).

$$\min_{(\theta,A^*)\in\mathcal{U}^L_{ad}} \left\{ J(\theta,A^*) = -\int_\Omega u(x)dx \right\},$$

where u is the solution of

$$\begin{cases} -\operatorname{div}(A^*\nabla u) = 1 & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega, \end{cases}$$

and the adjoint state is just $p = u$.
We solve in the domain $\Omega = (0,1)^2$ with the phases $\alpha = 1$ and $\beta = 2$. We fix a 50% volume constraint of α. We initialize with a constant value of $\theta = 0.5$ and a constant zero lamination angle. We perform 30 iterations.

Self-adjoint case $p = u$.

$$\nabla_{A^*} J(\theta, A^*) = \nabla u \otimes \nabla u \geq 0\,.$$

To minimize J we have to decrease A^*.

Any optimal A^* satisfies

$$A^* \nabla u = \lambda_\theta^- \nabla u$$

thus the optimal composite is the **worst possible conductor**.

Consequence. We can eliminate the angle ϕ and it remains to optimize with respect to θ only !

Convexity

We rewrite the optimization problem thanks to the primal energy

$$J(\theta, A^*) = \min_{v \in H_0^1(\Omega)} \int_\Omega A^* |\nabla v|^2 dx - 2 \int_\Omega v \, dx.$$

Thus, we obtain a double minimization

$$\min_{\theta, A^* \in G_\theta} J(\theta, A^*) = \min_{\theta, v} \int_\Omega \lambda_\theta^- |\nabla v|^2 dx - 2 \int_\Omega v \, dx.$$

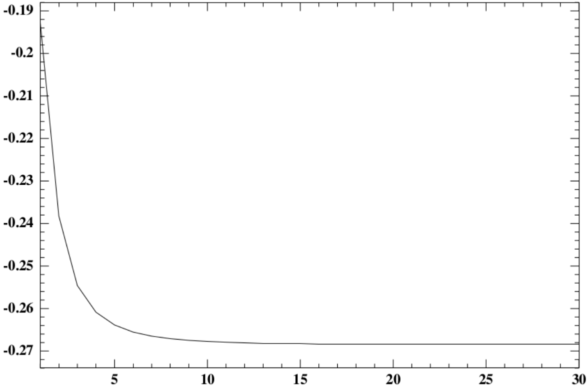
Remember: the function $(\theta, v) \to \lambda_\theta^- |\nabla v|^2$ is convex.

Consequence. There are only global minima !

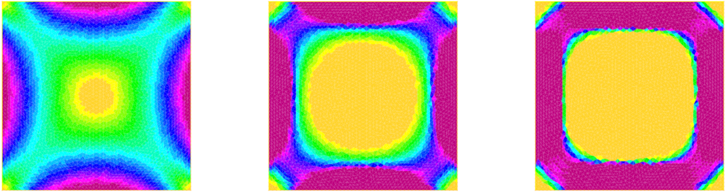
Numerically, we use an algorithm based on alternate direction minimization (see chapter 5).

Convergence history

objective function in terms of the iteration number.



Volume fraction θ (iterations 1, 5, and 30)



A second self-adjoint example

Compliance minimization.

$$\min_{(\theta, A^*) \in \mathcal{U}_{ad}^L} \left\{ J(\theta, A^*) = \int_\Omega u(x) dx \right\},$$

where u is the solution of

$$\begin{cases} -\operatorname{div}(A^* \nabla u) = 1 & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega, \end{cases}$$

and the adjoint state is just $p = -u$.
We solve in the domain $\Omega = (0,1)^2$ with the phases $\alpha = 1$ and $\beta = 2$. We fix a 50% volume constraint of α. We initialize with a constant value of $\theta = 0.5$ and a constant zero lamination angle. We perform 30 iterations.

Self-adjoint case $p = -u$.

$$\nabla_{A^*} J(\theta, A^*) = -\nabla u \otimes \nabla u \leq 0 \, .$$

To minimize J we have to increase A^*.

Any optimal A^* satisfies

$$A^* \nabla u = \lambda_\theta^+ \nabla u$$

thus the optimal composite is the **best possible conductor**.

Consequence. We can eliminate the angle ϕ and it remains to optimize with respect to θ only !

Convexity

We rewrite the optimization problem thanks to the dual energy

$$J(\theta, A^*) = \min_{\substack{\tau \in L^2(\Omega)^N \\ -\operatorname{div}\tau = 1 \text{ in } \Omega}} \int_\Omega (A^*)^{-1} |\tau|^2 dx \; .$$

Thus, we obtain a double minimization

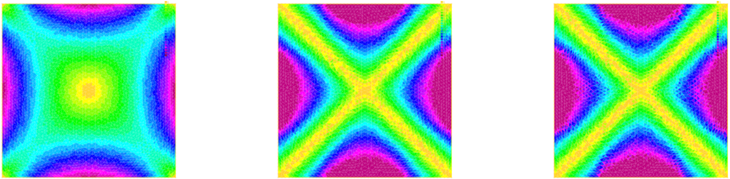
$$\min_{\theta, A^* \in G_\theta} J(\theta, A^*) = \min_{\theta, \tau} \int_\Omega (\lambda_\theta^+)^{-1} |\tau|^2 dx$$

Remember: the function $(\theta, \tau) \to \dfrac{|\tau|^2}{\lambda_\theta^+}$ is convex.

Consequence. There are only global minima !

Numerically, we use an algorithm based on alternate direction minimization (see chapter 5).

Minimal compliance membrane (iterations 1, 10, and 30)



Remarks

Convergence to a global minimum.

1. Numerical experiments with various initializations.
2. Convexity properties.

Shape optimization rather than two-phase optimization.

1. Numerically, holes can be mimicked by a very weak phase α ($\approx 10^{-3}\beta$).
2. Mathematically, when $\alpha \to 0$ we obtain Neumann boundary conditions on the holes boundaries.

Penalization

The previous algorithm computes composite shapes while we are rather interested by classical shapes.
Therefore we use a penalization process to force the density to take values close to 0 or 1.
Possible algorithms: after convergence to a composite shape,

1. either we add a penalization term to the objective function like

$$J(\theta, A^*) + c_{pen} \int_\Omega \theta(1-\theta)\, dx,$$

2. or we continue the previous algorithm with a modified "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 $\theta_{pen} > \theta_{opt}$.

Example

Optimal heater.

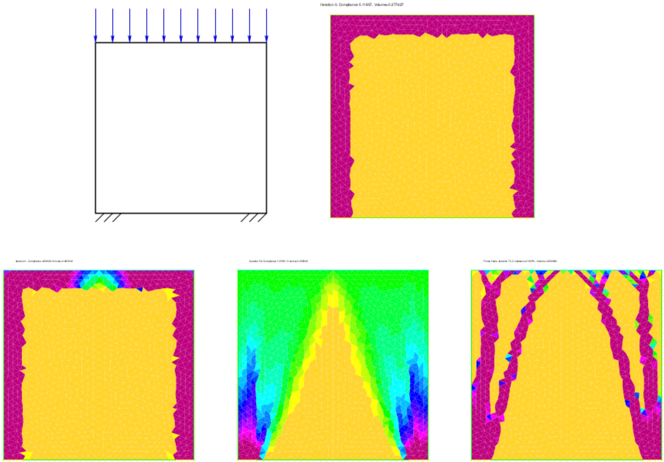
$$\begin{cases} -\operatorname{div}(A^*\nabla u) = 0 & \text{in } \Omega \\ A^*\nabla u \cdot n = 1 & \text{on } \Gamma_N \\ A^*\nabla u \cdot n = 0 & \text{on } \Gamma \\ u = 0 & \text{on } \Gamma_D. \end{cases}$$

We minimize the temperature where heating takes place

$$\min_{(\theta,A^*)\in\mathcal{U}^L_{ad}} \left\{ J(\theta, A^*) = \int_{\Gamma_N} u\, ds \right\}.$$

This is precisely the compliance ! Thus the problem is self-adjoint with $p = -u$.
Isotropic materials with conductivity $\alpha = 0.01$ and $\beta = 1$, in the domain $\Omega = (0,1)^2$.

Optimal heater



Initialization, iteration 1, iteration 50, iteration 70 (penalized)