A brief review of structural optimization: homogenization versus level set methods

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CMAP, Ecole Polytechnique

From Computational Fabrication to Material Design
GDR MePhy, June 22, 2021

Outline

- I - Introduction and geometric optimization
- II - Topology optimization: the homogenization method
- III - Topology optimization: the level set method
- IV - **New:** topology optimization of lattices

Shape optimization : minimize an objective function over a set of admissibles shapes Ω (including possible constraints)

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

The objective function is evaluated through the solution of a state equation

$$J(\Omega) = \int_\Omega j(u_\Omega)\, dx$$

where u_Ω is the solution of a partial differential equation

$$PDE(u_\Omega) = 0 \quad \text{in} \quad \Omega$$

The model of linear elasticity

A shape is a smoothdomain $\Omega \subset \mathbb{R}^d$ with boundary $\partial\Omega = \Gamma \cup \Gamma_N \cup \Gamma_D$.

For a given applied load $g : \Gamma_N \to \mathbb{R}^d$, the displacement $u : \Omega \to \mathbb{R}^d$ is the solution of

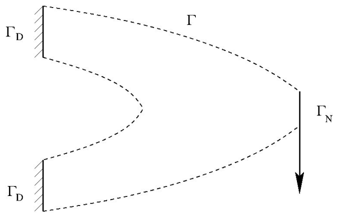
$$\begin{cases} -\operatorname{div}(A\, e(u)) = 0 & \text{in } \Omega \\ u = 0 & \text{on } \Gamma_D \\ \big(A\, e(u)\big)n = g & \text{on } \Gamma_N \\ \big(A\, e(u)\big)n = 0 & \text{on } \Gamma \end{cases}$$

with the strain tensor $e(u) = \frac{1}{2}(\nabla u + \nabla^t u)$, the stress tensor $\sigma = Ae(u)$, and $A = 2\mu I_4 + \lambda I_2 \otimes I_2$ an homogeneous isotropic elasticity tensor with $\lambda, \mu > 0$.

Typical objective function: the compliance

$$J(\Omega) = \int_{\Gamma_N} g \cdot u \, dx,$$

Admissible shapes



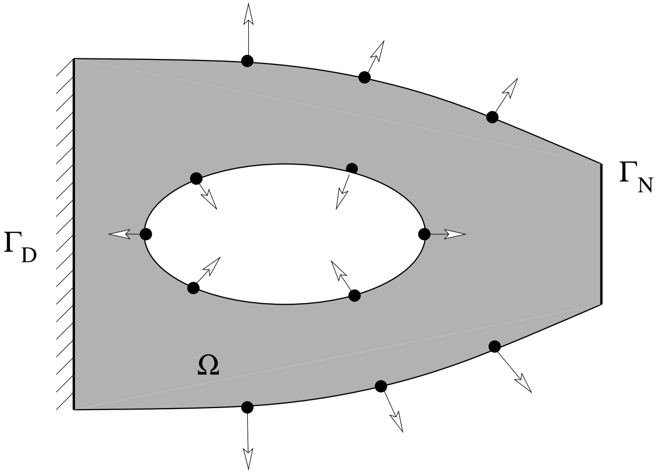
The **shape optimization** problem is $\inf_{\Omega \in \mathcal{U}_{ad}} J(\Omega)$, where the set of admissible shapes is typically

$$\mathcal{U}_{ad} = \left\{ \Omega \subset D \text{ open set such that } \Gamma_D \bigcup \Gamma_N \subset \partial\Omega \text{ and } \int_\Omega dx = V_0 \right\},$$

where $D \subset \mathbb{R}^d$ is given and V_0 is a prescribed volume.

Remark. The boundary subsets Γ_D and Γ_N are fixed. Only Γ is optimized (free boundary).

Classical geometrical optimization

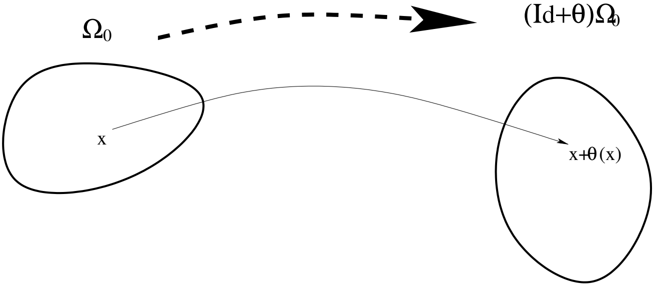


The boundary is parametrized by control nodes which are moved in the direction of the shape gradient (steepest descent algorithm).

Shape gradient: Hadamard method

Let Ω_0 be a reference domain. Consider its variations

$$\Omega = \big(\mathrm{Id} + \theta\big)\Omega_0 \quad \text{with} \quad \theta \in C^1(\mathbb{R}^d;\mathbb{R}^d).$$

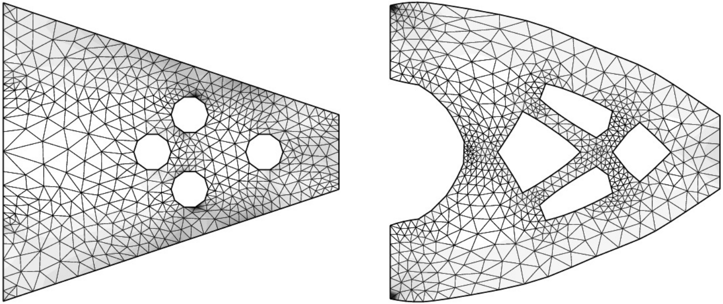


Definition: the shape derivative of $J(\Omega)$ at Ω_0 is the differential of $\theta \to J\big((\mathrm{Id} + \theta)\Omega_0\big)$ at 0.

Huge literature on how to compute shape gradients !

Classical geometrical optimization

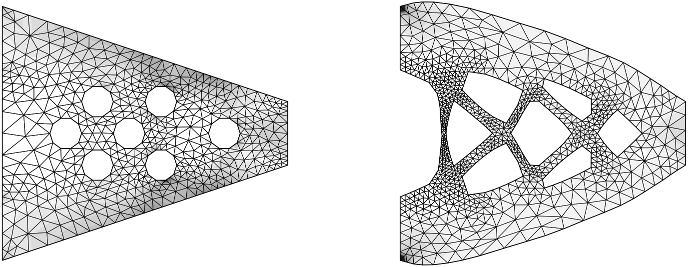
Numerical example for the cantilever:
initial shape (left), “optimal” shape (right)



- Convergence in 20 iterations.
- Global or local minimum ?
- No topology changes.

Classical geometrical optimization

Numerical example for the cantilever:
initial shape (left), “optimal” shape (right)



- No convergence ! Rather, problem with a thin bar...
- One more local minimum !

Topology optimization

- It is crucial to optimize, not only the geometry, but also the topology of shapes.
- In 2-d topology is the number of holes. A bit more complicated in 3-d...
- There are different approaches for topology optimization.
- We describe the two most popular ones:
  1. the homogenization method (and its simplified version, SIMP),
  2. the level set method.

II - Topology optimization: homogenization method

Fact: many small holes are better than just a few large holes. When they are so many tiny holes, the structure looks like a porous material.

Key idea: porous material, or **composite material**, are more optimal than classical shapes.

- Pionneer works in the 80's: Murat-Tartar, Lurie-Cherkaev, Kohn-Strang.
- First application to structural mechanics: Bendsoe-Kikuchi (1988).
- Reference books: Allaire (2001), Bendsoe-Sigmund (2003), Cherkaev (2000), Tartar (2000).

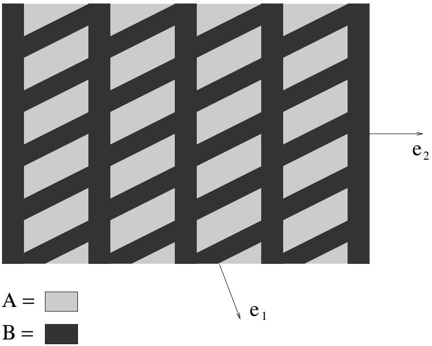
Homogenization method

Main idea: introduce generalized admissible shapes which are **composite materials**.

- At each point there is an underlying porous microstructure.
- **New design parameters**: density $0 \leq \theta \leq 1$, and homogenized Hooke' law A^* (depending on the microstructure).
- Generalized or "composite" shapes include "classical" shapes ($\theta = 0$ or 1).
- Topology changes will be allowed.

Composite materials

- Defined rigorously by homogenization as the "limits" of phase mixtures.
- Large body of work on the optimization of their properties.
- A class of (multi-scale) composites with explicit formulas: sequential laminates.
- Optimal composites can be found in this class.



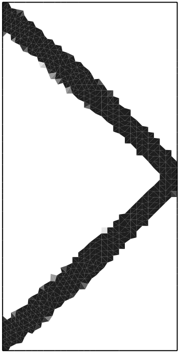
Algorithm for compliance minimization

First step: compute an optimal homogenized or composite design.

1. Designe variables: density θ, microstructure A^*.
2. Optimal composite: rank-d sequential laminate in dimension d, with directions aligned with the stress.

Second step: penalization to recover true shapes. After convergence of the first step; the material density θ is progressively forced to 0 or 1.

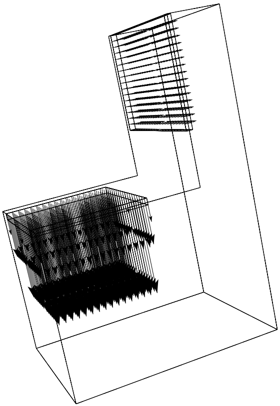
Short cantilever



Long cantilever

Long cantilever with a "politically correct" initialization

3-d chair



SIMP (Solid Isotropic Material with Penalization)

Idea. Homogenization introduces composites which are discarded at the end by penalization. Can we simplify the approach by introducing merely a density θ ?

- **Bendsoe:** replace the composite homogenized tensor A^* by $\theta^p A$ for some exponent $p > 1$ (for $p = 1$ this is convexification).
- It works very well in practice (the difficult part is the penalization: use some kind of continuation).
- Almost all softwares are base on SIMP.
- The homogenization method was "killed" by SIMP !
- One big default: no anisotropy (see later)...

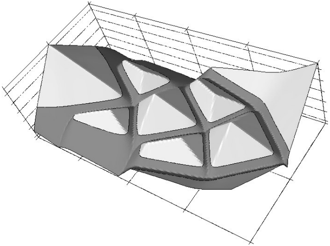
Homogenization is killed by SIMP !

A miracle: resurrection of homogenization !

And suddenly... a miracle happens, leading to the resurrection of the homogenization method !

The miracle is additive manufucturing (3-d printing) and its possibility of building composite materials, or more precisely achitectured materials, called lattice materials.

The concept of level set front propagation was introduced by Osher and Sethian.



A shape $\Omega \subset D$ is parametrized by a **level set** function

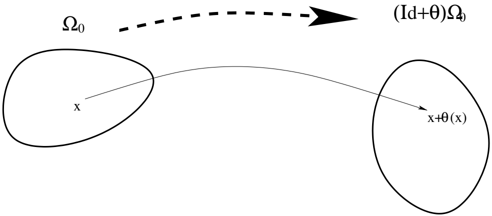
$$\psi(x) < 0 \Leftrightarrow x \in \Omega, \;\; \psi(x) > 0 \Leftrightarrow x \in (D \setminus \Omega)$$

Assume that the shape $\Omega(t)$ evolves in time t with a normal velocity $V(t,x)$. Then its motion is governed by the following Hamilton Jacobi equation

$$\frac{\partial \psi}{\partial t} + V |\nabla_x \psi| = 0 \quad \text{in } D.$$

Advection velocity = shape gradient

The velocity V is deduced from the shape gradient of the objective function.



Hadamard structure theorem: the shape derivative of $J(\Omega)$ can always be written

$$J'(\Omega_0)(\theta) = \int_{\partial\Omega_0} \theta(x) \cdot n(x)\, j(x)\, ds$$

The normal velocity $V = \theta \cdot n$ is chosen so that $J'(\Omega_0)(\theta) \leq 0$.
Simplest choice: $V = \theta \cdot n = -j$ (but other ones are possible).

Numerical algorithm

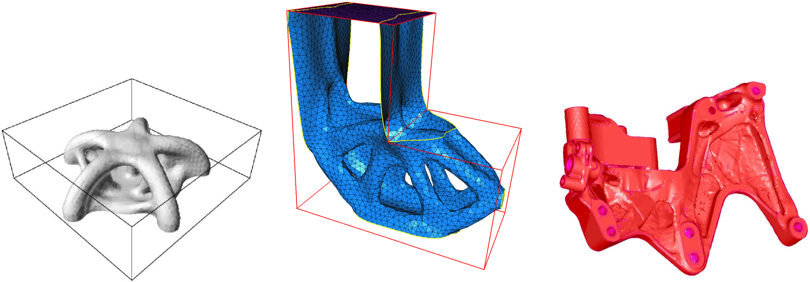
1. Initialization of the level set function ψ_0 (including holes).
2. Iteration until convergence for $k \geq 1$:
    1. Compute the elastic displacement u_k for the shape ψ_k. Deduce the shape gradient = normal velocity = V_k
    2. Advect the shape with V_k (solving the Hamilton Jacobi equation) to obtain a new shape ψ_{k+1}.

Optimization algorithms:

1. Lagrangian (possibly augmented) algorithm,
2. SLP (sequential linear programming).

Complex optimal topologies

Compliance minimization with a weight constraint



dome L-beam motor-support

Comparison between homogenization and level set methods

Homogenization (or SIMP) method:

1. almost insensitive to the initialization,
2. the penalization step may be tricky.

Level set method:

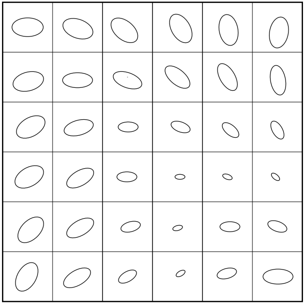
1. many local minima, depending on the initialization,
2. no penalization is required because the boundary is well captured.

IV - New: topology optimization of lattice materials

Lattice materials are periodic structures, with macroscopically varying parameters of the type

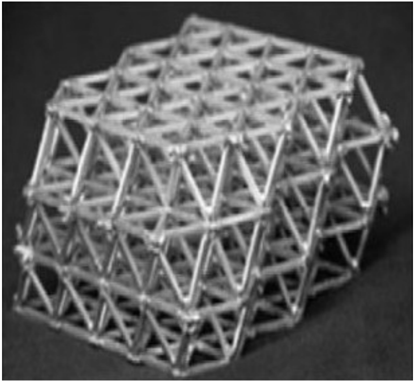
$$A\left(x, \frac{x}{\epsilon}\right)$$

where $y \to A(x, y)$ is periodic and $x \to A(x, y)$describes the macroscopic variations. Homogenization theory applies to this type of oscillating coefficients in pde's.



Lattice materials

Materials with graded (varying) microstructure can be built by additive manufacturing techniques.



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G. Allaire, P. Geoffroy-Donders, O. Pantz, *Topology optimization of modulated and oriented periodic microstructures by the homogenization method,* Computers & Mathematics with Applications, 78, 2197-2229 (2019).

P. Geoffroy-Donders, G. Allaire, O. Pantz, *3-d topology optimization of modulated and oriented periodic microstructures by the homogenization method,* to appear in J. Comp. Phys.

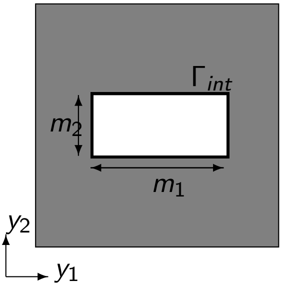
See also:

J. P. Groen and O. Sigmund, *Homogenization based topology optimization for high resolution manufacturable microstructures,* International Journal for Numerical Methods in Engineering, 113(8):1148-1163, 2018.

Pionneering paper:

O. Pantz and K. Trabelsi, *A post-treatment of the homogenization method for shape optimization,* SIAM J. Control Optim., 47(3):1380–1398, 2008.

Example: rectangular hole in a square cell (Bendsoe-Kikuchi)



Cell parameters: m_1, m_2 and angle α (applied to the cell).
Homogenized properties: $A^*(m_1, m_2, \alpha)$.
Good choice because it is close to the optimal rank-2 laminate.

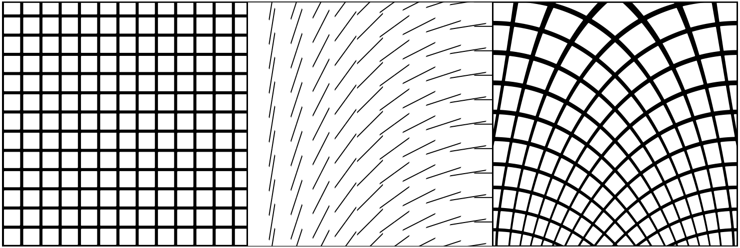
Remark: the same ideas apply to other geometries.

A three-step approach for optimization

1. Pre-compute (off-line). the homogenized properties $A^*(m_1, m_2, \alpha)$ for all values of the parameters.
2. Apply a simple parametric optimization process to the homogenized problem with design variables m_1, m_2, α, varying in space.
3. Choose a lengthscale ϵ and reconstruct a periodic domain $A\left(x, \frac{x}{\epsilon}\right)$ approximating the optimal A^*.
   (This is the delicate step of the approach !)

Orientation/reconstruction issue

The most delicate point is the combined problem of orientation of the microstructure and reconstruction of a macroscopically varying periodic lattice: the entire cell is rotated by an angle α.
It implies that the periodic grid must be deformed accordingly.

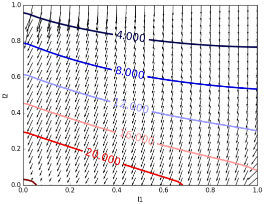


Regular grid (left), orientation field (middle), distorted grid (right).

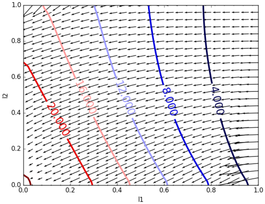
1st step: pre-computing the homogenized properties

Compute the homogenized properties $A^*(m_1, m_2)$ for a discrete sampling of $0 \leq m_1, m_2 \leq 1$ (with fixed 0 orientation).

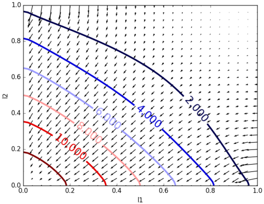
Rotate the cell by an angle α (in $2-d$). Analytic computation.



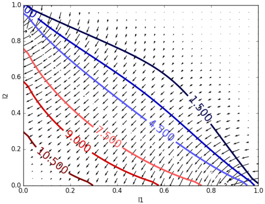
$(A_0^*(m))_{1111}$



$(A_0^*(m))_{2222}$



$(A_0^*(m))_{1122}$



$(A_0^*(m))_{1212}$

Isolines of the entries of the homogenized tensor A^* and their gradient (small arrows) depending on m_1 (x-axis) and m_2 (y-axis).

2nd step: parametric optimization of the homogenized problem

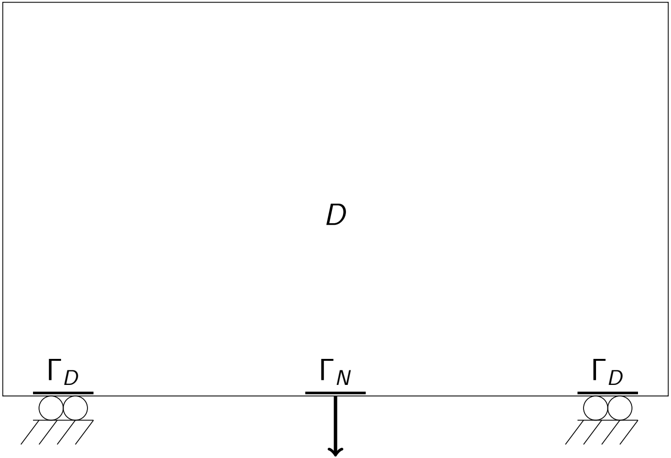
The homogenized equation in a box D (containing the lattice shape) is

$$\begin{cases} \operatorname{div} \sigma = 0 & \text{in } D, \\ \sigma = A^* e(u) & \text{in } D, \\ u = 0 & \text{on } \Gamma_D, \\ \sigma \cdot n = g & \text{on } \Gamma_N, \\ \sigma \cdot n = 0 & \text{on } \Gamma = \partial D \setminus (\Gamma_D \cup \Gamma_N). \end{cases}$$

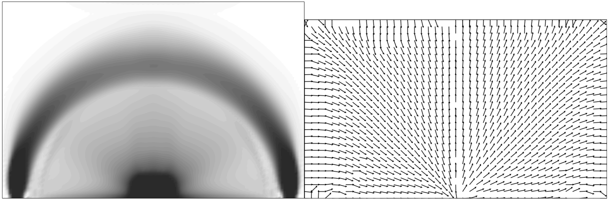
We consider compliance minimization

$$\min_{m_1, m_2, \alpha} J(A^*) = \int_{\Gamma_N} g \cdot u \, ds \, .$$

Bridge test case

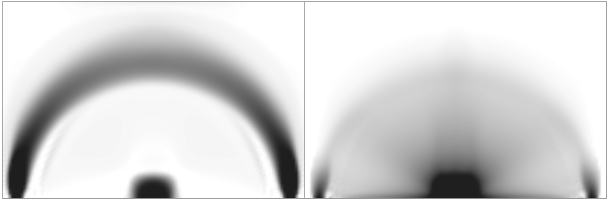


Results for the bridge



Density

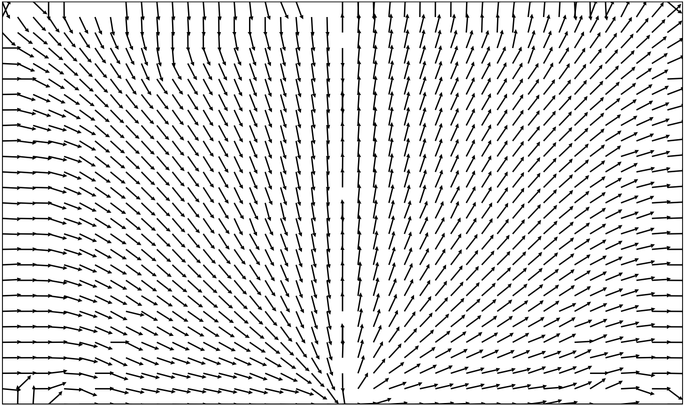
Cell orientation



m_1

m_2

Regularity issues for the optimal orientation



Remember: α or $\alpha + \pi$ are the same orientation. Singularities appear near the corners and at the bottom middle...

3rd step: reconstruction of an optimal periodic structure

- We computed an optimal homogenized design (with an underlying modulated periodic structure).
- Let us project it to obtain a lattice material !
- **This is a post-processing step.**
- We have to choose a lengthscale ε for this projection step.

Projection with orientation α

Main idea (Pantz and Trabelsi): find a map $\varphi = (\varphi_1, \varphi_2)$ from D into $\mathbb{R}^2$ which distorts a regular square grid in order to orientate each square at the optimal angle α.
Geometrically (in 2-d), the gradient matrix $\nabla\varphi$ should be proportional to the rotation matrix defined by

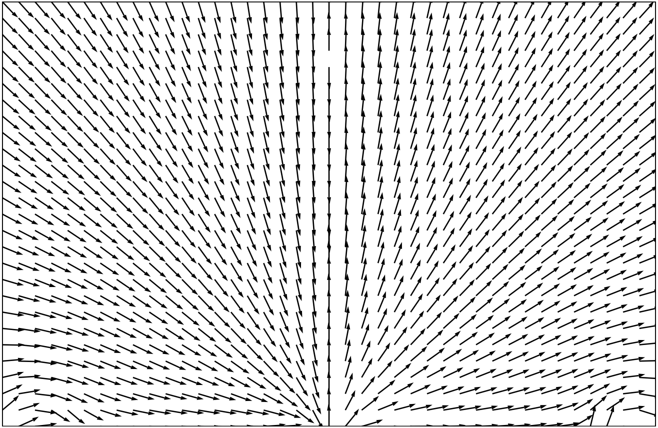
$$Q(\alpha) = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix}.$$

In other words, there should be a (scalar) dilation field r such that

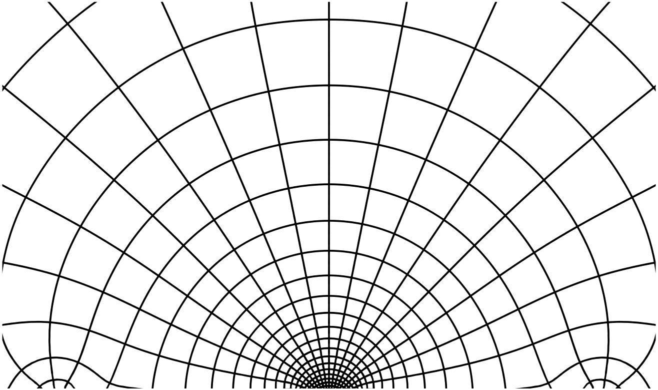
$$\nabla\varphi = e^r Q(\alpha) \quad \text{in } D.$$

This equation can be satisfied only if α is smooth and satisfies a conformality condition $\Delta\alpha = 0$.
This requires a regularization process for the angle α.

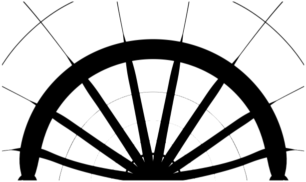
Regularized orientation α for the bridge case



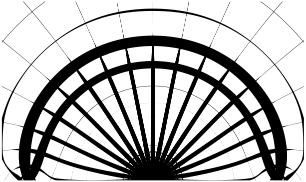
Projection of a regular grid through the map φ for the bridge case



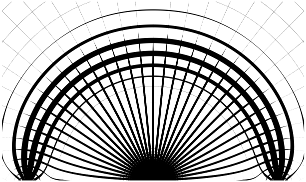
Reconstruction for several ε in the case of the bridge



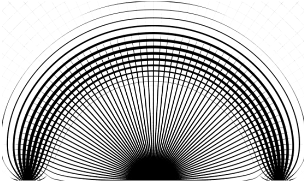
$\varepsilon = 0.4$



$\varepsilon = 0.2$



$\varepsilon = 0.1$



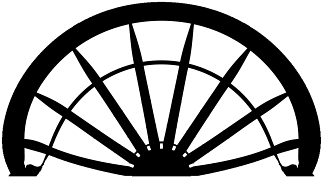
$\varepsilon = 0.05$

A final post-processing/cleaning of the lattice reconstruction

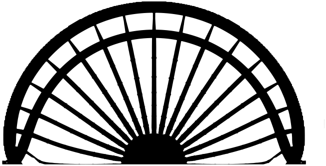
- There are disconnected components of the lattice structure to be removed.
- There are too thin members.

A final post-processing is made to cure these defects.

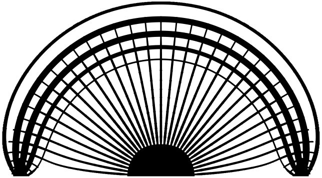
Post-processed structures for several ε



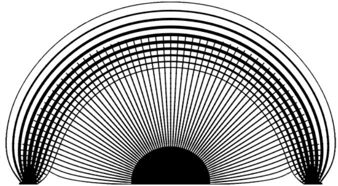
$\varepsilon = 0.4$



$\varepsilon = 0.2$

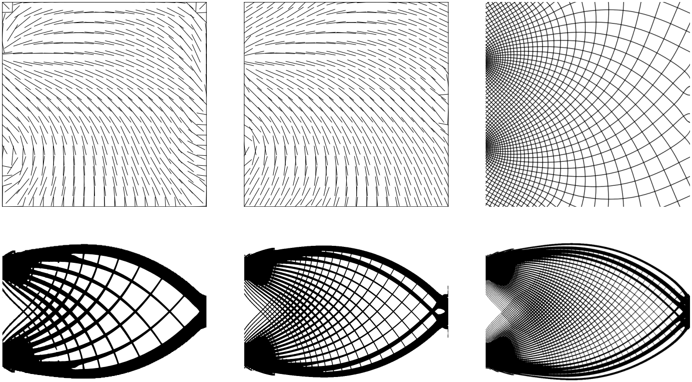


$\varepsilon = 0.1$

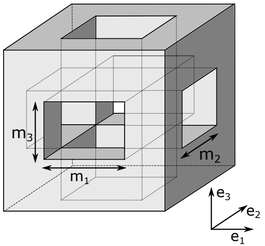


$\varepsilon = 0.05$

Cantilever case



3-d generalization

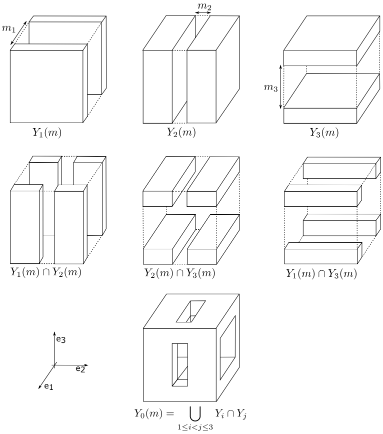


- Cell orientation by a direct rotation matrix $(\omega_1, \omega_2, \omega_3)$.
- No more conformality property (Liouville theorem).
- The map φ is computed direction by direction with 3 dilation fields:

$$\forall i \in \{1,2,3\} \quad \nabla \varphi_i = e^{r_i} \omega_i$$

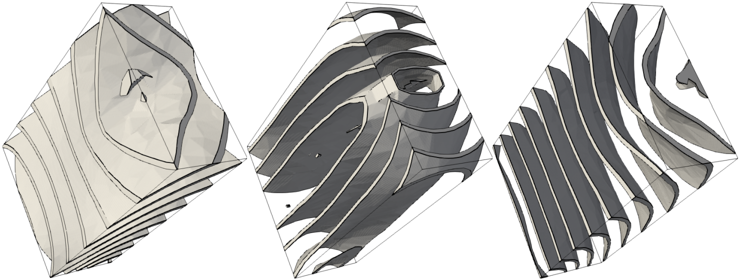
Cubes are transformed in rectangles...

3-d projection: construction of the cell from $Y_i(m_i)$

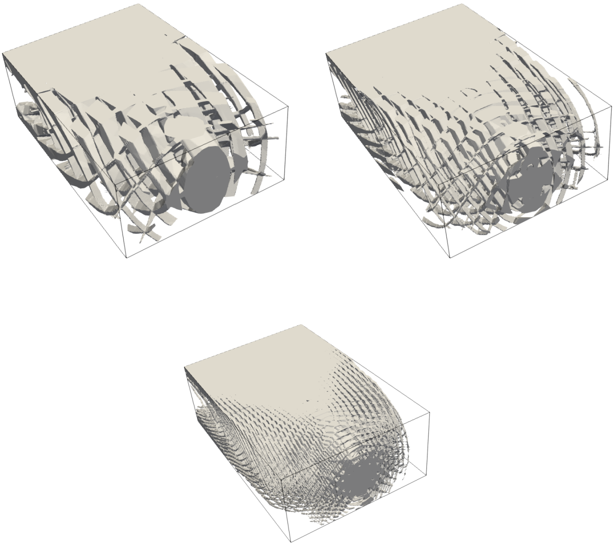


$$Y_0(m) = \cup_{1 \le i < j \le 3} \left(Y_i(m) \cap Y_j(m) \right)$$

3-d cantilever $Y_i(m_i)$



3-d cantilever



3-d bridge and mast