ECHOES

Extended Calculator of HOmogEnization Schemes

Jean-François Barthélémy

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Welcome

This manual aims at recalling some fundamental aspects of the theory of homogenization of random media along with a presentation of the main features of the library **ECHOES** as well as code examples.

The library **ECHOES** allows to implement various homogenization schemes involving different types of heterogeneities in the framework of elasticity, conductivity, viscoelasticity as well as tools to properly calculate the derivatives of macroscopic stiffness with respect to lower scale moduli (fundamental tool of the modified secant method in nonlinear homogenization).

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A Tensor algebra

B Hill polarization tensor in elasticity

This section recalls some results about the calculation of the Hill polarization tensors related to a matrix of stiffness $\mathbb{C}$ and an ellipsoid $\mathcal{E}_{\mathrm{A}}$ of equation

$$\underline{x} \in \mathcal{E}_{\mathrm{A}} \quad \Leftrightarrow \quad \underline{x} \cdot ({}^t\mathrm{A} \cdot \mathrm{A})^{-1} \cdot \underline{x} \leq 1$$

where A is an invertible second-order tensor so that ${}^t\mathrm{A} \cdot \mathrm{A}$ is a positive definite symmetric tensor associated to 3 radii (eigenvalues $a \geq b \geq c$ possibly written $\rho_1 \geq \rho_2 \geq \rho_3$ for convenience) and 3 angles (orientation of the frame of eigenvectors $\underline{e}_1, \underline{e}_2, \underline{e}_3$)

$$ {}^t\mathrm{A} \cdot \mathrm{A} = a^2 \underline{e}_1 \otimes \underline{e}_1 + b^2 \underline{e}_2 \otimes \underline{e}_2 + c^2 \underline{e}_3 \otimes \underline{e}_3 = \sum_{i=1}^{3} \rho_i \underline{e}_i \otimes \underline{e}_i \tag{B.1}$$

B.1 General expression

A general expression of the elastic polarization tensor is derived in (Willis, 1977) (see also (Mura, 1987))

$$\begin{aligned} \mathbb{P}(\mathrm{A}, \mathbb{C}) &= \frac{1}{4\pi} \int_{\|\underline{\zeta}\|=1} (\mathrm{A}^{-1} \cdot \underline{\zeta}) \overset{s}{\otimes} \Big((\mathrm{A}^{-1} \cdot \underline{\zeta}) \cdot \mathbb{C} \cdot (\mathrm{A}^{-1} \cdot \underline{\zeta}) \Big)^{-1} \overset{s}{\otimes} (\mathrm{A}^{-1} \cdot \underline{\zeta}) \, \mathrm{d}S_\zeta \\ &= \frac{\det \mathrm{A}}{4\pi} \int_{\|\underline{\xi}\|=1} \frac{\underline{\xi} \overset{s}{\otimes} (\underline{\xi} \cdot \mathbb{C} \cdot \underline{\xi})^{-1} \overset{s}{\otimes} \underline{\xi}}{\|\mathrm{A} \cdot \underline{\xi}\|^3} \, \mathrm{d}S_\xi \end{aligned} \tag{B.2}$$

When $\mathbb{C}$ is arbitrarily anisotropic, it is necessary to resort to numerical cubature to estimate $\mathbb{P}$ as proposed in (Ghahremani, 1977), (Gavazzi and Lagoudas, 1990) or (Masson, 2008). However in some cases of anisotropy, analytical solutions are available ((Withers, 1989), (Barthélémy, 2020)). The case of isotropic matrix is particularly developed in the next section.

B.2 Isotropic matrix

In this section, the matrix is assumed isotropic so that its stiffness tensor writes by means of a bulk k and shear μ or Lamé λ and μ moduli or even Young modulus E and Poisson ratio ν

with $k = \frac{E}{3(1-2\nu)}$ and $\mu = \frac{E}{2(1+\nu)}$.

$$\begin{aligned}\mathbb{C} =& 3k\mathbb{J} + 2\mu\mathbb{K} = 3\lambda\mathbb{I} + 2\mu\mathbb{K} \\ &\text{with} \quad J_{ijkl} = \frac{\delta_{ij}\delta_{kl}}{3}, I_{ijkl} = \frac{\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}}{2} \text{ and } \mathbb{K} = \mathbb{I} - \mathbb{J}\end{aligned} \tag{B.3}$$

Introducing Equation B.3 in Equation B.2 leads to after some algebra

$$\mathbb{P} = \frac{1}{\lambda + 2\,\mu}\mathbb{U} + \frac{1}{\mu}(\mathbb{V} - \mathbb{U})$$

where the tensors $\mathbb{U}$ and $\mathbb{V}$, depending only on the ellipsoidal tensor A of Equation B.1, are given by (see (Barthélémy, 2020))

$$\begin{aligned}\mathbb{U} &= \frac{\det \mathrm{A}}{4\pi}\int_{\|\underline{\xi}\|=1} \frac{\underline{\xi}\otimes\underline{\xi}\otimes\underline{\xi}\otimes\underline{\xi}}{\|\mathrm{A}\cdot\underline{\xi}\|^3}\,\mathrm{d}S_\xi \\ &= \frac{1}{4\pi}\int_{\|\underline{\zeta}\|=1} \frac{(\mathrm{A}^{-1}\cdot\underline{\zeta})\otimes(\mathrm{A}^{-1}\cdot\underline{\zeta})\otimes(\mathrm{A}^{-1}\cdot\underline{\zeta})\otimes(\mathrm{A}^{-1}\cdot\underline{\zeta})}{\|\mathrm{A}^{-1}\cdot\underline{\zeta}\|^4}\,\mathrm{d}S_\zeta\end{aligned}$$

and

$$\begin{aligned}\mathbb{V} &= \frac{\det \mathrm{A}}{4\pi}\int_{\|\underline{\xi}\|=1} \frac{\underline{\xi}\overset{s}{\otimes}1\overset{s}{\otimes}\underline{\xi}}{\|\mathrm{A}\cdot\underline{\xi}\|^3}\,\mathrm{d}S_\xi \\ &= \frac{1}{4\pi}\int_{\|\underline{\zeta}\|=1} \frac{(\mathrm{A}^{-1}\cdot\underline{\zeta})\overset{s}{\otimes}1\overset{s}{\otimes}(\mathrm{A}^{-1}\cdot\underline{\zeta})}{\|\mathrm{A}^{-1}\cdot\underline{\zeta}\|^2}\,\mathrm{d}S_\zeta\end{aligned}$$

For an arbitrary ellipsoid defined by Equation B.1, the components of $\mathbb{U}$ and $\mathbb{V}$ write

$$\begin{aligned}U_{iiii} &= \frac{3(I_i - \rho_i^2 I_{ii})}{2} \quad \forall\, i \in \{1,2,3\} \\ U_{iijj} = U_{ijij} = U_{ijji} &= \frac{I_j - \rho_i^2 I_{ij}}{2} = \frac{I_i - \rho_j^2 I_{ij}}{2} \quad \forall\, i \neq j \in \{1,2,3\}\end{aligned}$$

and

$$\begin{aligned}V_{iiii} &= I_i \quad \forall\, i \in \{1,2,3\} \\ V_{ijij} = V_{ijji} &= \frac{I_i + I_j}{4} \quad \forall\, i \neq j \in \{1,2,3\}\end{aligned}$$

where the coefficients I_i and I_{ij} are given by (note that I_i and I_{ij} are adapted from those provided in (Kellogg, 1929) and (Eshelby, 1957): they differ by a factor of $4\pi/3$ for I_{ij} with $i \neq j$ and by 4π for the others)

- if $a > b > c$

$$
\begin{aligned}
I_1 &= \frac{a\,b\,c}{(a^2-b^2)\sqrt{a^2-c^2}}\;(F-E) \\
I_3 &= \frac{a\,b\,c}{(b^2-c^2)\sqrt{a^2-c^2}}\;\left(\frac{b\sqrt{a^2-c^2}}{a\,c}-E\right) \\
I_2 &= 1-I_1-I_3 \\
I_{ij} &= \frac{I_j-I_i}{\rho_i^2-\rho_j^2} \quad \forall\, i \neq j \in \{1,2,3\} \\
I_{ii} &= \frac{1}{3}\left(\frac{1}{\rho_i^2}-\sum_{j\neq i} I_{ij}\right) \quad \forall\, i \in \{1,2,3\}
\end{aligned}
$$

where $F = F(\theta, \kappa)$ and $E = E(\theta, \kappa)$ are respectively the elliptic integrals of the first and second kinds (see (Abramowitz and Stegun, 1972)) of amplitude and parameter

$$
\theta = \arcsin\sqrt{1-\frac{c^2}{a^2}} \quad ; \quad \kappa = \sqrt{\frac{a^2-b^2}{a^2-c^2}}
$$

- if $a > b = c$ (prolate spheroid)

$$
\begin{aligned}
I_2 = I_3 &= a\,\frac{a\sqrt{a^2-c^2}-c^2\,\operatorname{arcosh}(a/c)}{2\,(a^2-c^2)^{3/2}} \\
I_1 &= 1-2\,I_3 \\
I_{1i} = I_{i1} &= \frac{I_i-I_1}{a^2-\rho_i^2} \quad \forall\, i \in \{2,3\} \\
I_{ij} &= \frac{1}{4}\left(\frac{1}{c^2}-I_{31}\right) \quad \forall\, i,j \in \{2,3\} \\
I_{11} &= \frac{1}{3}\left(\frac{1}{a^2}-2\,I_{31}\right)
\end{aligned}
$$

- if $a = b > c$ (oblate spheroid)

$$
\begin{aligned}
I_1 = I_2 &= c\,\frac{a^2\,\arccos(c/a)-c\sqrt{a^2-c^2}}{2\,(a^2-c^2)^{3/2}} \\
I_3 &= 1-2\,I_1 \\
I_{3i} = I_{i3} &= \frac{I_3-I_i}{\rho_i^2-c^2} \quad \forall\, i \in \{1,2\} \\
I_{ij} &= \frac{1}{4}\left(\frac{1}{a^2}-I_{31}\right) \quad \forall\, i,j \in \{1,2\} \\
I_{33} &= \frac{1}{3}\left(\frac{1}{c^2}-2\,I_{31}\right)
\end{aligned}
$$

- if $a = b = c$ (sphere)

$$I_1 = I_2 = I_3 = \frac{1}{3}$$
$$I_{ij} = \frac{1}{5\,a^2} \quad \forall\, i,j \in \{1,2,3\}$$

In this last case of spherical inclusion ($\mathrm{A} = 1$), $\mathbb{U}$ and $\mathbb{V}$ are simply decomposed as

$$\mathbb{U} = \frac{1}{3}\mathbb{J} + \frac{2}{15}\mathbb{K} \quad \text{and} \quad \mathbb{V} = \frac{1}{3}\mathbb{I}$$

B.3 Case of cracks

The case of cracks corresponds to ellipsoids for which the smallest radius is very small compared to the two others, in other words the characteristic tensor A Equation B.1 can be written here

$$\mathrm{A} = \underline{\ell} \otimes \underline{\ell} + \eta\, \underline{m} \otimes \underline{m} + \omega\, \underline{n} \otimes \underline{n} \quad \text{with} \quad \eta = \frac{b}{a} \quad \text{and} \quad \omega = \frac{c}{a}$$

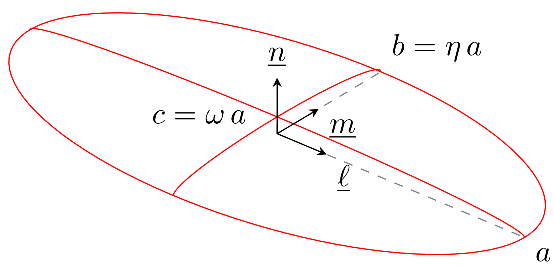

Figure B.1: Ellipsoidal crack

In the case of cracks, it is useful to introduce the second Hill polarization tensor defined as

$$\mathbb{Q} = \mathbb{C} - \mathbb{C} : \mathbb{P} : \mathbb{C}$$

and in particular $\lim_{\omega\to 0} \omega\, \mathbb{Q}^{-1}$ in which it is recalled that $\mathbb{P}$ and thus $\mathbb{Q}$ depend on ω such that the components Q_{nijk} (with n corresponding to the crack normal) behave as $1/\omega$ when ω tends towards 0. The analytical expressions of this limit are fully detailed in (Barthélémy et al., 2021) which recalls in particular that $\mathbb{L}$ actually derives from a symmetric second-order tensor B as

$$\mathbb{L} = \lim_{\omega\to 0} \omega\, \mathbb{Q}^{-1} = \frac{3}{4}\, \underline{n} \overset{s}{\otimes} \mathrm{B} \overset{s}{\otimes} \underline{n} \tag{B.4}$$

For an arbitrarily anisotropic matrix, an algorithm allowing to estimate the limit Equation B.4 is proposed in (Barthélémy, 2009) whereas in the isotropic case B writes

$$\mathrm{B} = B_{nn}\, \underline{n} \otimes \underline{n} + B_{mm}\, \underline{m} \otimes \underline{m} + B_{\ell\ell}\, \underline{\ell} \otimes \underline{\ell}$$

with

$$B_{nn} = \frac{8\,\eta\,(1-\nu^2)}{3\,E}\,\frac{1}{\mathcal{E}_\eta}$$
$$B_{mm} = \frac{8\,\eta\,(1-\nu^2)}{3\,E}\,\frac{1-\eta^2}{(1-(1-\nu)\,\eta^2)\;\mathcal{E}_\eta - \nu\,\eta^2\,\mathcal{K}_\eta}$$
$$B_{\ell\ell} = \frac{8\,\eta\,(1-\nu^2)}{3\,E}\,\frac{1-\eta^2}{(1-\nu-\eta^2)\,\mathcal{E}_\eta + \nu\,\eta^2\,\mathcal{K}_\eta}$$

where $\mathcal{K}_\eta = \mathcal{K}(\sqrt{1-\eta^2})$ and $\mathcal{E}_\eta = \mathcal{E}(\sqrt{1-\eta^2})$ are the complete elliptic integrals of respectively the first and second kind (see (Abramowitz and Stegun, 1972)). If the crack is circular, the components of B become

$$B_{nn} = \frac{16\,(1-\nu^2)}{3\,\pi\,E} \quad ; \quad B_{mm} = B_{\ell\ell} = \frac{B_{nn}}{1-\nu/2}$$

B.4 Application of Hill calculation

```
import numpy as np
from echoes import *
import matplotlib.pyplot as plt
```

B.4.1 Definition of the matrix tensor

```
C = stiff_Enu(1.,0.2) ; print(C)
```

```
Order 4 ISO tensor | Param(size=2)=[ 1.66667 0.833333 ] | Angles(size=0)=[ ]
[ 1.11111 0.277778 0.277778 0 0 0
  0.277778 1.11111 0.277778 0 0 0
  0.277778 0.277778 1.11111 0 0 0
  0 0 0 0.833333 0 0
  0 0 0 0 0.833333 0
  0 0 0 0 0 0.833333 ]
```

B.4.2 Calculation of the crack compliance $\mathbb{L} = \lim_{\omega\to 0}\omega\,\mathbb{Q}^{-1}$

Note that in *Echoes* it is necessary to provide an aspect ratio ω for the crack even if the crack compliance is actually calculated as a limit (not depending on ω)

```
ω = 1.e-4
L = crack_compliance(spheroidal(ω), C) ; print(L)
```

```
[[0.         0.         0.         0.         0.         0.        ]
 [0.         0.         0.         0.         0.         0.        ]
 [0.         0.         1.22230996 0.         0.         0.        ]
 [0.         0.         0.         0.67906109 0.         0.        ]
 [0.         0.         0.         0.         0.67906109 0.        ]
 [0.         0.         0.         0.         0.         0.        ]]
```

B.4.3 Checking the aspect ratio for which $\omega\,\mathbb{Q}^{-1} \approx \lim_{\omega\to 0} \omega\,\mathbb{Q}^{-1}$ is acceptable

```
tω = np.logspace(-5,1,20)
tabδ = []
for ω in tω:
    Q = hill_dual(spheroidal(ω), C)
    Lω = ω*np.linalg.inv(Q)
    δL = np.linalg.norm(Lω-L)/np.linalg.norm(L)
    tabδ.append(δL)
plt.figure(figsize=(8,3))
plt.loglog(tω,tabδ,'+-')
plt.xlabel(r"$\omega$")
plt.ylabel(r"$\frac{||\mathbb{L}-\omega\,\mathbb{Q}^{-1}||}{||\mathbb{L}||}$")
plt.grid(True,which='both')
plt.show()
```

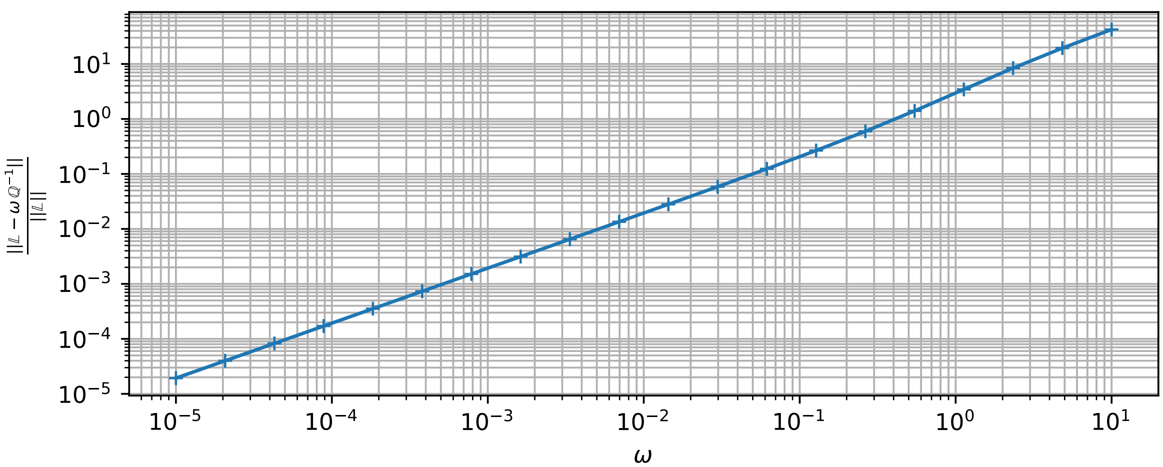

Figure B.2: Influence of the aspect ratio on the contribution tensor

C Hill polarization tensor in conductivity