

ECHOES

Extended Calculator of HOmogEnization Schemes

Jean-François Barthélémy

11/10/22

Table of contents

Welcome	4
Introduction	5
I Linear elasticity	6
1 Basic problem	7
2 Eshelby problem	8
3 Cracks	9
4 Morphologically representative patterns	10
5 Homogenization schemes	11
II Conductivity	12
6 Basic problem	13
7 Eshelby problem	14
8 Cracks	15
9 Morphologically representative patterns	16
10 Homogenization schemes	17
III Nonlinear homogenization	18
11 Second order moments	19
12 Differentiation of concentration tensors	20
13 Homogenization schemes	21

IV Viscoelasticity in frequency domain	22
14 Basic problem	23
15 Homogenization schemes	24
V Viscoelasticity in time domain	25
16 Basic problem	26
17 Homogenization schemes	27
VI Examples of implementation	28
18 Concrete strength	29
References	30
Appendices	30
A Tensor algebra	31
B Hill polarization tensor in elasticity	32
B.1 General expression	32
B.2 Isotropic matrix	32
B.3 Case of cracks	35
B.4 Application of Hill calculation	36
B.4.1 Definition of the matrix tensor	36
B.4.2 Calculation of the crack compliance $\mathbb{L} = \lim_{\omega \rightarrow 0} \omega \mathbb{Q}^{-1}$	36
B.4.3 Checking the aspect ratio for which $\omega \mathbb{Q}^{-1} \approx \lim_{\omega \rightarrow 0} \omega \mathbb{Q}^{-1}$ is acceptable	37
C Hill polarization tensor in conductivity	39

Welcome

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).

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.

Introduction

Part I

Linear elasticity

1 Basic problem

2 Eshelby problem

3 Cracks

4 Morphologically representative patterns

5 Homogenization schemes

Part II

Conductivity

6 Basic problem

7 Eshelby problem

8 Cracks

9 Morphologically representative patterns

10 Homogenization schemes

Part III

Nonlinear homogenization

11 Second order moments

12 Differentiation of concentration tensors

13 Homogenization schemes

Part IV

Viscoelasticity in frequency domain

14 Basic problem

15 Homogenization schemes

Part V

Viscoelasticity in time domain

16 Basic problem

17 Homogenization schemes

Part VI

Examples of implementation

18 Concrete strength

References

- Abramowitz, M., Stegun, I.A., 1972. Handbook of Mathematical Functions. National Bureau of Standards - Applied Mathematics Series - 55, Washington D.C.
- Barthélémy, J.-F., 2020. Simplified approach to the derivation of the relationship between Hill polarization tensors of transformed problems and applications. *International Journal of Engineering Science* 154, 103326. <https://doi.org/10.1016/j.ijengsci.2020.103326>
- Barthélémy, J.-F., 2009. Compliance and Hill polarization tensor of a crack in an anisotropic matrix. *International Journal of Solids and Structures* 46, 4064–4072. <https://doi.org/10.1016/j.ijsolstr.2009.08.003>
- Barthélémy, J.-F., Sevostianov, I., Giraud, A., 2021. Micromechanical modeling of a cracked elliptically orthotropic medium. *International Journal of Engineering Science* 161, 103454. <https://doi.org/10.1016/j.ijengsci.2021.103454>
- Eshelby, J.D., 1957. The determination of the elastic field of an ellipsoidal inclusion, and related problems. *Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences* 241, 376–396. <https://doi.org/10.1098/rspa.1957.0133>
- Gavazzi, A.C., Lagoudas, D.C., 1990. On the numerical evaluation of Eshelby's tensor and its application to elastoplastic fibrous composites. *Computational Mechanics* 7, 13–19. <https://doi.org/10.1007/BF00370053>
- Ghahremani, F., 1977. Numerical evaluation of the stresses and strains in ellipsoidal inclusions in an anisotropic elastic material. *Mechanics Research Communications* 4, 89–91. [https://doi.org/10.1016/0093-6413\(77\)90018-0](https://doi.org/10.1016/0093-6413(77)90018-0)
- Kellogg, O.D., 1929. Potential theory. Berlin : Springer-Verlag.
- Masson, R., 2008. New explicit expressions of the Hill polarization tensor for general anisotropic elastic solids. *International Journal of Solids and Structures* 45, 757–769. <https://doi.org/10.1016/j.ijsolstr.2007.08.035>
- Mura, T., 1987. *Micromechanics of Defects in Solids*, Second Edition. Kluwer Academic. <https://doi.org/10.1002/zamm.19890690204>
- Willis, J.R., 1977. Bounds and self-consistent estimates for the overall properties of anisotropic composites. *Journal of the Mechanics and Physics of Solids* 25, 185–202. [https://doi.org/10.1016/0022-5096\(77\)90022-9](https://doi.org/10.1016/0022-5096(77)90022-9)
- Withers, P.J., 1989. The determination of the elastic field of an ellipsoidal inclusion in a transversely isotropic medium, and its relevance to composite materials. *Philosophical Magazine A* 59, 759–781. <https://doi.org/10.1080/01418618908209819>

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}_A of equation

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

where A is an invertible second-order tensor so that ${}^t A \cdot A$ 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 $\underline{e}_1, \underline{e}_2, \underline{e}_3$)

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

B.1 General expression

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

$$\begin{aligned} \mathbb{P}(A, \mathbb{C}) &= \frac{1}{4\pi} \int_{\|\underline{\zeta}\|=1} (A^{-1} \cdot \underline{\zeta}) \overset{s}{\otimes} \left((A^{-1} \cdot \underline{\zeta}) \cdot \mathbb{C} \cdot (A^{-1} \cdot \underline{\zeta}) \right)^{-1} \overset{s}{\otimes} (A^{-1} \cdot \underline{\zeta}) dS_{\underline{\zeta}} \\ &= \frac{\det A}{4\pi} \int_{\|\underline{\xi}\|=1} \frac{\underline{\xi} \overset{s}{\otimes} (\underline{\xi} \cdot \mathbb{C} \cdot \underline{\xi})^{-1} \overset{s}{\otimes} \underline{\xi}}{\|A \cdot \underline{\xi}\|^3} dS_{\underline{\xi}} \end{aligned} \quad (\text{B.2})$$

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 $\mu = \frac{E}{2(1+\nu)}$.

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

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 \mathbf{A} of Equation B.1, are given by (see (Barthélemy, 2020))

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

and

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

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)

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

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

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

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

$$I_1 = I_2 = I_3 = \frac{1}{3}$$

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

In this last case of spherical inclusion ($A = 1$), \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

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

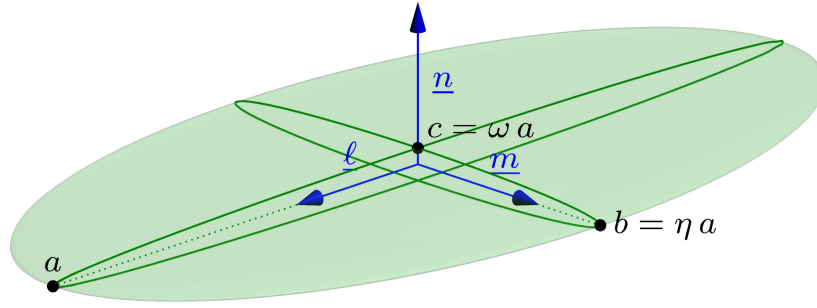


Figure B.1: Ellipsoidal crack

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 $\lim_{\omega \rightarrow 0} \omega \mathbb{Q}^{-1}$ 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

$$\mathbb{L} = \lim_{\omega \rightarrow 0} \omega \mathbb{Q}^{-1} = \frac{3}{4} \underline{n} \otimes \underline{n} B \otimes \underline{n} \otimes \underline{n} \quad (\text{B.4})$$

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

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

with

$$B_{nn} = \frac{8\eta(1-\nu^2)}{3E} \frac{1}{\mathcal{E}_\eta}$$

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

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

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 $\mathbb{L} = \lim_{\omega \rightarrow 0} \omega \mathbb{Q}^{-1}$

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 $\omega \mathbb{Q}^{-1} \approx \lim_{\omega \rightarrow 0} \omega \mathbb{Q}^{-1}$ is acceptable

```

tw = np.logspace(-5,1,20)
tabδ = []
for ω in tw:
    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(tw,tabδ,'+-')
plt.xlabel(r"$\omega$")
plt.ylabel(r"$\frac{||\mathbb{L}-\omega\mathbb{Q}^{-1}||}{||\mathbb{L}||}$")
plt.grid(True,which='both')
plt.show()

```

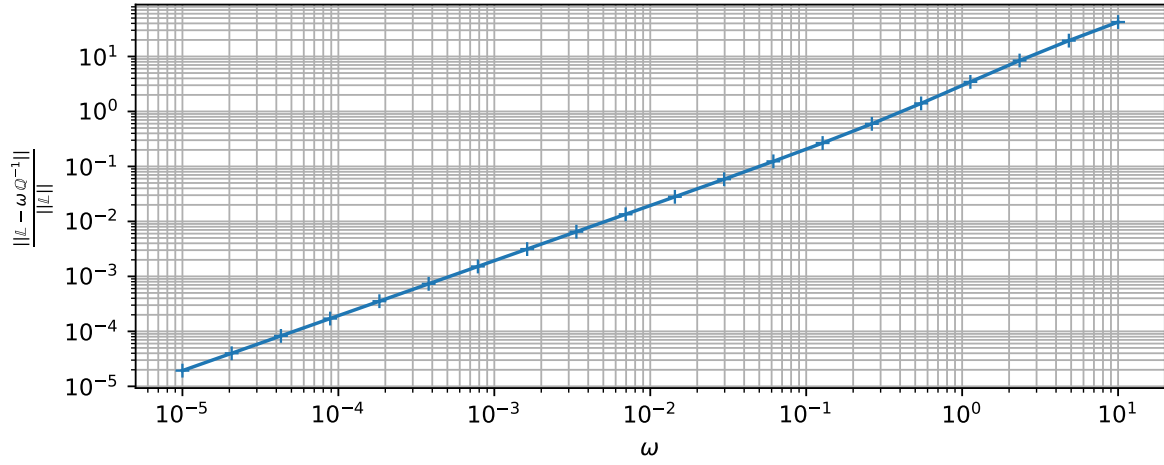


Figure B.2: Influence of the aspect ratio on the contribution tensor

C Hill polarization tensor in conductivity