Shape and topology optimization of structures built by additive manufacturing

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Outline of the course

- 1 - Introduction: a review of additive manufacturing
- 2 - Parametric optimization and the adjoint method
- 3 - Geometric optimization and Hadamard method
- 4 - Topology optimization and the level set method
- 5 - Typical constraints from additive manufacturing
- 6 - Optimization of lattice materials
- 7 - Coupled shape and laser path optimization

A "hot" topic with a lot of room for new ideas and modeling...

Outline of the sixth chapter

Chapter 6 - Optimization of lattice materials

- I - Introduction
- II - Modelling of lattice structures
- III - Proposed optimization method
- IV - 3-d generalization

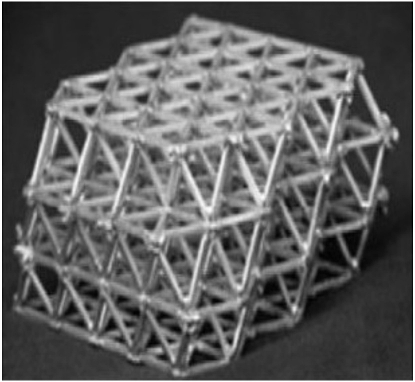
SOFIA

Sofia project: Add-Up, Michelin, Safran, ESI, etc. (2016-2022)

3-d printing enables structures made of composite materials or microscopically architectured (called lattice materials).

Example of lattice materials

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



- The homogenization method was the first (historically) method of topology optimization.
- However, it was complicated because it requires the knowledge of homogenized properties of composite materials.
- **Bendsoe** suggested a simpler method: SIMP (solid isotropic material with penalization). 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 based on SIMP.
- The homogenization method was "killed" by SIMP !
- One big default: no anisotropy (see later)...

Homogenization was killed by SIMP !

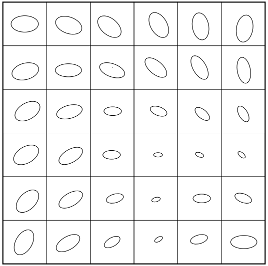
A miracle: resurrection of homogenization !

II - Modelling of lattice structures

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

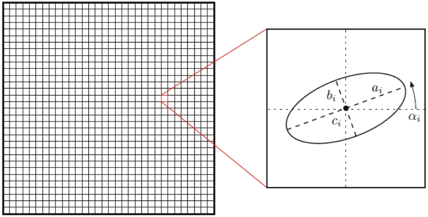
$$A\left(x, \frac{x}{\epsilon}\right)$$

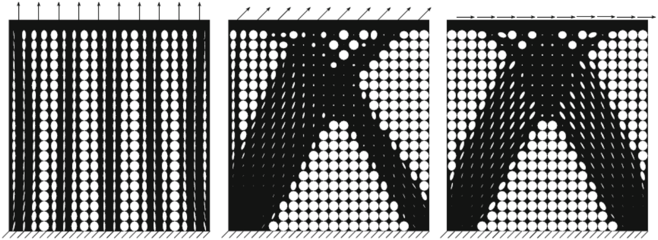
where $y \to A(x, y)$ is periodic and $x \to A(x, y)$ describes the macroscopic variations.



Homogenization theory applies !

Example of a macroscopically varying microstructure





From Geihe et al. (Math. Program. A, 2013, 141:383-403).

References

Joint work with P. Geoffroy-Donders and O. Pantz:
Computers & Mathematics with Applications, 78, 2197-2229 (2019).
J. Comp. Phys., 401, 108994 (2020).

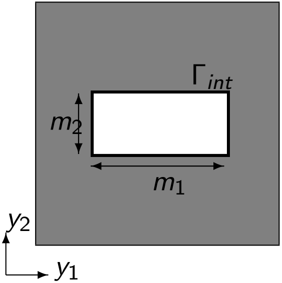
See also:
J. P. Groen and O. Sigmund, *Homogenization based topology optimization for high resolution manufacturable microstructures,* International Journal for Numerical Methods in Engineering, 113(8):1148-1163, 2018.

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.

Modelling issues for lattice materials

- For manufacturing reasons, a single microscopic scale is allowed. No sequential laminates !
- Choice of the period (square, rectangle, triangle, hexagon...).
- Choice of a parametrized cell (rectangular or ellipsoidal hole).
- Orientation of the cell is crucial because optimal microstructures are known to be anisotropic !
- No existence of optimal designs. It can be seen numerically for a "bad" choice of the cell...

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 difficult 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.

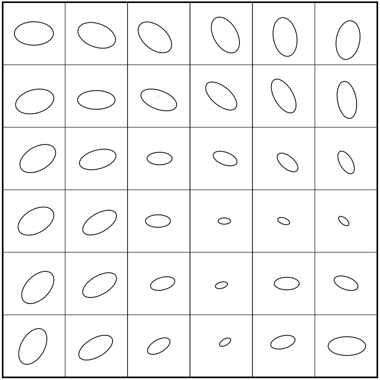
There are two possible approaches:

1. a "naive" approach,
2. a deeper approach (initiated by Pantz and Trabelsi, 2008).

Anisotropy is crucial for optimality !

A first naive approach

The periodic grid is **never** deformed like below.



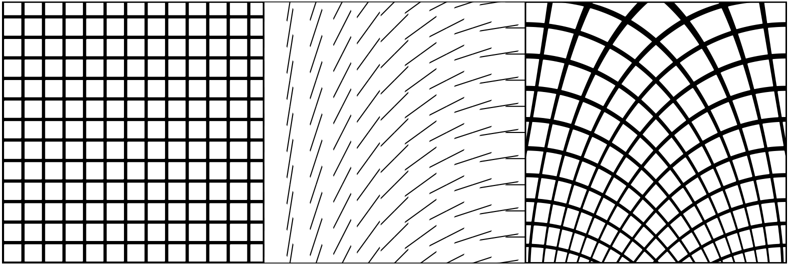
Only the holes are rotated.

Why is it naive ?

- The main advantage of the "naive" approach is that reconstruction of a periodic perforated structure is **very easy**.
- This approach is **naive** because, clearly, the "skeleton" of the reconstructed structure does not adapt to the supported stresses or forces.

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

If the cell is rotated by an angle α (in $2-d$), then the homogenized properties are given by

$$A^*(m_1, m_2, \alpha) = R(\alpha)^T A^*(m_1, m_2, 0) R(\alpha)$$

where $R(\alpha)$ is the fourth-order tensor defined by :

$$\forall \xi \in \mathcal{M}_2^s \quad R(\alpha)\xi = Q(\alpha)^T \xi Q(\alpha)$$

where $Q(\alpha)$ is the rotation matrix of angle α.

Cell problem. Let $(e_i)_{1\le i\le N}$ be the canonical basis of $\mathbb{R}^N$. Define

$$e_{ij} = \frac{1}{2}\left(e_i \otimes e_j + e_j \otimes e_i\right)$$

For each matrix e_{ij}, the *cell problem* is

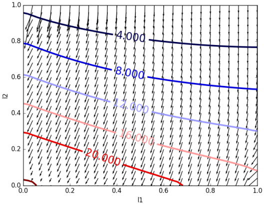
$$\begin{cases} -\operatorname{div}\left(A(y)\left(e_{ij} + e(w_{ij}(y))\right)\right) = 0 & \text{in } Y \setminus \mathrm{hole} \\ A(y)\left(e_{ij} + e(w_{ij}(y))\right) n = 0 & \text{on } \partial\mathrm{hole} \\ y \to w_{ij}(y) & Y\text{-periodic} \end{cases}$$

i.e. it gives the response of the microstructure under a given external strain e_{ij}. The homogenized tensor is then defined by

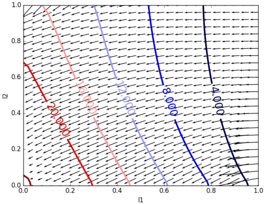
$$A^*_{ijkl} = \int_Y \left(A(y)e(w_{ij})_{kl} + A_{ijkl}(y)\right) dy.$$

or equivalently

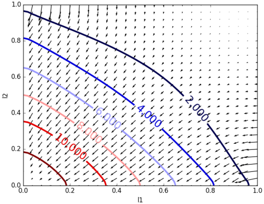
$$A^*_{ijkl} = \int_Y A(y)\left(e_{ij} + e(w_{ij})\right) \cdot \left(e_{kl} + e(w_{kl})\right) dy$$



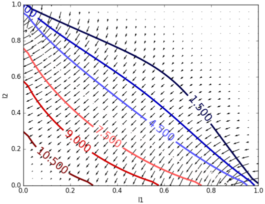
$(A_0^*(m))_{1111}$



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



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



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

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

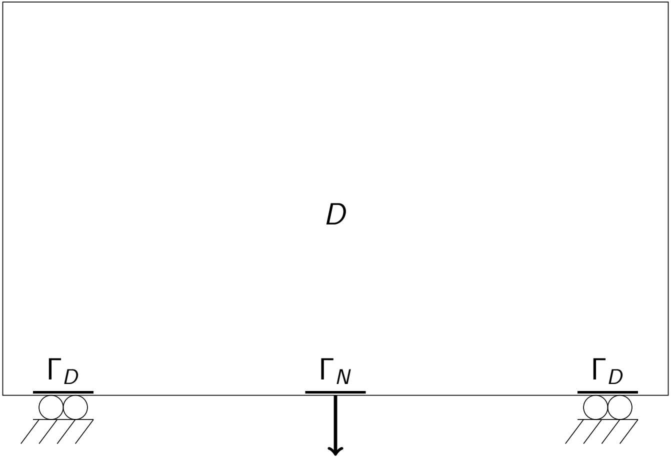
The homogenized equation in a box D (containing the lattice shape) is

$$\begin{cases} \operatorname{div} \sigma = 0 & \text{in } D, \\ \sigma = A^*(m_1, m_2, \alpha) e(u) & \text{in } D, \\ u = 0 & \text{on } \Gamma_D, \\ \sigma \cdot n = g & \text{on } \Gamma_N, \\ \sigma \cdot n = 0 & \text{on } \Gamma = \partial D \setminus (\Gamma_D \cup \Gamma_N). \end{cases}$$

We consider compliance minimization with a weight constraint

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

Bridge test case

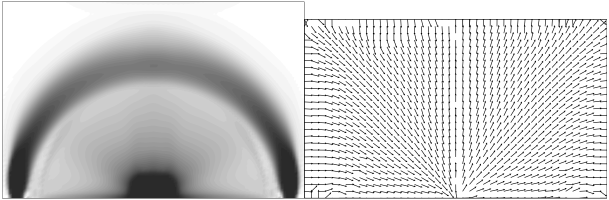


For compliance minimization, we use

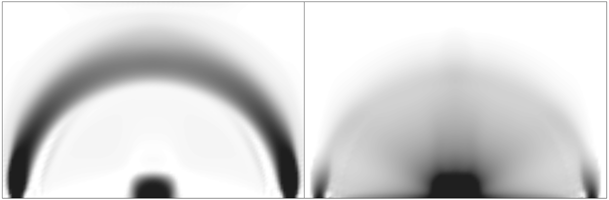
- an optimality criteria or alternate minimization algorithm for optimizing with respect to m_1, m_2,
- a result of Pedersen for orientation optimization: α is given by orienting A^* in the direction of the eigenvector of the largest (absolute) eigenstress,
- the weight constraint is enforced by a Lagrange multiplier.

Except when σ is proportional to the identity, the optimal orientation angle α is unique up to the addition of a multiple of π...

Non-uniqueness creates a regularity issue for α !

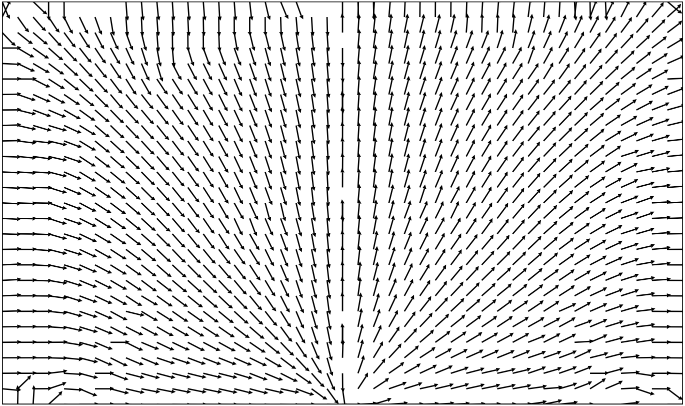


Density Cell orientation



m_1 m_2

Regularity issues for the optimal orientation



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

- α or $\alpha + \pi$ are the same orientation.
- Where the material density is close to 0 or 1, orientation does not play any role.
  (cf. the corners in the previous figure.)
- There are **real** singularities of the orientation, like a fan.
  (cf. the bottom middle in the previous figure.)
- If the value of m_1 and m_2 are exchanged, then the optimal orientation switches from α to $\alpha + \pi/2$.
  It does not seem to appear in our numerical results.

This is a source of numerical difficulties !
We shall come back to this point later...

- 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 satisfies a conformality condition.

Lemma. Let α be a regular orientation field and D be a simply connected domain. There exists a mapping function φ and a dilatation field r satisfying $\nabla\varphi = e^r Q(\alpha)$ if and only if

$$\Delta\alpha = 0 \text{ in } D.$$

Notation. For a vector field $u = (u_1, u_2)$ its curl is defined as $\mathrm{curl} u = \nabla \wedge u = \frac{\partial u_2}{\partial x_1} - \frac{\partial u_1}{\partial x_2}$, where $\wedge$ is the 2-d cross product of vectors.

Remark. Of course, $\mathrm{curl}\nabla\varphi = 0$.

Proof of the conformality condition

Proof. Since D is simply connected, a vector-valued map is a gradient if and only if its rotational vanishes.
Therefore, there exists φ if and only if $\mathrm{curl}\,(e^r Q(\alpha)) = 0$.
Let a_1, a_2 be the columns of $Q(\alpha)$. Then

$$\mathrm{curl}\,(e^r Q(\alpha)) = 0 \Leftrightarrow \nabla r \wedge a_i = -\nabla \wedge a_i \quad i = 1, 2.$$

Since (a_1, a_2) is a $\perp$-basis, $\nabla r = (-\nabla \wedge a_2)a_1 + (\nabla \wedge a_1)a_2$.
On the other hand

$$\nabla \wedge a_1 = \frac{\partial \alpha}{\partial x_1}\cos(\alpha) + \frac{\partial \alpha}{\partial x_2}\sin(\alpha)$$

and similarly for $\nabla \wedge a_2$. It leads to

$$\nabla r = \left(-\frac{\partial \alpha}{\partial x_2}, \frac{\partial \alpha}{\partial x_1}\right)^T.$$

Thus, the dilation factor r exists if and only if the above l.h.s. is curl free, which leads to the harmonic condition on α.

Is the orientation angle α harmonic ?

- Since α is a stress eigen-direction, it has no reason of being harmonic !
- Even worse, α is not smooth at some places...

Conclusion: we regularize the angle α and make it harmonic by a variational approach.

Working with the double angle $\beta = 2\alpha$ removes the indeterminate additive constant π.

At each iteration of the optimization algorithm, instead of minimizing locally (by using Pedersen result)

$$A^*(m_1, m_2, \beta)^{-1}\sigma : \sigma$$

we minimize globally

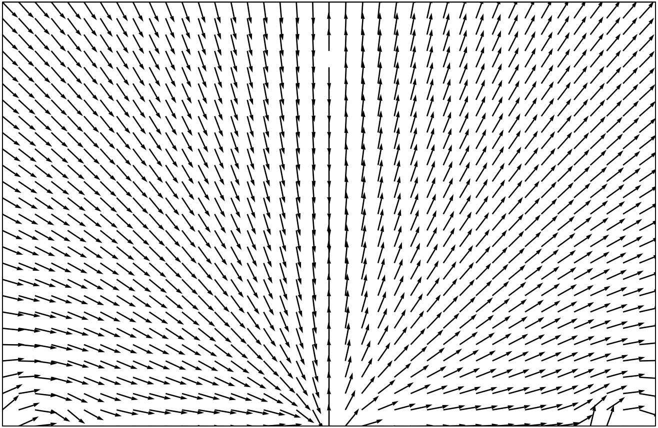
$$\int_D \left(A^*(m_1, m_2, \beta)^{-1}\sigma : \sigma + \eta^2 |\nabla\beta|^2 \right) dx,$$

under the harmonic constraint

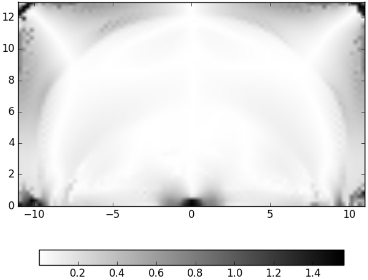
$$\int_D \nabla\beta \cdot \nabla q \, dx = 0 \quad \text{for all } q \in H^1_0(D).$$

Non-linear (non-quadratic) constrained optimization problem.

Regularized orientation α for the bridge case



Angle difference between optimized and regularized orientations



The regularization occurs mainly in areas where density is close to 0 or to 1, i.e. where the homogenized material is almost isotropic and the orientation has no significant impact.

Does this regularization process always work ?

In other words, does it always yield a smooth harmonic angle α ?

Answer: unfortunately, no... because of "true" singularities.

1. There may be singularities of the orientation that remain and thus the angle cannot be harmonic.
2. There are other regularization processes (e.g. minimizing a Ginzburg-Landau energy) which may help in removing singularities.

See the PhD thesis of P. Geoffroy-Donders for details.

Once an harmonic angle $\alpha = \beta/2$ has been found, one needs to compute r and φ such that

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

The dilation field r satisfies $\nabla r = (-\nabla \wedge a_2)a_1 + (\nabla \wedge a_1)a_2$, with $(a_1, a_2) = Q(\alpha)$, so it is a solution of

$$\min_{r \in H^1(D)} \int_D |\nabla r + (\nabla \wedge a_2)a_1 - (\nabla \wedge a_1)a_2|^2 dx.$$

Once r has been computed, a naive idea would be to compute φ as a minimizer in $H^1(D;\mathbb{R}^2)$ of

$$\int_D |\nabla\varphi - e^r Q(\alpha)|^2 \, dx.$$

However, we know that, even if β is smooth, α may have jumps of the type $\pm\pi$ and thus $Q(\alpha)$ may have jumps of its sign.

To compute φ there are two possibility.

1. Find a coherent orientation of α (i.e. choose between α and $\alpha + \pi$ at every point): this is possible only if there are no singularities (this is the approach of Groen and Sigmund).
2. Leave the angle α as it is and extend φ to be defined in an abstract manifold.
   This is the approach of A.-Geoffroy-Pantz and it works in the presence of singularities too.

Definition. Denote by T a rotation matrix field which is a candidate for being $Q(\alpha)$. We introduce the cover space of D

$$\mathcal{D} = \{(x, T) \in D \times \mathrm{SO}(2) \text{ such that } T^2 = Q(\beta)\},$$

where $\mathrm{SO}(2)$ is the set of rotations in $\mathbb{R}^2$.

Remarks.

1. At every point $x \in D$ the rotation satisifies $T(x)^2 = Q(\beta)(x)$.
2. Assuming that the angle α is globally orientable, then $T(x) = Q(\alpha)(x)$ or $T(x) = -Q(\alpha)(x)$, and thus $\mathcal{D}$ is simply the union of two copies of D, consisting of the two possible signs of $Q(\alpha)$.
3. If α is not globally orientable, see the PhD. of P. Geoffroy...

We minimize with respect to $\varphi(x,T)$ in the space of P_1 finite elements on $\mathcal{D}$, which are skew-symmetric $\varphi(x,-T) = -\varphi(x,T)$.

$$\int_{\mathcal{D}} |\nabla\varphi - e^r T|^2 \, dx$$

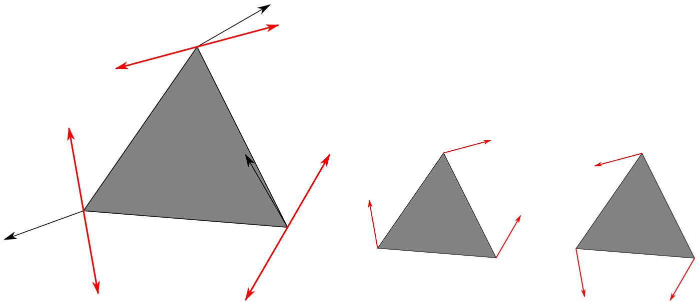
New idea: use non-conformal finite elements on D instead of continuous on $\mathcal{D}$!

On each triangle K of the mesh compute one continuous orientation T_K such that $T_K^2 = Q(\beta)$. Glue together these orientations (with P_1 discontinuous finite elements on D). Define a projection operator operator $\mathcal{I}$ from $\mathcal{D}$ to D with values ± 1 according to the local orientation T_K.

Then, minimize with respect to $\mathcal{I}\varphi$ in the space of P_1 discontinuous finite elements:

$$\int_{\mathcal{D}} |\nabla\varphi - e^r T|^2 \, dx = 2 \sum_K \int_K \left|\nabla \mathcal{I}\varphi(x) - e^{r(x)} T_K(x)\right|^2 \, dx.$$

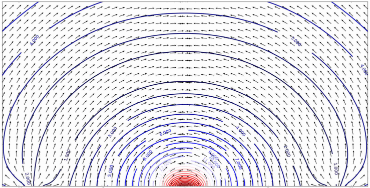
Discontinuous orientation, triangle by triangle

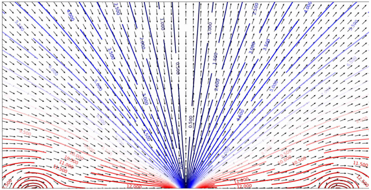


Left: orientation of β (black arrows) and of α (red arrows). Right: two possible coherent orientations of α.

Coherent: two by two, the scalar products of the vectors are positive.

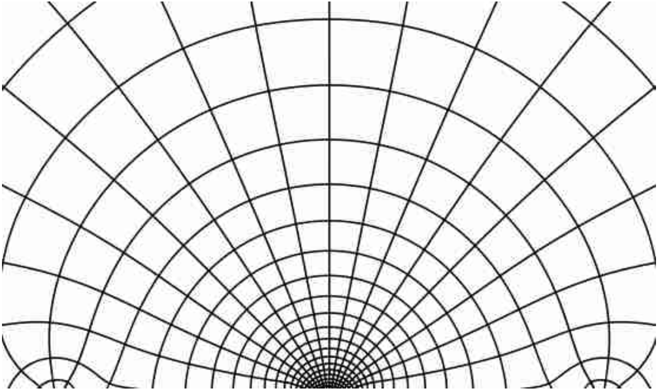
Map $|\varphi_i|$ (isolines) and the orientation vectors a_i (arrow for the bridge case





$|\varphi_1|$ and a_2 (left) $\qquad$ $|\varphi_2|$ and a_1 (right)

Mapping a regular grid with φ for the bridge case



Projection in the simple case where $\alpha \equiv 0$

When there is no varying orientation, $\alpha \equiv 0$, the projection is easy.
The unit cell (rectangular hole in a square) is defined by

$$Y(m) = \left\{ y \in [0,1]^2 \text{ s. t. } \begin{array}{c} \cos(2\pi y_1) \geq \cos(\pi(1 - m_1)) \\ \text{or} \\ \cos(2\pi y_2) \geq \cos(\pi(1 - m_2)) \end{array} \right\}.$$

The domain D is paved with cells $\varepsilon Y(m)$. The cell parameters $m(x)$ is varying in D, so we define a (macroscopically modulated) projected lattice shape $\Omega_\varepsilon(m)$

$$\Omega_\varepsilon(m) = \left\{ x \in D \text{ s. t. } \begin{array}{c} \cos\left(\frac{2\pi x_1}{\varepsilon}\right) \geq \cos(\pi(1 - m_1(x)) \\ \text{or} \\ \cos\left(\frac{2\pi x_2}{\varepsilon}\right) \geq \cos(\pi(1 - m_2(x)) \end{array} \right\},$$

with $m_1(x), m_2(x) : D \mapsto [0,1]$.

The cellular structures can be defined using level-sets. We introduce two functions $\psi^m_{\varepsilon,i}$, one for each direction

$$\psi^m_{\varepsilon,i}(x) = -\cos\left(\frac{2\pi x_i}{\varepsilon}\right) + \cos(\pi(1 - m_i(x))),$$

and a level-set function

$$\Phi^m_\varepsilon = \min(\psi^m_{\varepsilon,1}, \psi^m_{\varepsilon,2}).$$

The final structure $\Omega_\varepsilon(m)$ is then defined by

$$\Omega_\varepsilon(m) = \{x \in D \text{ such that } \Phi^m_\varepsilon(x) \leq 0\}.$$

Finally, we simply plot $\Omega_\varepsilon(m)$ for different values of ε.

Projection in the general case with orientation $\alpha \neq 0$

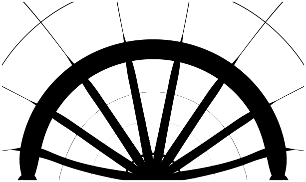
Once the map $\varphi = (\varphi_1, \varphi_2)$ from D into $\mathbb{R}^2$ is found, proceed as before !

The final shape, now denoted $\Omega_\varepsilon(\varphi, m)$, is still defined by a level set function:

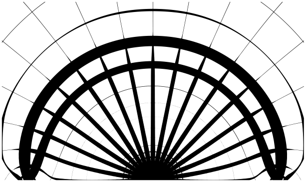
$$\Omega_\varepsilon(\varphi, m) = \{x \in D \text{ such that } \Phi_\varepsilon^{\varphi,m}(x) \leq 0\}$$

with $\Phi_\varepsilon^{\varphi,m} = \min(\psi_{\varepsilon,1}^{\varphi,m}, \psi_{\varepsilon,2}^{\varphi,m})$ and

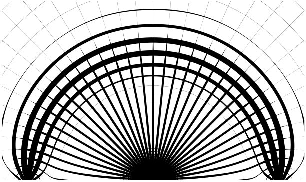
$$\psi_{\varepsilon,i}^{\varphi,m}(x) = -\cos\left(\frac{2\pi\varphi_i(x)}{\varepsilon}\right) + \cos(\pi(1 - m_i(x))).$$



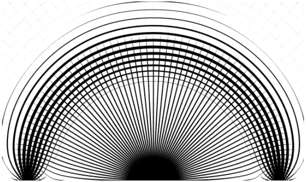
$\varepsilon = 0.4$



$\varepsilon = 0.2$



$\varepsilon = 0.1$



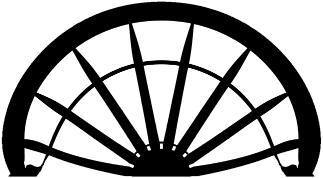
$\varepsilon = 0.05$

A final post-processing/cleaning of the lattice reconstruction

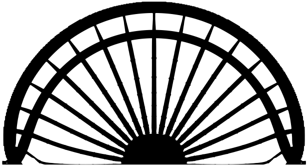
- There are disconnected components of the lattice structure to be removed.
- There are too thin members.

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

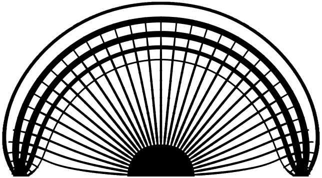
Post-processed structures for several ε



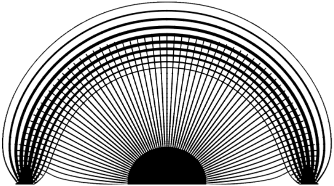
$\varepsilon = 0.4$



$\varepsilon = 0.2$

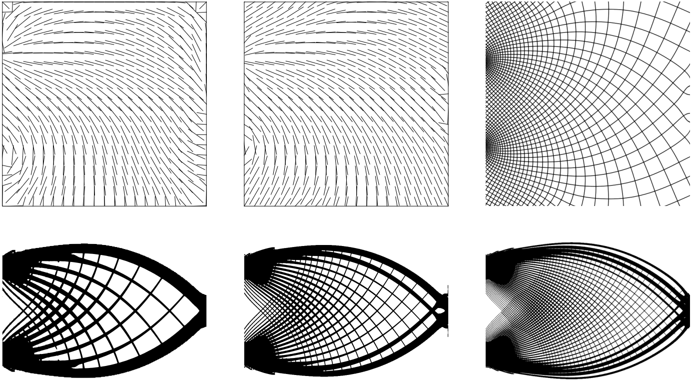


$\varepsilon = 0.1$

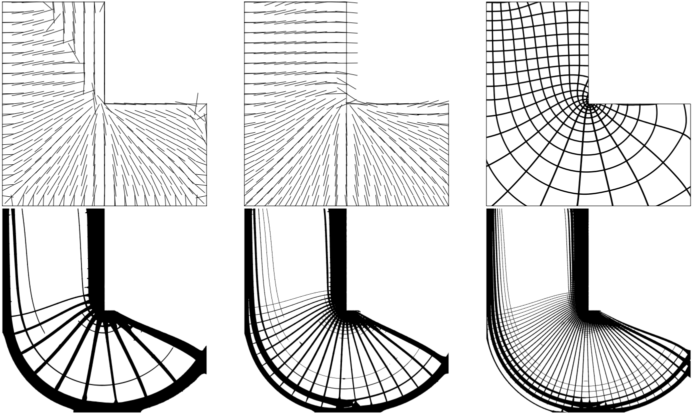


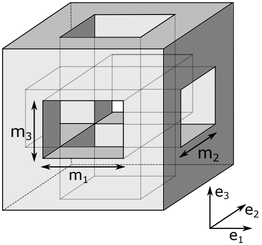
$\varepsilon = 0.05$

Cantilever case



L-beam

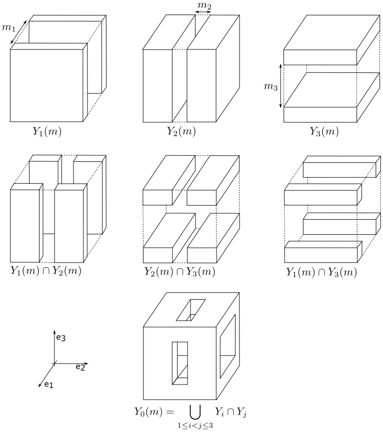




- Cell orientation by a direct rotation matrix $(\omega_1, \omega_2, \omega_3)$.
- No more conformality property (Liouville theorem).
- The map φ is computed direction by direction with 3 dilation fields:

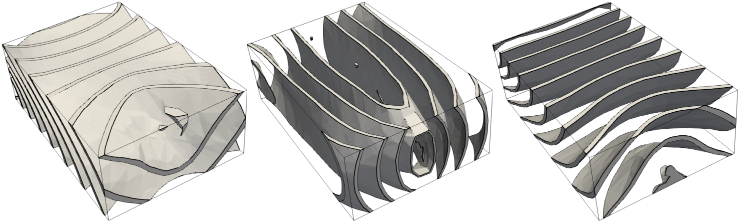
$$\forall i \in \{1,2,3\} \quad \nabla\varphi_i = e^{r_i}\omega_i$$

Cubes are transformed in rectangles...

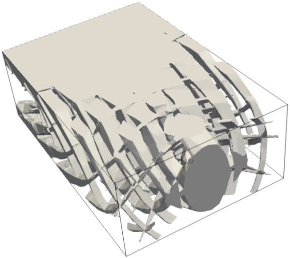


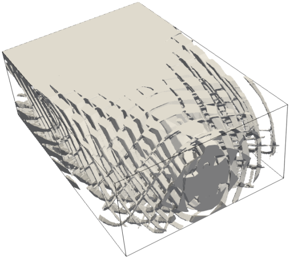
$$Y_0(m) = \cup_{1 \le i < j \le 3} \left(Y_i(m) \cap Y_j(m) \right)$$

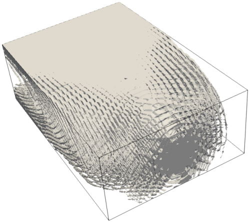
3-d cantilever $Y_i(m_i)$



3-d cantilever







3-d bridge and mast