Lecture 10: General results about shape optimization. Homogenization and relaxed designs. The SIMP method.

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Spring 2022 – Seminar for Applied Mathematics

ETH zürich

Outline

1. Counter examples for the non-existence of optimal designs
2. Relaxation of an optimal design problem by homogenization
3. The SIMP method
4. Inverse homogenization

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Proof.

Let $(x_n)_{n\in\mathbb{N}}$ be a minimizing sequence of J, i.e. $J(x_n) \to \inf_{x \in \mathbb{R}^n} J(x)$. Since $(J(x_n))_{n\in\mathbb{N}}$ is bounded, it follows that $(x_n)_{n\in\mathbb{N}}$ must also be bounded. Up to extracting a convergent subsequence, we can assume that $x_n \to x^*$ for some $x^* \in \mathbb{R}^n$. Then $J(x_n) \to J(x^*)$ and so $J(x^*) = \inf_{x \in \mathbb{R}^n} J(x)$. □

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This proof uses crucially that finite dimensional bounded sets are compact.

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with

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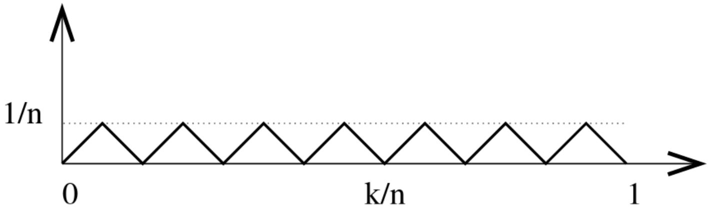

Figure: This sequence (f_n) converges to zero in $L^2(0,1)$ and satisfies $|f_n'| = 1$ for any $n \in \mathbb{N}$. Figure from the lecture of G. Allaire.

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Example: Consider the compliance minimization of the membrane problem

$$\min_{\Omega \subset D} J(\Omega) := \int_{\partial D} (\boldsymbol{e}_1 \cdot \boldsymbol{n}) u \mathrm{d}\sigma \qquad s.t. \quad \begin{cases} -\mathrm{div}(a(\Omega)\nabla u) = 0 \text{ in } D \\ a(\Omega)\nabla u \cdot \boldsymbol{n} = \boldsymbol{e}_1 \cdot \boldsymbol{n} \text{ on } \partial D \\ \dfrac{1}{|D|} \displaystyle\int_\Omega \mathrm{d}x = \theta \end{cases} \tag{1}$$

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Proposition 2

There is no minimizing shape Ω *to the compliance minimization problem eq.* (2). *However, it holds*

$$\inf_{\Omega \subset D} J(\Omega) = (\alpha\theta + (1 - \theta)\beta)^{-1} |D|.$$

Non-existence of optimal designs

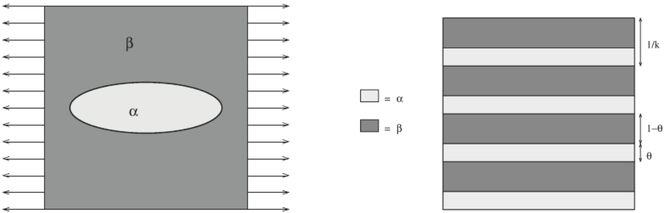

Figure: A minimizing sequence for the problem 1. It is advantageous to distribute the weakest material in horizontal strips to reduce the strain in the $\boldsymbol{e}_2$ direction while being stiff in the $\boldsymbol{e}_1$ direction. Figure from Allaire.

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- the lack of a minimizer comes from the fact that it is often advantageous to refine the shape with more details
- in practice, numerically optimized designs are dependent on the mesh (size, type of elements), and on the initialization.

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- under a perimeter constraint
- under a constraint on the number of holes
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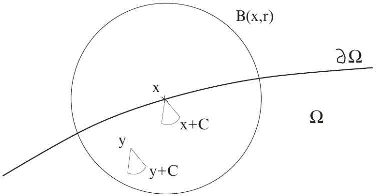

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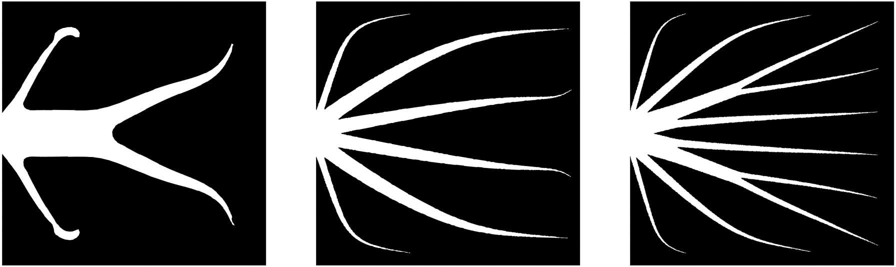

Figure: Optimized designs for the same heat conduction problem with coarse to fine meshes

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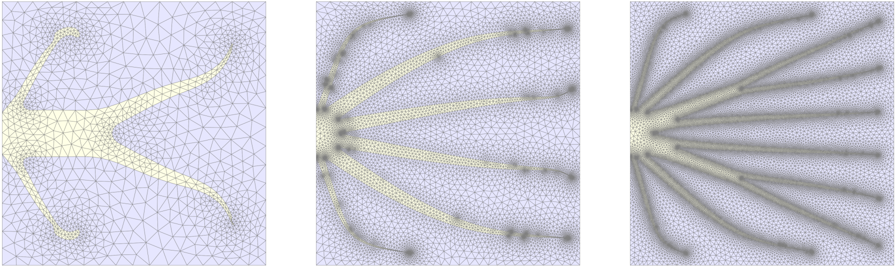

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for $J : E \to \mathbb{R}$ a continuous functional on some Hilbert space satisfying $J(x) \to +\infty$ as $|x| \to +\infty$, and $A \subset E$ the set of admissible candidates.

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Let $\bar{A}$ the weak closure of A. If J is weakly lower semi-continuous, then there exists a minimizer to the relaxed minimization problem

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- Such functions $\rho : D \to (0,1)$ can be interpreted as density functions in the set D: $\rho(x)$ is the local volume fraction of material around the point x.

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A key idea for topology optimization: replace the optimal design problem

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- It turns out that this "weak closure" and the appropriate notion of convergence of shapes depends on the PDE model used, and on the shape functionals.

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Consider the compliance minimization problem for the conductivity equation:

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Proposition 3 (Tartar compactness theorem)

Let $(\Omega_n)_{n\in\mathbb{N}}$ a sequence of domains and (u_n) the associated solutions. There exists a subsequence $(\Omega_{\phi(n)})_{n\in\mathbb{N}}$ and $(u_{\phi(n)})_{n\in\mathbb{N}}$ such that $u_{\phi(n)}$ converges weakly in $H^1(D)$ to the solution u^* of the homogenized *problem*

$$\begin{cases} -\mathrm{div}(a^*(x)\nabla u^*) = 0 \ in\ D \\ a^*(x)\nabla u^*\cdot\boldsymbol{n} = \boldsymbol{e}_1\cdot\boldsymbol{n} \ on\ \partial D. \end{cases}$$

where $a^*(x)\in\mathbb{R}^{d\times d}$ is a positive symmetric effective matrix-valued conductivity.

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where $a^*(x) \in \mathbb{R}^{d\times d}$ is a positive symmetric effective matrix-valued conductivity. Furthermore, the characteristic functions $(1_{\Omega_{\phi(n)}})_{n\in\mathbb{N}}$ converge weakly to some density field $\rho : D \to (0,1)$.

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- Both limits $a^*(x)$ and $\rho(x)$ can be seen as an **effective description** of a limiting microstructure.

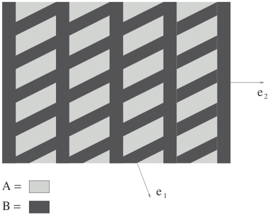

Figure: An anisotropic composite microstructure with two principal directions. Figure from Allaire.

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- *any minimizing sequence of shapes* $(\Omega_n)_{n\in\mathbb{N}}$ *converges in the homogenization sense to some optimal solution* (a^*,ρ) *to eq.* (3)

Relaxation by homogenization

$$\min_{(a^*,\rho)\in G} J^*(a^*,\rho) := \int_{\partial D} (\boldsymbol{e}_1 \cdot \boldsymbol{n}) u \mathrm{d}\sigma \qquad s.t. \quad \begin{cases} -\mathrm{div}(a^* \nabla u) = 0 \text{ in } D \\ a^* \nabla u \cdot \boldsymbol{n} = \boldsymbol{e}_1 \cdot \boldsymbol{n} \text{ on } \partial D \\ \dfrac{1}{|D|} \displaystyle\int_D \rho \mathrm{d}x = \theta \end{cases} \tag{3}$$

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- *any optimal solution to eq.* (3) *is the limit of a minimizing sequence* $(\Omega)_{n\in\mathbb{N}}$.

Relaxation by homogenization

In order to solve numerically the relaxed formulation

$$\min_{(a^*,\rho)\in G} J^*(a^*,\rho) := \int_{\partial D} (\boldsymbol{e}_1 \cdot \boldsymbol{n}) u \, \mathrm{d}\sigma \qquad s.t. \quad \begin{cases} -\mathrm{div}(a^* \nabla u) = 0 \text{ in } D \\ \quad a^* \nabla u \cdot \boldsymbol{n} = \boldsymbol{e}_1 \cdot \boldsymbol{n} \text{ on } \partial D \\ \dfrac{1}{|D|} \displaystyle\int_D \rho \, \mathrm{d}x = \theta \end{cases}$$

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This can be done through periodic homogenization.

Consider a rectangular domain D with periodic boundary conditions filled with periodic inclusions distributed with a period $\epsilon > 0$.

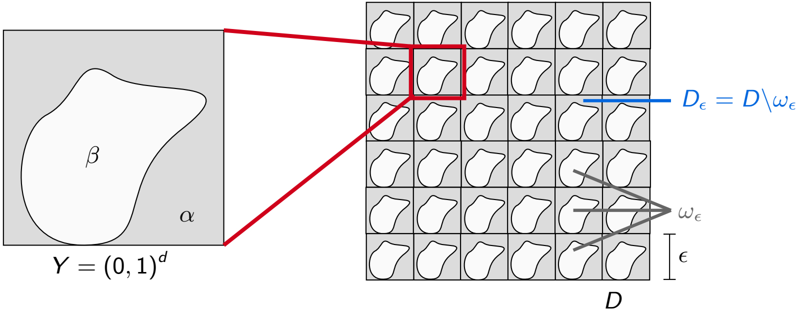

Figure: The composite domain and the unit cell Y filled with two materials α and β.

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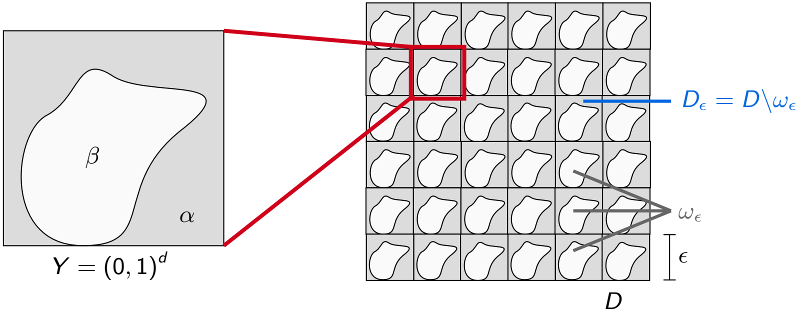

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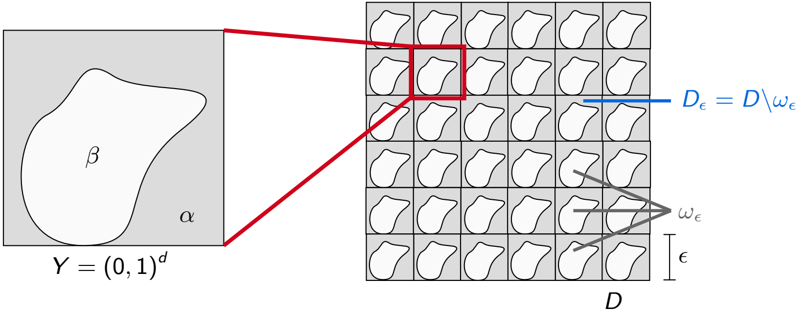

Figure: The composite domain and the unit cell Y filled with two materials α and β.

Let $a : Y \to \{\alpha I, \beta I\}$ the Y–periodic matrix with values αI or βI in the inclusions. Let Ω the phase associated to the material α. Then

$$A(\Omega)(y) = a(y/\epsilon).$$

Relaxation by homogenization

Consider the conductivity problem with periodic boundary conditions.

$$\begin{cases} -\mathrm{div}(a(y/\epsilon)\nabla u_\epsilon) = f \text{ in } D \\ \qquad\qquad u_\epsilon \text{ is } D\text{–periodic} \end{cases} \tag{4}$$

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Proposition 5

Assume that f is a compatible right-hand side (i.e. $\int_D f \mathrm{d}x = 0$). There exists a unique solution u_ϵ satisfying $\int_D u_\epsilon \mathrm{d}x = 0$. Moreover,

$$u_\epsilon \to u^* \textit{ in } H^1(D)$$

where u^* is the unique solution to

$$\begin{cases} -\mathrm{div}(a^* \nabla u^*) = f \textit{ in } D \\ u^* \textit{ is } D\text{–periodic} \\ \int_D u^* \mathrm{d}x = 0, \end{cases}$$

and $1_{\Omega_\epsilon} \rightharpoonup \theta$ in $L^2(D)$.

Proposition 6

The matrix a^* is given by

$$a^*_{ij} = \int_Y a(y)(\boldsymbol{e}_i + \nabla w_i(y)) \cdot (\boldsymbol{e}_j + \nabla w_j(y)) \mathrm{d}y$$

where $(w_i(y))_{1 \leq i \leq d}$ are the solutions to the cell-problem

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Proof.

This can be proved with the method of two-scale expansions: we seek

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

where $u_i(x, y)$ is D–periodic in the x variable and Y periodic in the y variable. We find that u_0 is the limit u^* predicted. □

Relaxation by homogenization

In order to solve numerically the relaxed formulation

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Proposition 7

Let G_θ the set of all matrices a^* that can be obtained by periodic homogenization of the phases α and β in proportion θ and $1-\theta$. Then the set G is the set of all matrix valued fields and densities $(a^*(y),\rho(y))$ such that $a^*(y)\in G_{\rho(y)}$.

It is possible to compute explicitly a^* for particular shapes of inclusions call sequential laminates.

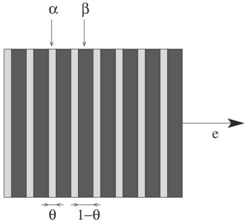

Figure: Figure from Allaire

Proposition 8

Assume that Y is given by two strips orthogonal to the $\boldsymbol{e}$ direction of width θ and $1-\theta$, filled with two materials A and B. Then the associated homogenized tensor A^* is given explicitly by the formula

$$(A^* - B)^{-1} = (A - B)^{-1} + \frac{(1-\theta)}{B\boldsymbol{e}\cdot\boldsymbol{e}}\boldsymbol{e}\otimes\boldsymbol{e}.$$

The procedure can be iterated for several directions of lamination.

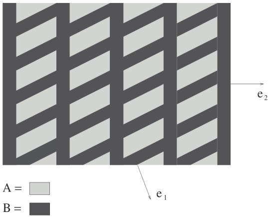

Figure: Figure from Allaire

Proposition 9

Let $\mathbf{e}_1, \ldots, e_p$ *be a set of unit vectors,* $\theta \in (0,1)$ *and* $m_i \in (0,1)$, $1 \leq i \leq p$ *the laminate of rank* p *with lamination parameters* m_i *defined by*

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

The matrix A_p^* *corresponds to a homogenized tensor obtained by sequentially laminating the phase* B *with the phase* A *in proportions* $m_1 \ldots m_p$, *with a total proportion of* A *being* θ.

The optimum value for the relaxed compliance minimization problems is attained by rank–1 laminates.

Proposition 10

There exists (a^*, ρ) *a global minimizer to* J^* *which is a rank one laminate.*

Relaxation by homogenization

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In dimension 2, we can parametrize such laminate by the direction of lamination ϕ and the volume fraction θ:

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

where

$$\lambda_\theta^- = \alpha\theta + (1-\theta)\beta, \qquad \lambda_\theta^- = (\alpha^{-1}\theta + \beta^{-1}(1-\theta))^{-1}$$

Relaxation by homogenization

It becomes then possible to rephrase the optimization problem as

$$\min_{(\rho,\phi)\in L^\infty(D,(0,1)\times\mathbb{R})} J^*(\rho,\phi) := \int_{\partial D} (\boldsymbol{e}_1 \cdot \boldsymbol{n}) u \mathrm{d}\sigma$$

$$s.t. \quad \begin{cases} -\mathrm{div}(A^*(\rho(y),\phi(y))\nabla u) = 0 \text{ in } D \\ A^*(\rho(y),\phi(y))\nabla u \cdot \boldsymbol{n} = \boldsymbol{e}_1 \cdot \boldsymbol{n} \text{ on } \partial D \\ \dfrac{1}{|D|}\displaystyle\int_D \rho \mathrm{d}x = \theta \end{cases}$$

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This is a **parametric** optimization problem with respect to ρ and ϕ. It can be solved with gradient methods as in shape optimization on a fixed mesh.

Relaxation by homogenization

Using standard derivation, one finds indeed that

$$\frac{\partial J}{\partial(\rho,\phi)} = \int_{\partial D} \boldsymbol{e}_1 \cdot \boldsymbol{n} \frac{\partial \boldsymbol{u}}{\partial(\rho,\phi)} \mathrm{d}\sigma = \int_D A^*(\rho,\phi) \nabla \frac{\partial \boldsymbol{u}}{\partial(\rho,\sigma)} \cdot \nabla \boldsymbol{u} \mathrm{d}x$$
$$= -\int_D \frac{\partial A^*}{\partial(\rho,\phi)} \nabla \boldsymbol{u} \cdot \nabla \boldsymbol{u} \mathrm{d}x.$$

Relaxation by homogenization

Remark 1

- One needs to take into account **point-wise bound constraints**

$$0 \leq \rho(y) \leq 1 \text{ for all } y \in D,$$

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- For the linear elasticity system, the optimum value is achieved by rank d sequential laminates, requiring some adaptations.
- In order to obtain a true shape, one can try to **penalize** intermediate densities with

$$\rho_{n+1} \leftarrow \frac{1 - \cos(\pi \rho_{n+1})}{2}$$

which "forces" values of ρ_{n+1} to become closer to the values 0 or 1.

Figure: Iteration 0 (Reprint from Allaire)

Relaxation by homogenization

Figure: Iteration 1 (Reprint from Allaire)

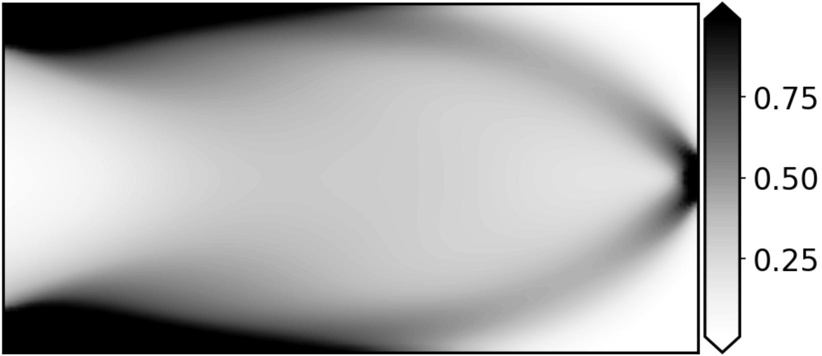

Figure: Iteration 10 (Reprint from Allaire)

Relaxation by homogenization

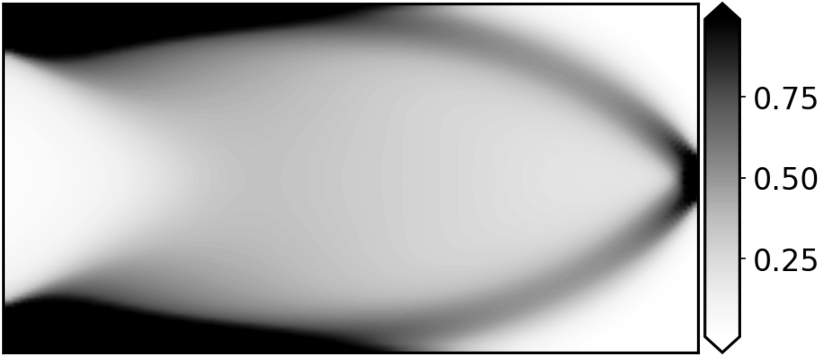

Figure: Iteration 20 (Reprint from Allaire)

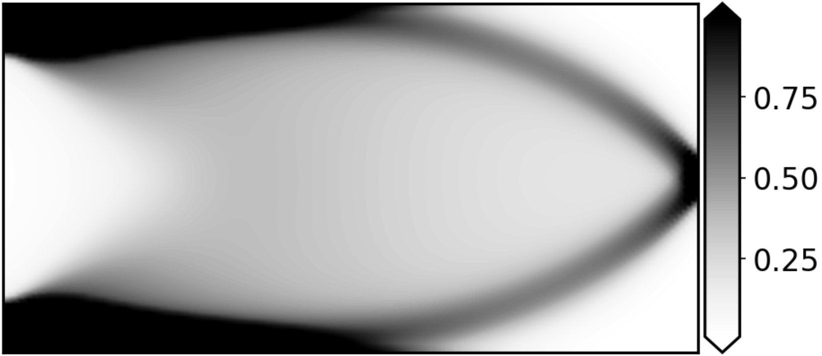

Figure: Iteration 40 (Reprint from Allaire)

Figure: Iteration 45 (Reprint from Allaire)

Relaxation by homogenization

Figure: Iteration 55 (Reprint from Allaire)

Relaxation by homogenization

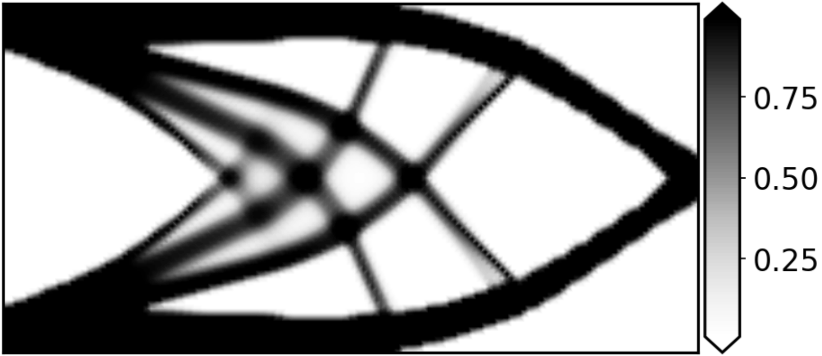

Figure: Iteration 60 (Reprint from Allaire)

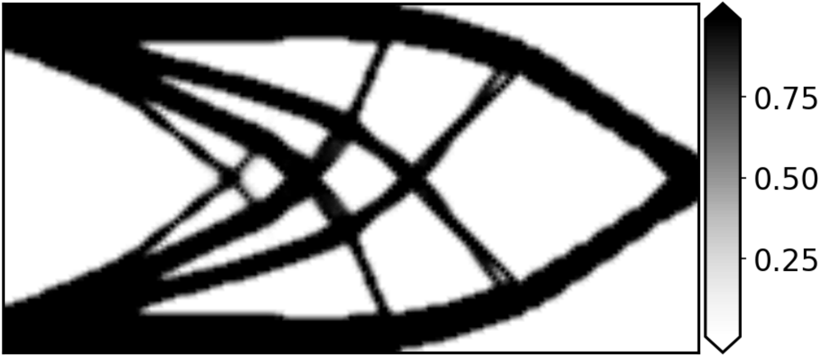

Figure: Iteration 60 (Reprint from Allaire)

Outline

1. Counter examples for the non-existence of optimal designs
2. Relaxation of an optimal design problem by homogenization
3. The SIMP method
4. Inverse homogenization

The SIMP method

- SIMP: Solid Isotropic Material Penalization
- Simplification of homogenization method: interpolate the stress tensor with the density:

$$\min_{\Omega \subset D} J(\Omega) := \int_{\partial D} (\boldsymbol{e}_1 \cdot \boldsymbol{n}) u \mathrm{d}\sigma \qquad s.t. \quad \begin{cases} -\mathrm{div}(a(\Omega)\nabla u) = 0 \text{ in } D \\ a(\Omega)\nabla u \cdot \boldsymbol{n} = \boldsymbol{e}_1 \cdot \boldsymbol{n} \text{ on } \partial D \\ \dfrac{1}{|D|} \displaystyle\int_\Omega \mathrm{d}x = \theta \end{cases}$$

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- It is not guaranteed that $(a(\rho), \rho) \in G$. The method uses **fictitious materials** and optimized densities might not be interpretable.
- However, we can select $(a(\rho), \rho) \in G$ by taking $p = 3$ (for the conductivity), or to make them satisfy suitable bounds.

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However, it is popular because simple to implement, works on fixed meshes, and yields good results.

The SIMP method

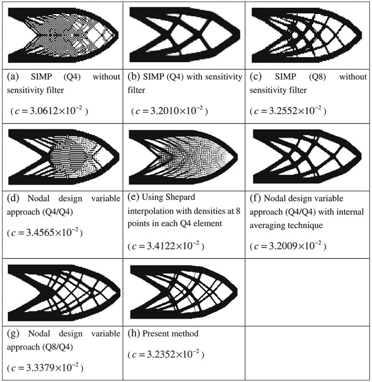

Figure: Filters for the SIMP method. Figure from Kang (2011)

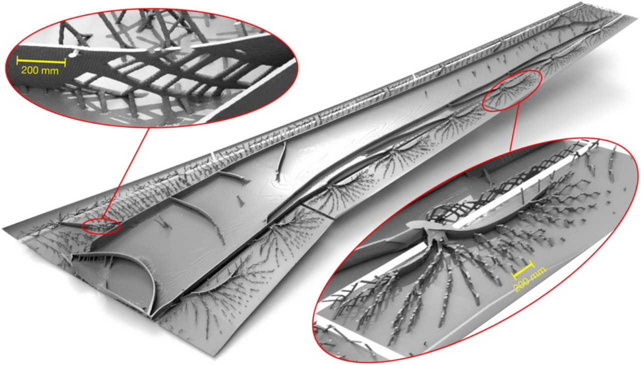

Figure: Large scale computations in structural design with the SIMP method. Figure from Aage et. al. (2017)

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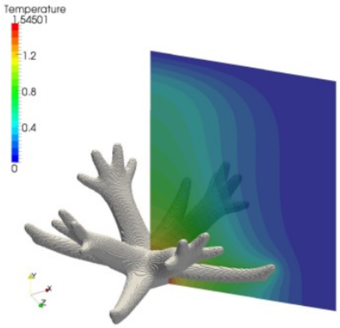

(b) $Gr = 10^4$

Figure: Large scale computations in convective cooling design with a density method. Figure from Alexandersen et. al. (2016)

Outline

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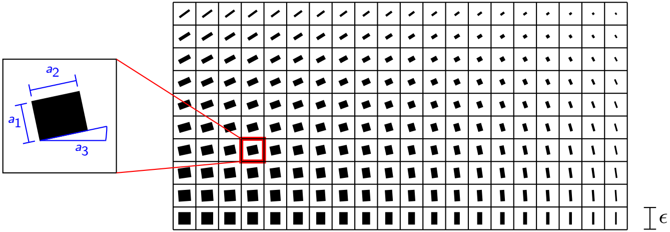
Inverse homogenization

A recent trend (Geoffroy Donders (2019), and Groen (2019)): inverse homogenization.

Parametrize the microstructure of the composite material Ω:



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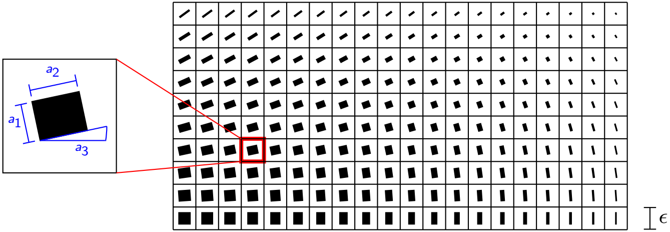

$$\min_{(a_1,\ldots,a_m)\in L^\infty(D,\mathbb{R}^d)} \quad J^*(a_1,\ldots,a_m,\boldsymbol{u}(a_1,\ldots,a_m))$$

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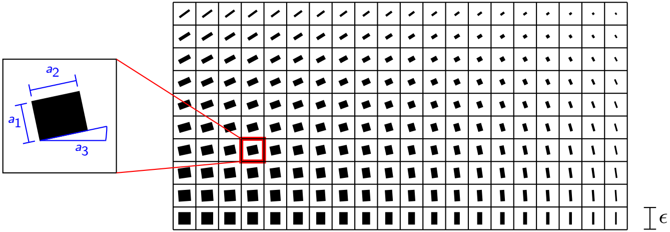

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$A^*(a_1,\ldots,a_m)$ is the effective material tensor.

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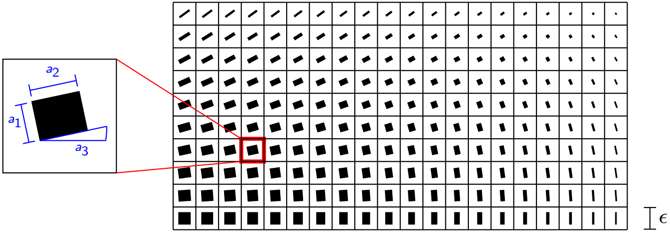

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$A^*(a_1,\ldots,a_m)$ is the effective material tensor. Optimize then $a_1(x),\ldots a_m(x)$ instead of Ω!

Inverse homogenization

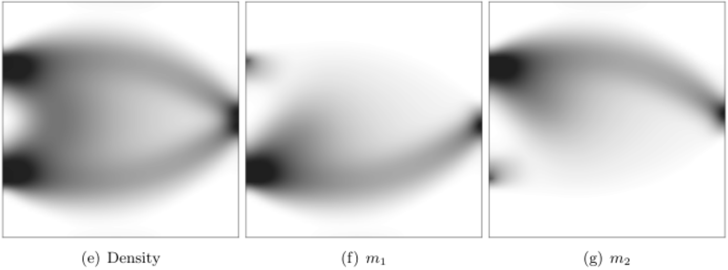
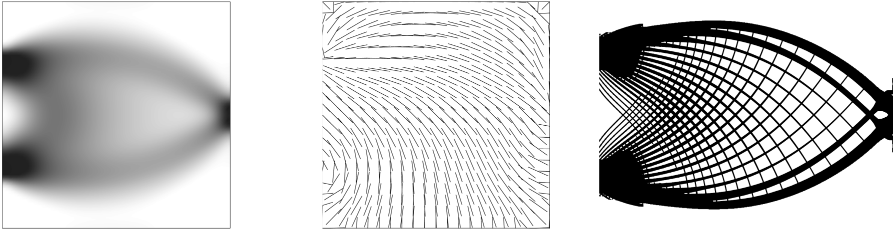


Figure: Optimized microstructure parameters. Figure from Donders (2019).

Inverse homogenization



(a) Optimized density

(b) Optimized orientation

(c) Interpreted shape

Figure: Topology optimization of a 2-d cantilever beam by a homogenization method. Figure from Donders (2019).

Inverse homogenization

The procedure involves the computation of a diffeomorphism projecting a cartesian grid according to the orientation:

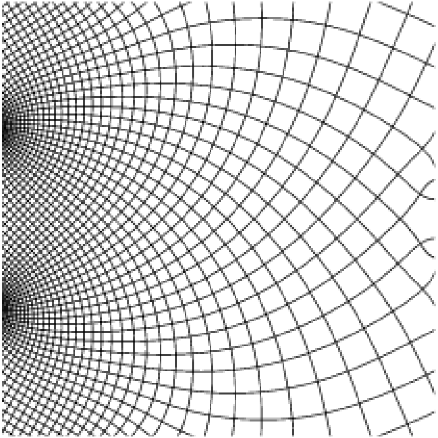
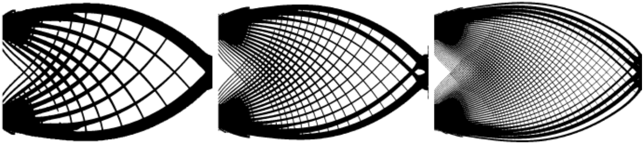


Figure: Reconstructed grid. Figure from Donders (2019).

From the knowledge of the parameters, it is easy to reconstruct a **minimizing sequence of shapes**



(k) $\tilde{\Omega}_\varepsilon(\varphi, \tilde{m})$, $\varepsilon = 0.2$ (l) $\tilde{\Omega}_\varepsilon(\varphi, \tilde{m})$, $\varepsilon = 0.1$ (m) $\tilde{\Omega}_\varepsilon(\varphi, \tilde{m})$, $\varepsilon = 0.05$

Figure: Reconstructed shapes. Figure from Donders (2019).

Also works in 3D:

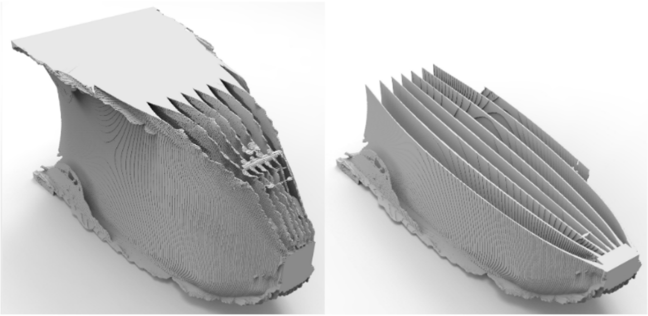


Figure: Reconstructed shapes. Figure from Groen (2019).

Inverse homogenization

- Right now, rather restricted to structural design for compliance minimization
- However, lots of potentialities offered in the future for other physics.