Nonperiodic homogenization for material optimization

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Control of PDE, Benasque
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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.
Motivation: structurally graded materials

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

\[ E_{ijkl}^S(x) := \chi_S(x) E_{ijkl}^0, \quad \chi_S(x) := \begin{cases} 1 \text{ if } x \in S, \\ \eta \text{ if } x \notin S, \end{cases} \quad \text{with } \eta > 0 \text{ small.} \]
Given a linear elasticity tensor $E(x) = (E_{ijkl}(x))_{1 \leq i,j,k,l \leq d}$, using Einstein’s notation,

$$\begin{cases} 
\text{find } u^E \in (H^1_0(\Omega))^d \text{ such that} \\
\forall v \in (H^1_0(\Omega))^d, \quad \int_\Omega E_{ijkl}(x)e_{ij}(u^E) e_{kl}(v) \, dx = \int_\Omega f \cdot v,
\end{cases}$$

For all $1 \leq i,j \leq d$, $v \in H^1_0(\Omega)$,

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

Abuse of notation: $Eu^E = f$. 
Typical optimization problem

\[ \begin{align*}
S_{\text{opt}} & \in \mathop{\arg\min}_{S} c(I(S)) \\
S & \in S \\
E^S u^E = f \\
c_l(u^E) & \leq C_u
\end{align*} \]

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

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

Typical example of constraints: Linear displacement constraint: \( c_l(u) = \int_{\Omega} d \cdot u \)
Relaxation of the optimization problem by the homogenization method

Find $S_{\text{opt}} \in \text{argmin} \quad J(u^{E^H,S}, S)$, \hspace{1cm} (1)

where

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

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Limitations

Problem with the periodic homogenization method

For a given periodic structure $S$, the homogenized elastic tensor $E^H_S$ is constant over all the domain $\Omega$.

**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...]

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Free material optimization

\[ E_{\text{opt}}^H \in \underset{E^H \in \mathcal{E}}{\arg\min} \mathcal{J}(\mathbf{u}^{E^H}, E^H), \quad (3) \]

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:
\[ \mathcal{J}(E^H) = \int_{\Omega} \text{Tr}E^H(x) \, dx. \]
**Theorem**

Let $C_1, C_2 > 0$ and

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

and

$$ \int_{\Omega} \text{Tr} E^H(x) \, dx \leq C_2 \}. $$

Then, (3) has a solution.

Proof of [Haslinger, Kocvara, Leugering, Stingl, 2011]: H-convergence introduced by Murat, Tartar.
Goal: find a microstructure, which yields desired macroscopic material properties.

Idea:

Macroscopic material
Representative base structure?
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 $\chi_{\text{per}} \in L^\infty_{\text{per}}(Y)$.

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

where

$$g : \left\{ \begin{array}{c} \Omega \\
\xrightarrow{\rightarrow} \mathbb{R}^d \\
\x \mapsto g(x) = (g_j(x))_{1 \leq j \leq d}. \end{array} \right.$$ 

is a continuous function.

Idea: optimize on the function $g(x)$ which describes the structure.
Examples for g
Gradient matrix

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

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

For all $G = (G_{ij})_{1 \leq i,j \leq d} \in \mathbb{R}^{d \times d}$, all $u \in H^1(\Omega)$ and all $1 \leq i \leq d$, 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 $u \in (H^1_0(\Omega))^d$, $1 \leq i,j \leq d$,

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

\[
\begin{align*}
\text{find } u^{\varepsilon,g} \in (H^1_0(\Omega))^d & \text{ such that} \\
\forall v \in (H^1_0(\Omega))^d, \quad \int_\Omega E^{\varepsilon,g}_{ijkl} e_{ij}(u^{\varepsilon,g}) e_{kl}(v) \, dx &= \int_\Omega f \cdot v,
\end{align*}
\]

\[E^{\varepsilon,g}_{ijkl}(x) = \chi_{\text{per}} \left( \frac{g(x)}{\varepsilon} \right) E^0_{ijkl}\]

Assumptions on \( g \)

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

(A2) There exists \( \kappa > 0 \) such that for all \( x \in \Omega \), \( G(x)^T G(x) \geq \kappa \cdot \text{id} \).

N.B.: Standard periodic homogenization: \( g = \text{id} \)
Homogenization result

**Theorem (slight extension of Bensoussan, Lions, Papanicolaou, general $g$)**

Under assumptions (A1)-(A2), the sequence $(u^{\varepsilon}, g)^{\varepsilon > 0}$ converges weakly in $(H^1_0(\Omega))^d$ and strongly in $(L^2(\Omega))^d$ towards $u^{H,g} \in (H^1_0(\Omega))^d$ the unique solution of

$$
\forall v \in (H^1_0(\Omega))^d, \quad \int \Omega E^{H,g}_{ijkl}(x) e_{ij}(u^{H,g}) e_{kl}(v) \, dx = \int \Omega f \cdot v,
$$

where for all $1 \leq i, j, k, l \leq d$, and $x \in \Omega$, $E^{H,g}_{ijkl}(x) = \tilde{E}(G(x))$, where for all $1 \leq i, j \leq d$, all $G \in \mathbb{R}^{d \times d}$ invertible matrix, the corrector function $w^G_{kl} \in (H^1_{\text{per}}(Y))^d$ is the unique solution (up to an additive constant) of:

$$
\forall v \in (H^1_{\text{per}}(Y))^d,
$$

$$
\int_Y E^{0}_{ijmn} \chi_{\text{per}}(y) e^{G}_{ij}(w^G_{kl}) e^G_{mn}(v) \, dy = \int_Y E^{0}_{klmn} \chi_{\text{per}}(y) e^G_{mn}(v) \, dy,
$$

(4)

and

$$
\tilde{E}(G) = \int_Y E^{0}_{ijkl} \chi_{\text{per}}(y) \, dy - \int_Y E^{0}_{ijmn} \chi_{\text{per}}(y) e^G_{mn}(w^G_{kl}) \, dy.
$$
Optimization problem

\[ g_{opt} \in \arg\min_{g \in G} \mathcal{J}(u^{E^H,g}, g), \]

\[ E^H g u^{E^H,g} = f \]

\[ c_I \left( u^{E^H,g} \right) \leq C_u \]

where

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

\begin{equation}
G_{opt}(x) \in \arg \min \mathcal{J}(u^{E(G(x))}, G(x)), \quad \mathcal{J}(G(x)) \in \tilde{\mathcal{G}} \\
\tilde{E}(G(x))u^{\tilde{E}(G(x))} = f \\
c_I \left( u^{\tilde{E}(G(x))} \right) \leq C_u
\end{equation}

where

- \( \tilde{\mathcal{G}} \subset \{ G : \Omega \to \mathbb{R}^{d \times d}, \text{ satisfying (A1) and (A2)} \) such that \( \exists g : \Omega \to \mathbb{R}^d, G(x) = \nabla g(x) \) for a.a. \( x \in \Omega \};

- \( \mathcal{J} \) is a cost functional to minimize;

- \( c_I \) denotes some constraints which must be satisfied on \( u^{E^{H,g}} \).

N.B.: In the optimization loop, need to compute \( \tilde{E}(G) \) for a significant number of matrices \( G \in \mathbb{R}^{d \times d} \): need for a reduced-order model to compute the corrector problem (4) for several values of \( G \): greedy algorithms.
For all $G \in \mathbb{R}^{d \times d}$ such that $\det G > 0$, it holds that

$$G = R_1 D R_2,$$

where

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

**Example in 2D:**

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

\[
\forall \mathbf{g} \cdot \mathbf{n} = G_{opt} \cdot \mathbf{n} \text{ on } \partial \Omega.
\]

Unique solution $\mathbf{g}$ up to an additive constant! This is our “approximate” optimal mapping.
Result using model reduction
Open questions and current research

- Optimize on $\chi_{\text{per}}$?
- 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
References on homogenization and structure optimization


References on greedy algorithms


