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Optimization of bodies with locally periodic microstructure

Cristian Barbarosie
CMAF, Universidade de Lisboa

jointly with

Anca-Maria Toader
CMAF, Universidade de Lisboa
**Goal**: Optimize the macroscopic properties (e.g. compliance) of a two-dimensional body made of a linearly elastic material and presenting locally periodic (quasi-periodic) microscopic perforations.
Main ingredient: a code for optimizing the properties of a periodic microstructure, by varying the shape and topology of the hole in the periodicity cell.


Finite element code for the macroscopic analysis, collaboration of Paulo Vieira (C++, libMesh) and of Sérgio Lopes (FreeFem++)

Interface (written in Python) between macroscopic and microscopic codes.

Linear elasticity

\[
\begin{aligned}
- \text{div} (C \nabla u) &= f \quad \text{in} \quad \Omega \\
 u &= 0 \quad \text{on} \quad \Gamma_D \\
(C \nabla u) n &= g \quad \text{on} \quad \Gamma_N
\end{aligned}
\]

Non-homogeneous material: \( C \) depends on \( x \in \Omega \).

Small scale \( \varepsilon \). Sequence \( C^\varepsilon \) of tensor fields.

\[
\begin{aligned}
- \text{div} (C^\varepsilon \nabla u^\varepsilon) &= f \quad \text{in} \quad \Omega \\
 u^\varepsilon &= 0 \quad \text{on} \quad \Gamma_D \\
(C^\varepsilon \nabla u^\varepsilon) n &= g \quad \text{on} \quad \Gamma_N
\end{aligned}
\]

\[
C^\varepsilon_{ijkl} \in L^\infty(\Omega)
\]

Which is the behaviour of the body (macroscopic behaviour)?
Definition We say that a sequence \( C^\varepsilon \) of elastic tensors \( H \)-converges to \( C^H \) if, for any \( f \in L^2(\Omega) \) and for any \( g \in H^{1/2}(\Gamma_N) \), the solution \( u^\varepsilon \in H^1(\Omega) \) of problem

\[
\begin{align*}
-\text{div}(C^\varepsilon \nabla u^\varepsilon) &= f & \text{in} & & \Omega \\
u^\varepsilon &= 0 & \text{on} & & \Gamma_D \\
(C^\varepsilon \nabla u^\varepsilon)n &= g & \text{on} & & \Gamma_N
\end{align*}
\]

converges, weakly in \( H^1(\Omega) \), to the solution \( u \) of problem

\[
\begin{align*}
-\text{div}(C^H \nabla u) &= f & \text{in} & & \Omega \\
u &= 0 & \text{on} & & \Gamma_D \\
(C^H \nabla u)n &= g & \text{on} & & \Gamma_N
\end{align*}
\]
For given $\alpha$ and $\beta$, $0 < \alpha < \beta$, we define $T_{\alpha,\beta}(\Omega)$ as the space of all tensor functions $C$ whose components belong to $L^\infty(\Omega)$ and such that

$$\|C\xi\| \leq \beta\|\xi\|, \ \forall \ \xi \ \text{matrix}$$

$$\langle C\xi, \xi \rangle \geq \alpha\|\xi\|^2, \ \forall \ \xi \ \text{symmetric matrix}$$

**Theorem** The $H$-convergence defines a metrizable topology on $T_{\alpha,\beta}(\Omega)$. The $H$-convergence has local character. Moreover, $T_{\alpha,\beta}(\Omega)$ is a compact space when endowed with the $H$-topology.
Periodic microstructure: \( C^\varepsilon(x) = C^*(\frac{x}{\varepsilon}), \; x \in \Omega. \)

\( C^* : \mathbb{R}^n \rightarrow \mathbb{R}^{n \times n \times n \times n} \) periodic tensor field

\( \mathcal{G} \) periodicity group: \( C^*(x + \vec{v}) = C^*(x), \; \forall \; x \in \Omega, \; \forall \vec{v} \in \mathcal{G} \)
For a periodic microstructure, the homogenized tensor $C^H$ is constant in $\Omega$ and can be defined in terms of cellular problems. For an arbitrary matrix $A \in \mathbb{R}^{n \times n}$

\[
\begin{align*}
\begin{cases}
-\text{div} (C^* \nabla w) = 0 & \text{in } \mathbb{R}^n \\
w(x) = Ax + \varphi(x), & \varphi \text{ } \mathcal{G}-\text{periodic}
\end{cases}
\end{align*}
\]

\[w(y + \vec{v}) = w(y) + A\vec{v}, \forall y \in \mathbb{R}^n, \forall \vec{v} \in \mathcal{G}\]

\[
A = \frac{1}{|Y|} \int_Y \nabla w_A \quad \quad C^H A = \frac{1}{|Y|} \int_Y C^* \nabla w_A
\]

\[
\langle C^H A, B \rangle = \frac{1}{|Y|} \int_Y \langle C^* \nabla w_A, \nabla w_B \rangle
\]
\[ \begin{cases} 
-\text{div} (C^*(A + \nabla \varphi_A)) = 0 \quad \text{in } \mathbb{R}^n \\
\varphi_A \text{ } \mathcal{G}\text{-periodic} 
\end{cases} \]

\[ \begin{cases} 
-\text{div} (C^* \nabla \varphi_A) = \text{div} (C^* A) \quad \text{in } \mathbb{R}^n \\
\varphi_A \text{ } \mathcal{G}\text{-periodic} 
\end{cases} \]

\[ C^H A = \frac{1}{|Y|} \int_Y C^*(A + \nabla \varphi_A) \]

\[ \langle C^H A, B \rangle = \frac{1}{|Y|} \int_Y \langle C^*(A + \nabla \varphi_A), (B + \nabla \varphi_B) \rangle \]

\[ \begin{cases} 
-\text{div} (C^* \nabla \varphi_A) = \text{div} (C^* A) \quad \text{in } Y \\
\varphi_A \text{ } \mathcal{G}\text{-periodic} 
\end{cases} \]
Quasi-periodic microstructure: $C^\varepsilon(x) = C^*(x, \frac{x}{\varepsilon}), \ x \in \Omega$.

$C^* : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}^{n \times n \times n \times n}$ pattern tensor field, periodic in the second argument

$\mathcal{G}$ periodicity group: $C^*(x, y + \vec{v}) = C^*(x, y) , \ \forall \ x \in \Omega , \ \forall y \in \mathbb{R}^n , \ \forall \vec{v} \in \mathcal{G}$
For a quasi-periodic microstructure, the homogenized tensor $C^H$ is no longer constant. It each point $x \in \Omega$, the tensor $C^H(x)$ is defined in terms of a different set of cellular problems, given by the pattern tensor field $C^*(x, \cdot)$:

\[
\begin{cases}
-\text{div}_y(C^*(x, y) \nabla_y w) = 0 & \text{in } \mathbb{R}^n \\
w(y) = Ay + \varphi(y), & \varphi \text{ } G-\text{periodic}
\end{cases}
\]

\[
A = \frac{1}{|Y|} \int_Y \nabla w_A \\
C^H(x)A = \frac{1}{|Y|} \int_Y C^*(x, \cdot) \nabla w_A
\]

\[
\langle C^H(x)A, B \rangle = \frac{1}{|Y|} \int_Y \langle C^*(x, \cdot) \nabla w_A, \nabla w_B \rangle
\]
Macroscopic problem

\[
\begin{cases}
-\text{div}(C^H \nabla u) = f \quad \text{in} \quad \Omega \\
u = 0 \quad \text{on} \quad \Gamma_D \\
(C^H \nabla u)n = g \quad \text{on} \quad \Gamma_N
\end{cases}
\]

Objective functional (e.g.)

\[
\Phi = \int_{\Gamma_N} gu = 2 \int_{\Gamma_N} gu - \int_{\Omega} \langle C^H \nabla u, \nabla u \rangle
\]

Constraint on the volume of material :

\[
V = \int_{\Omega} \theta
\]
Chain of dependencies:

\[ C^*(x, y) \rightarrow C^H(x) \rightarrow \Phi \]
\[ \delta C^* \rightarrow \delta C^H \rightarrow \delta \Phi \]

Macroscopic level:

\[ \Phi = 2 \int_{\Gamma_N} g u - \int_{\Omega} \langle C^H \nabla u, \nabla u \rangle \]
\[ \delta \Phi = 2 \int_{\Gamma_N} g \delta u - \int_{\Omega} \langle \delta C^H \nabla u, \nabla u \rangle - 2 \int_{\Omega} \langle C^H \nabla u, \nabla \delta u \rangle \]
\[ \delta \Phi = - \int_{\Omega} \langle \delta C^H \nabla u, \nabla u \rangle \]
\[ \delta V = \int_{\Omega} \delta \theta \]
Microscopic level – fixed $x \in \Omega$:

Isotropic elastic tensor $C^*(x, y)$, of Lamé coefficients $\lambda$ and $\mu$.

Shape variations:

\[
\langle D_S C^H A, B \rangle = \frac{1}{|Y|} \int_{\partial T} \left[ 2\mu \langle e(w_A), e(w_B) \rangle + \lambda \text{tr}(e(w_A))\text{tr}(e(w_B)) \right] \langle \vec{\tau}, \vec{n} \rangle
\]

\[
D_S C^H = \int_{\partial T} S \langle \vec{\tau}, \vec{n} \rangle
\]
Topology variations:

\[
\langle DTCH A, B \rangle (y) = -\frac{\pi}{|Y|} \frac{\lambda + 2\mu}{\lambda + \mu} \left[ 4\mu \langle e(w_A), e(w_B) \rangle + \frac{\lambda^2 + 2\lambda\mu - \mu^2}{\mu} \text{tr}(e(w_A)) \text{tr}(e(w_B)) \right] (y)
\]

\[
DTCH(y) = \mathcal{T}(y)
\]
The macroscopic domain $\Omega$ is divided in finite elements $K_1, K_2, \ldots, K_n$. In each $K_e$, a periodic pattern tensor field $C^*_e(y)$ is considered, which gives rise to the homogenized elastic tensor $C^H_e$, with local material density $\theta_e$.

Each periodic microstructure $C^*_e$ is optimized, by using the chain of derivatives presented above. Shape optimization and topology optimization steps (at the cellular level) are alternated.
For the case of (microscopic) shape variations, in each macroscopic finite element $K_e$ consider a deformation field $\vec{\tau}_e$. The corresponding changes in the homogenized tensor $C^H_e$ and in the local density $\theta_e$ are:

$$\delta C^H_e = \frac{1}{|Y|} \int_{\partial T_e} S_e \langle \vec{\tau}_e, \vec{n} \rangle \quad \delta \theta_e = \frac{1}{|Y|} \int_{\partial T_e} \langle \vec{\tau}_e, \vec{n} \rangle$$

This gives, for the macroscopic functional:

$$\delta (\Phi + \Lambda V) = - \int_{\Omega} \langle \delta C^H \nabla u, \nabla u \rangle + \Lambda \int_{\Omega} \delta \theta$$

$$= - \sum_e \int_{\partial T_e} \langle S_e, \int_{K_e} \nabla u \otimes \nabla u \rangle \langle \vec{\tau}_e, \vec{n} \rangle + \Lambda \sum_e |K_e| \int_{\partial T_e} \langle \vec{\tau}_e, \vec{n} \rangle$$

$$= \sum_e |K_e| \int_{\partial T_e} \gamma_e \langle \vec{\tau}_e, \vec{n} \rangle$$

$\gamma_e$ are computable functions, depending on the macroscopic strain $\nabla u$ and on the microscopic solutions $w_A$ in the periodicity cell in $K_e$.

For a steepest descent method, simply choose deformation fields $\vec{\tau}_e = -\gamma_e \vec{n}$.
For (microscopic) topology variations, pick a macroscopic finite element $K_e$; consider a virtual nucleation of a small hole at location $y$ in the periodicity cell $Y$. Then the corresponding variation in the lagrangean is

$$
\delta(\Phi + \Lambda V) = -\int_{\Omega} \langle \delta C^H \nabla u, \nabla u \rangle + \Lambda \int_{\Omega} \delta \theta
$$

$$
= -\langle T_e(y), \int_{K_e} \nabla u \otimes \nabla u \rangle \rho^2 + \Lambda |K_e| \rho^2 = |K_e| \eta_e(y) \rho^2
$$

Find the minimum point of the scalar function $\eta_e$ defined in the periodicity cell $Y$. If the minimum value is negative, nucleate a small hole at the minimum point.
Initiate process with (globally) periodic microstructure

- compute homogenized elastic coefficients and material density

- solve macroscopic elastic problems(s)
  - compute sensitivities
  \[ \int_{K_e} \nabla u \otimes \nabla u \]

- perform a shape optimization or topology optimization step in each periodicity cell

convergence ?

- no

- yes: stop
The image contains a schematic representation of a structure with labeled axes and graphs. The graph on the right shows a red line labeled 'Lagrangean' declining from 190 to 130, with the x-axis ranging from 0 to 300. The graph below shows another red line labeled 'convex combination of compliances' with a Y-axis ranging from 0 to 45 and an X-axis ranging from 0 to 300. The graph on the left shows a red line labeled 'volume' with a Y-axis ranging from 0.7 to 1.3 and an X-axis ranging from 0 to 300.
\[
\int_{K_e} \nabla u \otimes \nabla u
\]
First version (parallel, naive): the code launches \( m \) microscopic optimization processes, keeps a list of running processes, waits for the first one to finish, launches one more process and appends it to the list and so on.

```python
import subprocess
list_of_procs = []
while True:
    while (len(list_of_procs)<m) and (...there still are undealt cells...):
        p = subprocess.Popen((optim_cell_executable, cell_name),
                             stdin=subprocess.PIPE, stdout=subprocess.PIPE)
        p.stdin.write(...data, parameters,...)
        list_of_procs.append(p)
    if len(list_of_procs) == 0: break
    p = list_of_procs[0]
    for line in p.stdout.readlines():
        ...manipulate the output: extract from line relevant informations...
        ...e.g. homogenized elastic tensor and density...
    del list_of_procs[0]
```
Second version (parallel): the code launches $m$ microscopic optimization processes, keeps a list of running processes, selects the one which ends first, launches one more process and appends it to the list and so on.

```python
import select
c
list_of_pipes = []
while True:
    while (len(list_of_pipes) < m) and (...there still are undealt cells...) :
        p = subprocess.Popen(...same arguments...)
        p.stdin.write(...data, parameters,...)
        list_of_pipes.append(p.stdout)
    if len(list_of_pipes) == 0 : break
    a,b,c = select.select(list_of_pipes,[],[])
    selected_pipe = a[0]
    line = selected_pipe.readline()
    ...manipulate the output from line...
    if ...the selected process has ended... :
        list_of_pipes.remove(selected_pipe)
```
Third version (distributed): the script connects to several machines and spreads microscopic optimization processes.

```python
import getpass, pexpect, pxssh

password = getpass.getpass()
for m in list_of_machines:
    ssh_m = pxssh.pxssh()
    ssh_m.login (m,'user_name',password)
    sftp_m = pexpect.spawn('sftp',[m])
    sftp_m.expect ('password: ')
    sftp_m.sendline (password)
```

It keeps track of execution times for each process in each machine, thus re-evaluating constantly the performance of each machine. It then migrates cellular processes from less performant machines towards faster ones.
Conclusions:

- Code on two levels: macroscopic analysis (provides sensitivities) and microscopic optimization and analysis (provides homogenized tensor)
- Heavy problem: hundreds/thousands of cellulars problems, each with its finite element mesh (on torus)
- Easy to treat in parallel
- The scripting language Python is appropriate for managing many processes and for distributing them among different machines linked through the internet
- Limitations: two-dimensional code (for periodic microstructures) fixed periodicity group

Question: is this really different from optimizing directly 600 holes in the macroscopic domain?

The complexity is roughly the same.