OPTIMAL DESIGN OF STRUCTURES (MAP 562)

CHAPTER VII

Topology optimization by the homogenization method (second part)

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Topology optimization in the elasticity setting

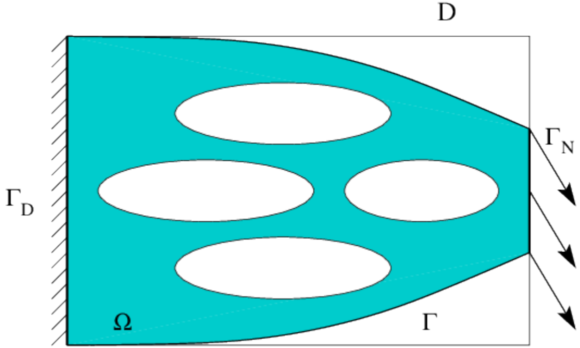
Very similar to the conductivity setting but there are some additional hurdles.

We shall review the results without proofs.

The basic ingredients of the homogenization method are the same:

- introduction of composite designs characterized by (θ, A^*),
- Hashin-Shtrikman bounds for composites,
- sequential laminates are optimal microstructures in important cases.

Model problem: compliance minimization



Bounded working domain $D \subset \mathbb{R}^N$ ($N = 2, 3$).
Linear isotropic elastic material, with Hooke's law A

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

(κ, μ)=bulk / shear moduli = eigenvalues of A, $\qquad \kappa = \lambda + \dfrac{2\mu}{N}$

Admissible shape = subset $\Omega \subset D$.

Boundary $\partial\Omega = \Gamma \cup \Gamma_N \cup \Gamma_D$ with Γ_N and Γ_D fixed.

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

Weight is minimized and stiffness is maximized. Let $\ell > 0$ be a Lagrange multiplier, the objective function is

$$\inf_{\Omega \subset D} \left\{ J(\Omega) = \int_{\Gamma_N} g \cdot u \, ds + \ell \int_{\Omega} dx \right\}.$$

This shape optimization problem can be approximated by a two-phase optimization problem: the original material A and the holes of Hooke's law $B \approx 0$.
The Hooke's law of the medium in D is

$$\chi_\Omega(x)A + \big(1 - \chi_\Omega(x)\big)B.$$

The admissible set is

$$\mathcal{U}_{ad} = \Big\{\chi \in L^\infty\left(D; \{0, 1\}\right)\Big\}.$$

As in the conductivity/membrane case, one can apply the relaxation approach based on the homogenization theory.
The homogenization method can be generalized to the elasticity setting.

Homogenized formulation of shape optimization

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

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

The homogenized compliance is defined by

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

The relaxed or homogenized optimization problem is

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

Major inconvenient: in the elasticity setting an explicit characterization of G_θ is still lacking !
Fortunately, for compliance one can replace G_θ by its explicit subset of laminated composites.

The key argument to overcome the incomplete knowledge of G_θ is that, by the complementary energy, the 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 (we already used this argument in chapter 5).

Exchanging the order of minimizations

The shape optimization problem is

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

Since the order of minimization is irrelevant, and the minimization with respect to the design parameters (θ, A^*) is local, it can be rewritten

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

For a given stress tensor σ, the minimization of complementary energy

$$\min_{A^* \in G_\theta} A^{*-1}\sigma \cdot \sigma$$

is a classical problem in homogenization, of finding optimal bounds on the effective properties of composite materials.
It turns out that we can restrict ourselves to sequential laminates which form an explicit subset L_θ of G_θ.
Such a simplification is made possible because compliance is the objective function.

Sequential laminates in elasticity

Two materials with Hooke's laws

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

with $\kappa_{A,B} = \lambda_{A,B} + 2\mu_{A,B}/N$. 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. The Hooke's law A^* of a simple laminate of A and B in proportions θ and $(1-\theta)$, respectively, in the direction e, satisfies

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

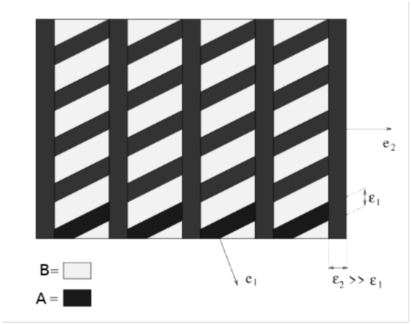
with $f_A^c(e)$ the symmetric tensor defined, for any symmetric matrix ξ, by

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

Reiterated lamination formula

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

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



Proposition. Let G_θ be the set of all homogenized elasticity tensors obtained by mixing the two phases A and B in proportions θ and $(1-\theta)$. Let L_θ be the subset of G_θ made of sequential laminated composites. For any stress σ,

$$HS(\sigma) := \min_{A^* \in G_\theta} {A^*}^{-1}\sigma \cdot \sigma = \min_{A^* \in L_\theta} {A^*}^{-1}\sigma \cdot \sigma.$$

Furthermore, the minimum is attained by a rank-N sequential laminate with lamination directions given by the eigendirections of σ.

Remark.

- An optimal tensor A^* can be interpreted as the most rigid composite material in G_θ able to sustain the stress σ.
- $HS(\sigma)$ is called Hashin-Shtrikman optimal energy bound.
- In the conductivity setting, a rank-1 laminate was enough...
- Practical conclusion: G_θ can be replaced by L_θ.

Homogenized formulation of shape optimization ($B \approx 0$)

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

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

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

with in 2-D (more complicated formulas in 3-D)

$$m_{1/2} = \frac{|\sigma_{2/1}|}{|\sigma_1| + |\sigma_2|}, \qquad \theta_{opt} = \min\left(1, \sqrt{\frac{\kappa+\mu}{4\mu\kappa\ell}}\,(|\sigma_1| + |\sigma_2|)\right),$$

where σ is the solution of the homogenized equation.

Numerical algorithm

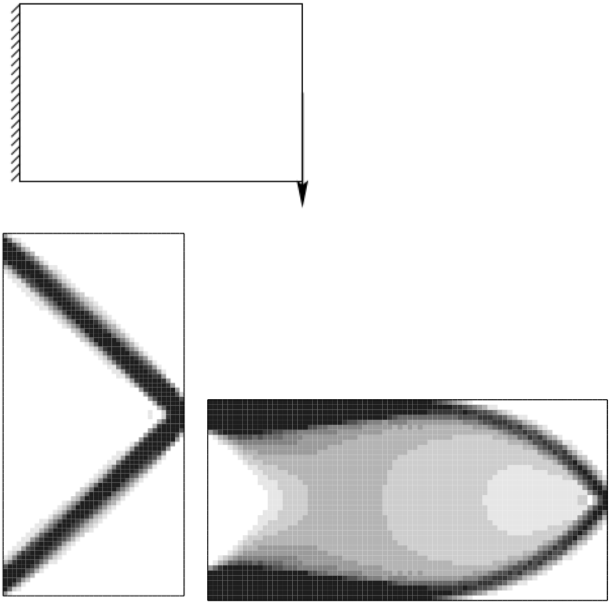
Double "alternating" minimization in σ and in (θ, A^*).

- 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.

- The objective function always decreases.
- Algorithm of the type "optimality criteria".
- Algorithm 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 cantilevers



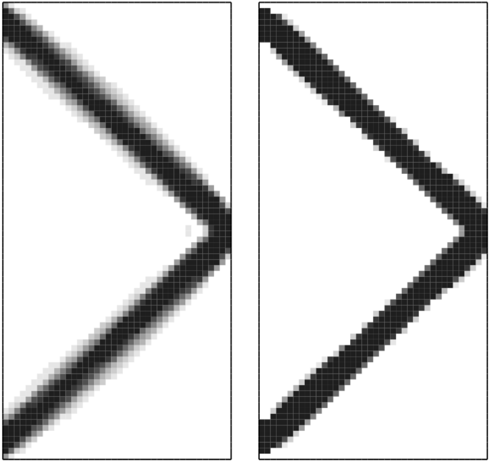
Optimal densities for the short and long cantilevers

Penalization

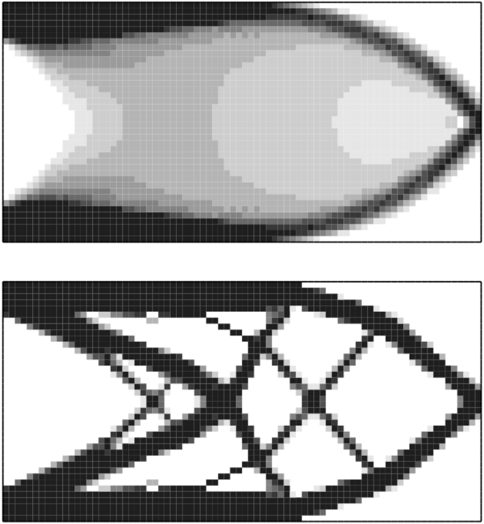
The previous algorithm computes **composite** shapes instead of **classical** shapes.
We thus use a penalization technique to enforce density values close to 0 or 1.
Algorithm: after convergence to a composite shape, we perform a few more iterations with a penalized density

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

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

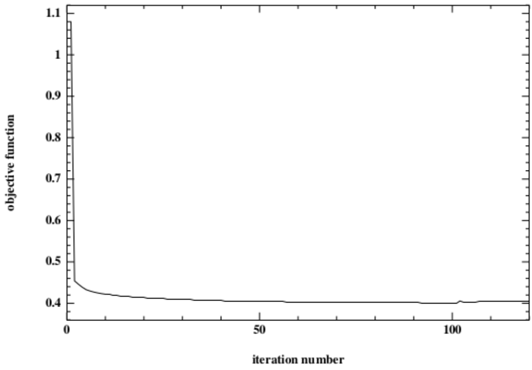


Short cantilever without / with penalty

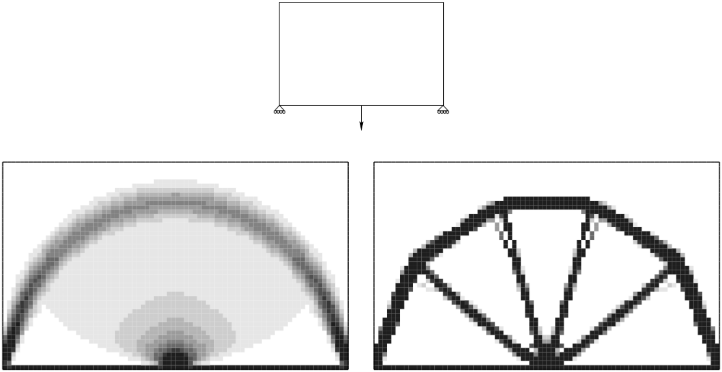


Long cantilever without / with penalty

Convergence history



Another example: wheel bridge



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, then we look for $\theta(x) \in [0, 1]$.

The Hooke law, which was $\chi(x)A$, becomes $\theta(x)A$, or more generally $\varphi(\theta(x))A$ (φ is called interpolation profile). We also call this **fictitious materials** because in general one cannot guarantee that they can be realized by a true homogenization process.

For the self-penalizing profile $\varphi(\theta) = \theta^p$, this method is called **SIMP** (Solid Isotropic Material with Penalization).

Convexified formulation with linear interpolation

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

Consider compliance minimization

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

$$
\text{with} \quad c(\theta) = \int_{\Gamma_N} g \cdot u dx = \int_D (\theta(x) A)^{-1} \sigma \cdot \sigma dx
$$

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

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

Existence of solutions

Theorem. The convexified formulation

$$\min_{0\le\theta(x)\le1}\ \min_{\substack{div\tau=0 \text{ in } D\\ \tau n=g \text{ on } \Gamma_N\\ \tau n=0 \text{ on } \partial D\setminus\Gamma_N\cup\Gamma_D}} \int_D (\theta(x)A)^{-1}\tau\cdot\tau\,dx+\ell\int_D\theta\,dx$$

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

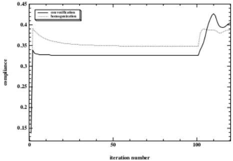
- intialization of the shape θ_0
- iterations $k \geq 1$ until convergence
  - given a shape θ_{k-1}, we compute the stress σ_k by solving an elasticity problem (by a finite element method)
  - given a stress field σ_k, we update the new material density θ_k with the explicit optimality formula in terms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

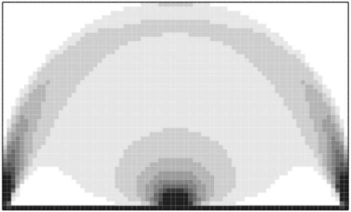
Penalization: we use a penalized density

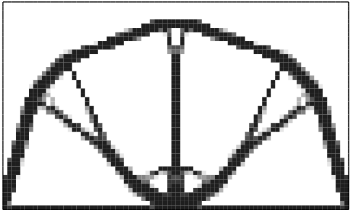
$$\theta_{pen} = \frac{1 - \cos(\pi \theta_{opt})}{2}.$$

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

Optimal bridge by the convexification method







A standard nonlinear interpolation: SIMP

It simply consists in choosing

$$\boxed{\varphi(\theta) = \theta^p, \qquad p > 1}$$

for interpolating the Hooke law. The volume is still defined by $\int_D \theta(x)dx$.

Penalizing effect: $0 < \theta(x) < 1$ yields a poor stiffness.

The typical (mainly empirical) choice is $p = 3$. However it may help convergence to start with the value $p = 1$ and increase it gradually with the iterations.

Even for compliance existence is lost (no more convexity). We can apply a projected gradient method where θ is the single design parameter (it works also in non self-adjoint cases).

Remarks on SIMP

- SIMP is very simple and **very popular** (many commercial softwares are using it).
- SIMP uses very few informations on composites !
- 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.
- It can be delicate to monitor the penalization parameter p.

Perimeter penalization

Add to the cost function c_{pen} times

$$P_\varepsilon(\theta) = \frac{1}{\varepsilon}\int_D (1 - w_\varepsilon)\theta dx$$

with

$$\begin{cases} -\varepsilon^2 \Delta w_\varepsilon + w_\varepsilon = \theta \text{ in } D \\ \frac{\partial w_\varepsilon}{\partial n} = 0 \text{ on } \partial D. \end{cases}$$

When $\varepsilon \to 0$,

$$P_\varepsilon(\theta) \to \begin{cases} \frac{1}{2}|\partial\Omega \cap D| \text{ if } \theta = \chi_\Omega \text{ for some } \Omega \subset D \\ +\infty \text{ if } \theta \text{ is not a characteristic function.} \end{cases}$$

$\rightsquigarrow$ meaningful penalization + existence of optimal shapes at the limit (see chapter 6)

We also have the primal energy formulation (easy to check)

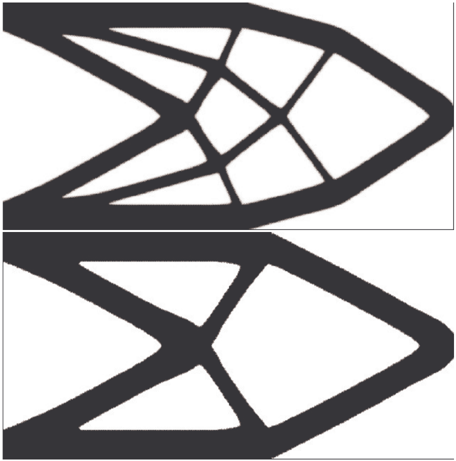
$$P_\varepsilon(\theta) = \inf_{w \in H^1(D)} \int_D \left(\varepsilon |\nabla w|^2 + \frac{1}{\varepsilon}(w^2 + \theta - 2\theta w) \right) dx.$$

Algorithm

- Consider a decreasing sequence $\varepsilon_k \to 0$ (typically ranging from the size of D to the size of the mesh)
- For each ε_k minimize $J(\theta, A^*) + c_{\mathrm{pen}} P_{\varepsilon_k}(\theta)$ (homogenization) or $J(\theta) + c_{\mathrm{pen}} P_{\varepsilon_k}(\theta)$ (convexification), taking as initialization the density obtained with ε_{k-1}.
  Classical methods apply:
  - projected gradient (it requires the computation of an other pair of direct / adjoint states);
  - alternating minimizations for compliance, based on the energy formulation (it requires a third minimization).

For the 2-D homogenized compliance the update of θ becomes

$$\theta_{opt} = \min\left(1, \sqrt{\frac{\kappa+\mu}{4\mu\kappa} \frac{1}{\ell + \frac{c_{\mathrm{pen}}}{\varepsilon}(1-2w_\varepsilon)}}(|\sigma_1| + |\sigma_2|)\right).$$



Cantilever of minimal compliance with perimeter penalization for $c_{\mathrm{pen}} = 0.1$ and $c_{\mathrm{pen}} = 2$. Homogenization method.

Inverse homogenization

Goal: find a microstructure (material distribution within the RVE) that yields target macroscopic properties

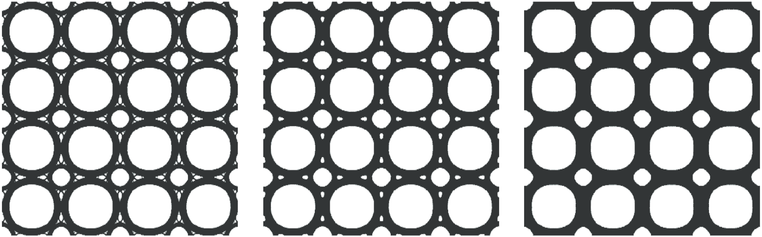
This can be formulated as

$$\min_{A^*} J(A^*) \text{ with } A^* \text{ obtained by homogenization of } A \text{ and } B.$$

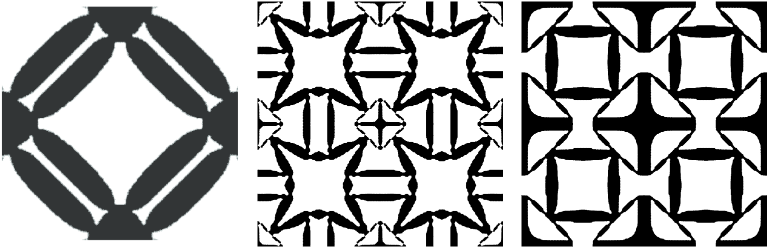
For instance $J(A^*) = \|A^* - A^{\mathrm{target}}\|^2$.

When the obtained A^* enjoys unusual properties one speaks of **metamaterial**.

In the following examples the topology optimization of the RVE is done by a variant of SIMP (level-set method + topological derivative).



Bulk modulus maximization without (left) and with (middle and right) perimeter penalization.



Poisson ratio maximization (left) and minimization without (middle) and with (right) perimeter penalization.
Negative Poisson ration $\equiv$ auxetic (meta)material.