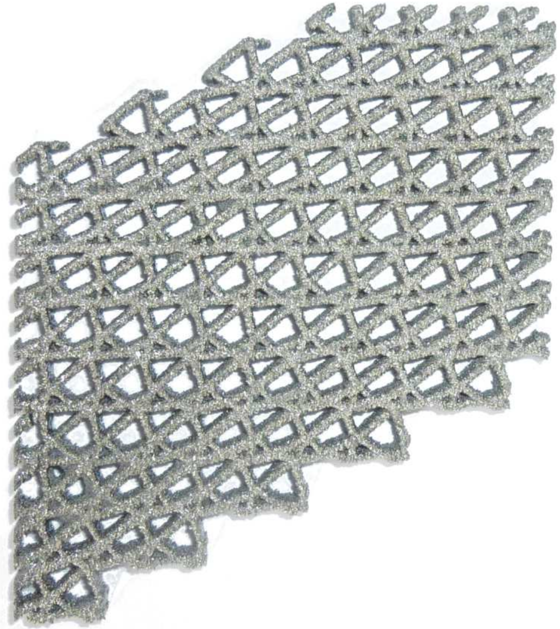
Nonperiodic homogenization for material optimization

V. Ehrlacher, C. Le Bris, F. Legoll, G. Leugering,
M.Stingl

Control of PDE, Benasque
28.08.2013

FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG
Department MATHEMATIK
CONTINUOUS OPTIMIZATION

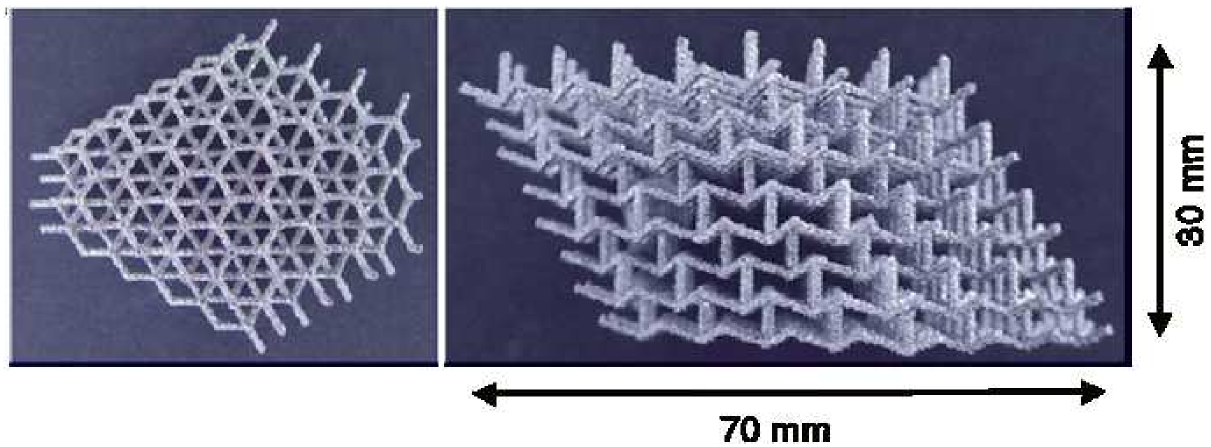
Motivation: structurally graded material



- Varying structural properties
- Typically continuous changes
- Applications: bone replacement, light weight design, support structure of catalyst...

Goal: Identify optimal structure with respect to given loading scenarios and boundary conditions.

Structurally graded materials



$\Omega \subset \mathbb{R}^d$ macroscopic domain: $S \subset \Omega$. For all $x \in \Omega$, all $1 \leq i, j, k, l \leq d$,

$$E^S_{ijkl}(x) := \chi_S(x) E^0_{ijkl}, \quad \chi_S(x) := \begin{cases} 1 \text{ if } x \in S, \\ \eta \text{ if } x \notin S, \end{cases} \quad \text{with } \eta > 0 \text{ small.}$$

Elasticity problem

External forces $\mathbf{f} \in \left(L^2(\Omega)\right)^d$.

Given a linear elasticity tensor $E(x) = (E_{ijkl}(x))_{1\le i,j,k,l\le d}$, using Einstein's notation,

$$\begin{cases} \text{find } \mathbf{u}^E \in \left(H_0^1(\Omega)\right)^d \text{ such that} \\ \forall \mathbf{v} \in \left(H_0^1(\Omega)\right)^d, \quad \int_\Omega E_{ijkl}(x) e_{ij}\left(\mathbf{u}^E\right) e_{kl}(\mathbf{v})\, dx = \int_\Omega \mathbf{f}\cdot\mathbf{v}, \end{cases}$$

For all $1 \le i,j \le d$, $\mathbf{v} \in H_0^1(\Omega)$,

$$e_{ij}(\mathbf{v}) = \frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right).$$

Abuse of notation: $E\mathbf{u}^E = \mathbf{f}$.

Typical optimization problem

Find $S_{opt} \in \mathcal{S}$ such that

$$S_{opt} \in \operatorname*{argmin}_{\substack{S \in \mathcal{S} \\ E^S \mathbf{u}^{E^S} = \mathbf{f} \\ c_l\left(\mathbf{u}^{E^S}\right) \leq C_u}} \mathcal{J}(\mathbf{u}^{E^S}, S),$$

where

- $\mathcal{S}$ is an admissible set of structures S: contains structural constraints;
- $\mathcal{J}$ is a cost functional to minimize;
- c_l denotes some constraints which must be satisfied on $\mathbf{u}^{E^S}$.

Typical examples of $\mathcal{J}$:

- tracking functional: $\mathcal{J}(\mathbf{u}) = \int_\Omega (\mathbf{u} - \mathbf{u}_d)^2 \, dx$
- compliance functional: $\mathcal{J}(\mathbf{u}) = \int_\Omega \mathbf{f} \cdot \mathbf{u} \, dx$
- $\mathcal{J}(S) = \int_\Omega \chi_S(x) \, dx$ is the mass of the structure.

Relaxation by homogenization

Find $S_{opt} \in \mathcal{S}$ such that

$$S_{opt} \in \underset{\substack{S \in \mathcal{S} \\ E^{H,S}\mathbf{u}^{E^{H,S}} = \mathbf{f} \\ c_l\left(\mathbf{u}^{E^{H,S}}\right) \leq C_u}}{\operatorname{argmin}} \mathcal{J}(\mathbf{u}^{E^{H,S}}, S), \tag{1}$$

where

- $\mathcal{S}$ is an admissible set of structures S: contains structural constraints;
- $\mathcal{J}$ is a cost functional to minimize;
- c_l denotes some constraints which must be satisfied on $\mathbf{u}^{E^{H,S}}$.
- $E^{H,S}$ is an "approximate" linear elasticity tensor, associated to the structure S, obtained usually through an homogenization process.

Limitations

For a given periodic structure S, the homogenized elasticity tensor $E^{H,S}$ is constant over all the domain Ω!

Goal: Allow for elasticity tensors $E^{H,S}(x)$ whose value can depend on $x \in \Omega$: need for non-periodic optimization!

[Allaire, Briane,Chenais, Kikuchi, Bendsoe, Lipton etc...]

Free material optimization

Find $E^H_{opt} \in \mathcal{E}$ such that

$$E^H_{opt} \in \underset{\substack{E^H \in \mathcal{E} \\ E^H \mathbf{u}^{E^H} = \mathbf{f} \\ c_l\left(\mathbf{u}^{E^H}\right) \leq C_u}}{\operatorname{argmin}} \mathcal{J}(\mathbf{u}^{E^H}, E^H), \qquad (3)$$

where

- $\mathcal{E}$ is an admissible set of linear elasticity tensors E^H: contains structural constraints;
- $\mathcal{J}$ is a cost functional to minimize;
- c_l denotes some constraints which must be satisfied on $\mathbf{u}^{E^H}$.

Minimization of the mass replaced by the minimization of the total stiffness: $\mathcal{J}(E^H) = \int_\Omega \mathrm{Tr} E^H(x)\, dx$.

Free material optimization

Theorem

Let $C_1, C_2 > 0$ *and*

$$\mathcal{E} := \{E^H(x) \text{ such that a.e. in } \Omega,\ E^H(x) \geq \eta Id,\ TrE^H(x) \leq C_1 \text{ and } \int_\Omega TrE^H(x)\,dx \leq C_2\}.$$

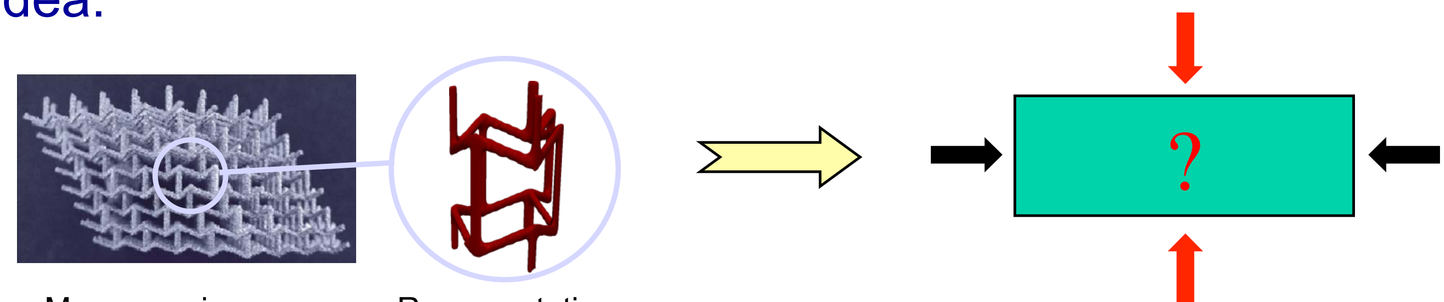
Then, (3) has a solution.

Proof of [Haslinger, Kocvara,Leugering, Stingl, 2011]: H-convergence introduced by Murat, Tartar.

Material design

Goal: find a microstructure, which yields desired macroscopic material properties

Idea:



Macroscopic material

Representative base structure

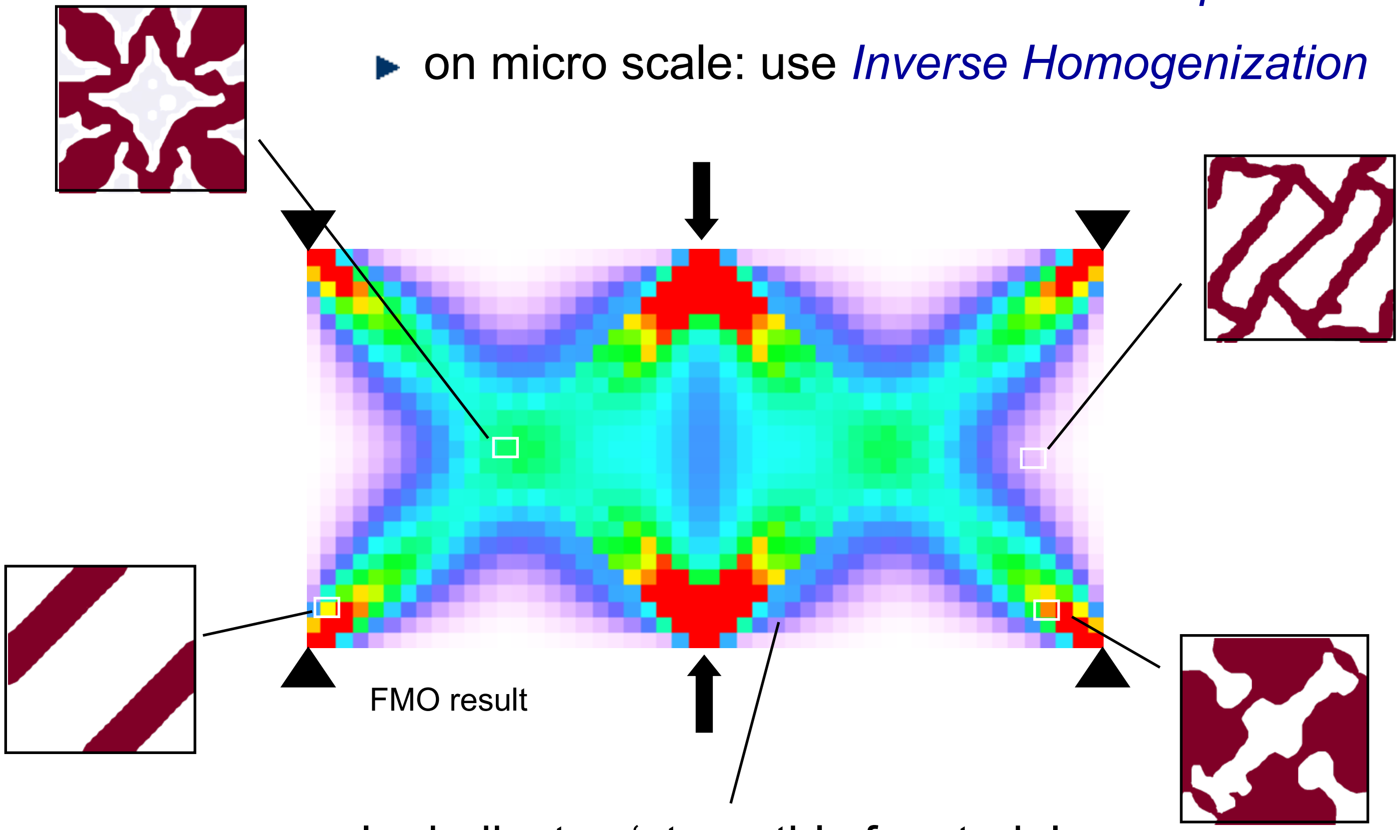
S ← material design — $E_H(S)$

$$\text{For given } E \text{ find } S \text{ s.t. } \|E - E_H(S)\| \to \min$$

In particular, E may be given by the FMO-optimized matrix!

A two-scale approach: example

- on macro scale: use *Free Material Optimization*
- on micro scale: use *Inverse Homogenization*



color indicates ‘strength’ of material

Alternative approach

[Pantz, Trabelsi, 2009]

Fix some $\varepsilon > 0$ small, and $\chi_{\rm per} \in L^\infty_{\rm per}(Y)$.

$$E^{\mathbf{g},\varepsilon}_{ijkl}(x) = \chi_{\rm per}\left(\frac{\mathbf{g}(x)}{\varepsilon}\right) E^0_{ijkl} = E^{\rm per}_{ijkl}\left(\frac{\mathbf{g}(x)}{\varepsilon}\right)$$

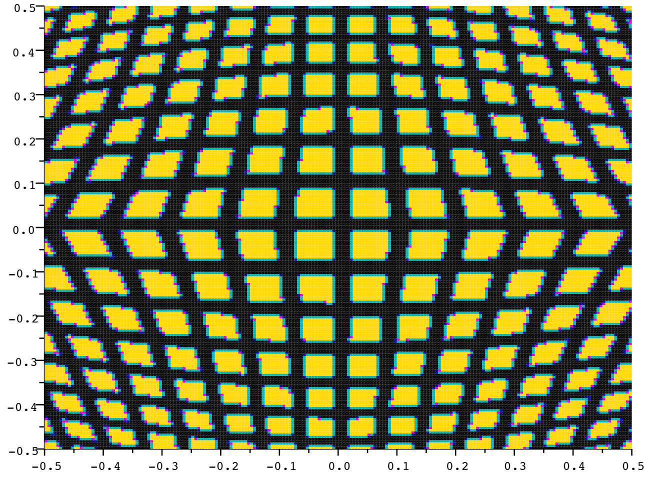
where

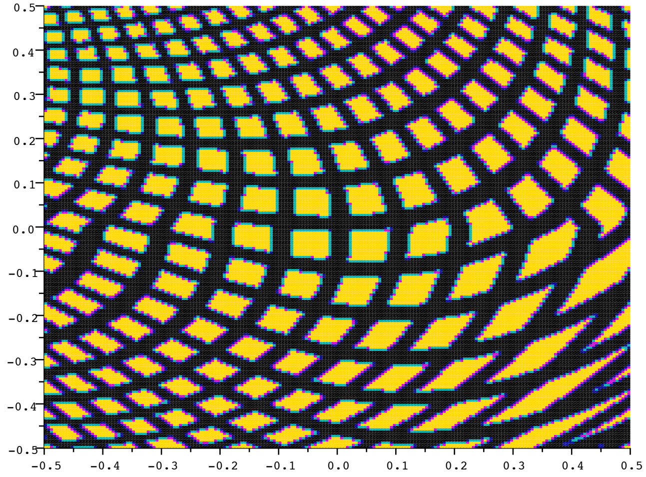
$$\mathbf{g} : \begin{cases} \Omega & \longrightarrow & \mathbb{R}^d \\ x & \longmapsto & \mathbf{g}(x) = (g_j(x))_{1\le j\le d}. \end{cases}$$

is a continuous function.

Idea: optimize on the function $\mathbf{g}(x)$ which describes the structure.

Examples for g





Gradient matrix

For all $x \in \Omega$, we denote by

$$G(x) := \left(\frac{\partial g_j}{\partial x_i}(x) \right)_{1 \le i,j \le d} \in \mathbb{R}^{d \times d}.$$

For all $G = (G_{ij})_{1 \le i,j \le d} \in \mathbb{R}^{d \times d}$, all $u \in H^1(\Omega)$ and all $1 \le i \le d$, we denote by

$$\frac{\partial^G u}{\partial x_i} = \sum_{j=1}^{d} G_{ij} \frac{\partial u}{\partial x_j},$$

and for all $\mathbf{u} \in \left(H_0^1(\Omega) \right)^d$, $1 \le i, j \le d$,

$$e_{ij}^G(\mathbf{u}) = \frac{1}{2} \left(\frac{\partial^G u_i}{\partial x_j} + \frac{\partial^G u_j}{\partial x_i} \right).$$

Linear elasticity

$$\begin{cases} \text{find } \mathbf{u}^{\varepsilon,\mathbf{g}} \in \left(H_0^1(\Omega)\right)^d \text{ such that} \\ \forall \mathbf{v} \in \left(H_0^1(\Omega)\right)^d, \quad \int_\Omega E_{ijkl}^{\varepsilon,\mathbf{g}} e_{ij}\left(\mathbf{u}^{\varepsilon,\mathbf{g}}\right) e_{kl}(\mathbf{v})\, dx = \int_\Omega \mathbf{f}\cdot\mathbf{v}, \end{cases}$$

$$E_{ijkl}^{\varepsilon,\mathbf{g}}(x) = \chi_{\mathrm{per}}\left(\frac{\mathbf{g}(x)}{\varepsilon}\right) E_{ijkl}^0$$

Assumptions on $\mathbf{g}$

(A1) The function $G : \Omega \to \mathbb{R}^{d\times d}$ is continuous;

(A2) There exists $\kappa > 0$ such that for all $x \in \Omega$, $G(x)^T G(x) \geq \kappa Id$.

N.B.: Standard periodic homogenization: $\mathbf{g} = \mathbf{Id}$

Homogenization result

Theorem ((slight) extension of Bensoussan, Lions, Papanicolaou, general $\mathbf{g}$)

Under assumptions (A1)-(A2), the sequence $(\mathbf{u}^{\varepsilon,\mathbf{g}})_{\varepsilon>0}$ *converges weakly in* $\left(H_0^1(\Omega)\right)^d$ *and strongly in* $\left(L^2(\Omega)\right)^d$ *towards* $\mathbf{u}^{H,\mathbf{g}} \in \left(H_0^1(\Omega)\right)^d$ *the unique solution of*

$$\forall \mathbf{v} \in \left(H_0^1(\Omega)\right)^d, \quad \int_\Omega E_{ijkl}^{H,\mathbf{g}}(x) e_{ij}\left(\mathbf{u}^{H,\mathbf{g}}\right) e_{kl}(\mathbf{v})\, dx = \int_\Omega \mathbf{f}\cdot\mathbf{v},$$

where for all $1 \le i,j,k,l \le d$, *and* $x \in \Omega$, $E_{ijkl}^{H,\mathbf{g}}(x) = \widetilde{E}(G(x))$, *where for all* $1 \le i,j \le d$, *all* $G \in \mathbb{R}^{d\times d}$ *invertible matrix, the corrector function* $\mathbf{w}_{kl}^G \in \left(H_{\mathrm{per}}^1(Y)\right)^d$ *is the unique solution (up to an additive constant) of:* $\forall \mathbf{v} \in \left(H_{\mathrm{per}}^1(Y)\right)^d$,

$$\int_Y E_{ijmn}^0 \chi_{\mathrm{per}}(y) e_{ij}^G\left(\mathbf{w}_{kl}^G\right) e_{mn}^G(\mathbf{v})\, dy = \int_Y E_{klmn}^0 \chi_{\mathrm{per}}(y) e_{mn}^G(\mathbf{v})\, dy, \qquad (4)$$

and

$$\widetilde{E}(G) = \int_Y E_{ijkl}^0 \chi_{\mathrm{per}}(y)\, dy - \int_Y E_{ijmn}^0 \chi_{\mathrm{per}}(y) e_{mn}^G\left(\mathbf{w}_{kl}^G\right)\, dy.$$

Optimization problem

Find $\mathbf{g}_{opt} \in \mathcal{G}$ such that

$$\mathbf{g}_{opt} \in \operatorname*{argmin}_{\substack{\mathbf{g} \in \mathcal{G} \\ E^{H,\mathbf{g}} \mathbf{u}^{E^{H,\mathbf{g}}} = \mathbf{f} \\ c_l\left(\mathbf{u}^{E^{H,\mathbf{g}}}\right) \leq C_u}} \mathcal{J}(\mathbf{u}^{E^{H,\mathbf{g}}}, \mathbf{g}), \tag{5}$$

where

- $\mathcal{G}$ is an admissible set of mapping $\mathbf{g}$ (satisfying (A1) and (A2));
- $\mathcal{J}$ is a cost functional to minimize;
- c_l denotes some constraints which must be satisfied on $\mathbf{u}^{E^{H,\mathbf{g}}}$.

Reformulation in terms of gradient

Actually, $E^{H,\mathbf{g}}(x) = \widetilde{E}\left(G(x)\right)$ only depends locally on the value of the gradient matrix...

Find $G_{opt}(x) \in \widetilde{\mathcal{G}}$ such that

$$G_{opt}(x) \in \operatorname*{argmin}_{\substack{G(x) \in \widetilde{\mathcal{G}} \\ \widetilde{E}(G(x))\mathbf{u}^{\widetilde{E}(G(x))} = \mathbf{f} \\ c_l\left(\mathbf{u}^{\widetilde{E}(G(x))}\right) \leq C_u}} \mathcal{J}(\mathbf{u}^{\widetilde{E}(G(x))}, G(x)), \tag{6}$$

where

- $\widetilde{\mathcal{G}} \subset \begin{array}{l}\{G : \Omega \to \mathbb{R}^{d\times d}, \quad \text{satisfying (A1) and (A2)} \\ \text{such that } \exists \mathbf{g} : \Omega \to \mathbb{R}^d, \; G(x) = \nabla \mathbf{g}(x) \text{ for a.a. } x \in \Omega\};\end{array}$
- $\mathcal{J}$ is a cost functional to minimize;
- c_l denotes some constraints which must be satisfied on $\mathbf{u}^{E^{H,\mathbf{g}}}$.

Parametrization of G

For all $G \in \mathbb{R}^{d\times d}$ such that $\det G > 0$, it holds that

$$G = R_1 D R_2, \quad \text{where}$$

- R_1, R_2 are rotation matrices;
- D is a diagonal matrix with positive coefficients.

Example in 2D:

$$G = G(\theta, \phi, \lambda_1, \lambda_2) = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \begin{pmatrix} \cos\phi & \sin\phi \\ -\sin\phi & \cos\phi \end{pmatrix}.$$

Apply a reduced basis method (greedy POD, emperical interpolation DEIM).....
Patera, Ohlberger, Maday, Le Bris et al.........ongoing research!

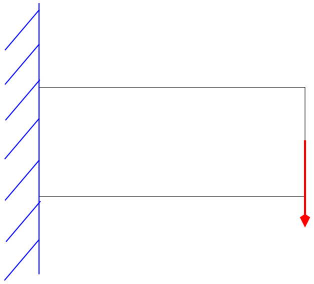
Retrieve the mapping form G

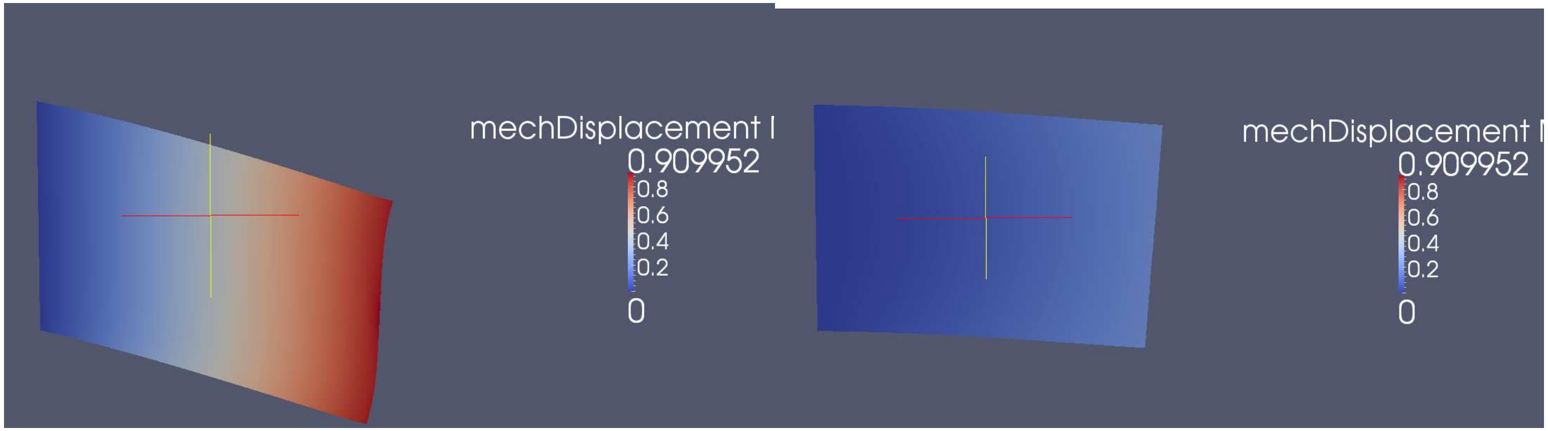
Resolution of a Laplace problem with Neumann boundary conditions

$$\begin{cases} -\Delta \mathbf{g} = -\mathrm{div} G_{opt} \text{ in } \mathcal{D}'(\Omega) \\ \nabla \mathbf{g} \cdot \mathbf{n} = G_{opt} \cdot \mathbf{n} \text{ on } \partial\Omega. \end{cases}$$

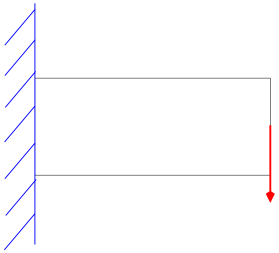
Unique solution $\mathbf{g}$ up to an additive constant! This is our "approximate" optimal mapping.

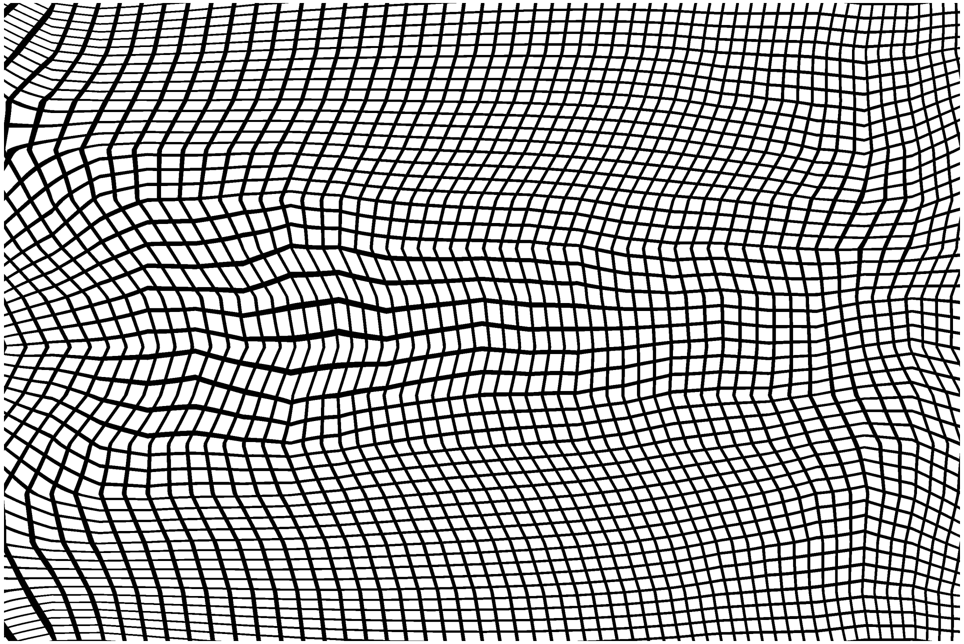
Example




mechDisplacement I
0.909952
0.8
0.6
0.4
0.2
0
mechDisplacement I
0.909952
0.8
0.6
0.4
0.2
0

Result using model reduction





Open questions and current reserach

- 3D computations
- Optimize on χ_{per}?
- Use in addition a level-set method in order to optimize the shape of the macroscopic domain?
- Take into account possible (random) defects which could occur during manufacturing ([Blanc, Le Bris, Lions, 2007]...)
- Alternative to the reconstruction of a structure computed with Free Material Optimization

Selected literature

- G. Allaire, *Shape Optimization by the Homogenization method*, Springer-Verlag, 2002.
- M. P. Bendsoe and O. Sigmund, *Topology Optimization. Theory, Methods and Applications*, Springer-Verlag, Heidelberg, 2002.
- G. Allaire, *Homogenization and two-scale convergence*, SIAM J. Math. Anal., vol. 23, no. 6, pp. 1482-1518, 1992.
- M. Briane, *Homogenization of a non-periodic material*, Journal de mathmatiques pures et appliques, vol. 73, no. 1, pp. 47-66, 1994.
- A. Bensoussan, J.-L. Lions, G. Papanicolaou, *Asymptotic Analysis for Periodic Structures*, Elsevier, 1978.
- D. Chenais, M.L. Mascarenhas and L. Trabucho, *Optimization of non periodic homogenized microstructures*, ESAIM Proc., vol. 2, pp. 165-172, 1997.
- J. Haslinger, G. Leugering, M. Kocvaraz and M. Stingl, *Multidisciplinary Free Material Optimization*, SIAP, 2010.
- F. Schury, M. Stingl, F. Wein, *Slope constrained material optimization*, SISC, 2012.
- O. Pantz and K. Trabelsi, *A Post-treatement of the homogenization method in shape optimization*, 8th World Congress on Structural and Multidisciplinary Optimization, 2009.

- R.E. Bellman. Dynamic Programming. Princeton University Press, 1957.
- A. Ammar, B. Mokdad, F. Chinesta, and R. Keunings. A new family of solvers for some classes of multidimensional partial differential equations encountered in kinetic theory modeling of complex fluids. J. Non-Newtonian Fluid Mech., 139:153-176, 2006.
- E. Cancès, VE, T. Lelièvre Convergence of a greedy algorithm for high-dimensional convex nonlinear problems, M3AS, 2433-2467, 2011.
- E. Cancès, VE, T. Lelièvre Greedy algorithms for high-dimensional linear eigenvalue problems, arXiv, 2013.
- C. Le Bris, T. Lelièvre and Y. Maday. Results and questions on a nonlinear approximation approach for solving high-dimensional partial differential equations, Constructive Approximation 30(3):621-651, 2009.
- A. Nouy, A. Falco, Proper Generalized Decomposition for Nonlinear Convex Problems in Tensor Banach Spaces, Numerische Mathematik, 2011.
- V.N. Temlyakov. Greedy approximation. Acta Numerica, 17:235-409, 2008.
- A. Ammar and F. Chinesta, Circumventing Curse of Dimensionality in the Solution of Highly Multidimensional Models Encountered in Quantum Mechanics Using Meshfree Finite Sums Decompositions, Lecture notes in Computational Science and Engineering, 65, 1-17, 2010.