Echoes

Extended Calculator of HOmogEnization Schemes

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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

This book does not aim at providing an exhaustive presentation of the theory of random medium homogeneization (see (Milton, 2002), (Torquato, 2002) or (Kachanov and Sevostianov, 2018) among others) but it is rather intended to recall some of the basic notations and results related to the implementation of the **Echoes** library.

Part I

Linear elasticity

1 Basic problem of elasticity homogenization

1.1 System of equations

Consider a representative volume element (RVE) Ω composed of a heterogeneous material. Neglecting body forces in a problem posed at the scale of a RVE is consistent with the fact that the order of magnitude of mechanical effects induced by body forces is in general much lower than that of the macroscopic strain E or stress Σ effects accounting for interactions with particles surrounding the RVE (see (Dormieux et al., 2006)). The hypothesis of quasi-static equilibrium is also invoked here to write the balance law involving the Cauchy stress field σ

$$\underline{\mathrm{div}}\,\sigma = \underline{0} \quad (\Omega) \tag{1.1}$$

In the sequel, the small perturbation hypothesis is adopted so that the strain field ε derives from the displacement one $\underline{u}$ as the symmetrical part of its gradient

$$\varepsilon = \frac{\mathrm{grad}\,\underline{u} + {}^t\mathrm{grad}\,\underline{u}}{2} \quad (\Omega) \tag{1.2}$$

In the framework of random media homogenization, two types of conditions applied at the boundary $\partial\Omega$ of a RVE Ω are usually considered:

- *homogeneous strain boundary conditions* corresponding to prescribed displacements $\underline{u}^g$ at $\partial\Omega$

$$\underline{u}^g = \mathrm{E}\cdot\underline{x} \quad (\partial\Omega) \tag{1.3}$$

  It is noticeable that in this case the divergence theorem implies the following relationship between the microscopic and macroscopic strain tensors

$$<\varepsilon>_\Omega = \frac{1}{|\Omega|}\int_\Omega \varepsilon\,\mathrm{d}\Omega = \frac{1}{|\Omega|}\int_{\partial\Omega} \underline{u}\overset{s}{\otimes}\underline{n}\,\mathrm{d}S = \mathrm{E} \tag{1.4}$$

  where the spatial average over a domain ω is denoted by $<\bullet>_\omega$ and $\underline{n}$ is the unit outward normal at the boundary. The macroscopic stress tensor is then simply defined as the average

$$\Sigma = <\sigma>_\Omega = \frac{1}{|\Omega|}\int_\Omega \sigma\,\mathrm{d}\Omega \tag{1.5}$$

- *homogeneous stress boundary conditions* corresponding to prescribed surface tractions $\underline{T}^g$ at $\partial\Omega$

$$\underline{T}^g = \Sigma \cdot \underline{n} \quad (\partial\Omega) \tag{1.6}$$

Now owing to the remarkable identity $(x_i\sigma_{jk})_{,k} = \sigma_{ij}$ resulting from (1.1) and the symmetry of σ, the relationship between the microscopic and macroscopic stress is ensured by the divergence theorem

$$< \sigma >_\Omega = \frac{1}{|\Omega|}\int_\Omega \sigma \,\mathrm{d}\Omega = \frac{1}{|\Omega|}\int_{\partial\Omega} \underline{x} \overset{s}{\otimes} (\sigma \cdot \underline{n})\,\mathrm{d}S = \Sigma \tag{1.7}$$

The macroscopic stress tensor is then simply defined as the average

$$\mathrm{E} = < \varepsilon >_\Omega = \frac{1}{|\Omega|}\int_\Omega \varepsilon \,\mathrm{d}\Omega \tag{1.8}$$

Hill lemma

Note that whatever the choice of boundary conditions between (1.3) and (1.6), the consistency between the microscopic and macroscopic works is ensured by

$$< \sigma : \varepsilon >_\Omega = \frac{1}{|\Omega|}\int_\Omega \sigma : \varepsilon \,\mathrm{d}\Omega = \frac{1}{|\Omega|}\int_{\partial\Omega} \underline{u} \cdot \sigma \cdot \underline{n}\,\mathrm{d}S = \Sigma : \mathrm{E} \tag{1.9}$$

which results from the application of the divergence theorem to $(u_i\sigma_{ij})_{,k} = u_{i,j}\sigma_{ij} = \varepsilon_{ij}\sigma_{ij}$.

The set of equations defining the problem posed on the RVE is finally completed by the local constitutive law relating the strain and stress fields. The hypothesis of linear elasticity is adopted in this part so that

$$\sigma = \mathbb{c} : \varepsilon \quad (\Omega) \tag{1.10}$$

where $\mathbb{c}(\underline{x})$ denotes the heterogeneous (positive definite fourth-order) stiffness tensor field satisfying the conditions of minor ($c_{jikl} = c_{ijlk} = c_{ijkl}$) and major ($c_{klij} = c_{ijkl}$) symmetries. The compliance tensor field is introduced as the inverse $\mathbb{s} = \mathbb{c}^{-1}$ in the sense of fourth-order tensors operating over symmetrical second-order tensors.

In short, the system of equations posed on the RVE is given by (1.1), (1.2), (1.3) or (1.6) and (1.10).

1.2 Macroscopic stiffness or compliance tensors

Whatever the boundary condition of homogeneous strain or stress type (1.3) or (1.6), the linearity of the problem allows to invoke the existence of concentration tensors relating the microscopic strain ε and stress σ fields to the macroscopic strain E or stress Σ tensors

$$\begin{aligned}
&\varepsilon = \mathbb{A}_E : \mathrm{E} \\
&\sigma = \mathbb{B}_E : \mathrm{E} \quad \text{with} \quad \mathbb{B}_E = \mathbb{c} : \mathbb{A}_E \\
&\sigma = \mathbb{B}_\Sigma : \Sigma \\
&\varepsilon = \mathbb{A}_\Sigma : \Sigma \quad \text{with} \quad \mathbb{A}_\Sigma = \mathbb{s} : \mathbb{B}_\Sigma
\end{aligned} \tag{1.11}$$

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A Tensor algebra

A.1 Conventions of tensor algebra

This appendix presents some conventions regarding tensor algebra in the usual three-dimensional euclidean space $E = \mathbb{R}^3$. In the sequel, tensor components are associated to an orthonormal frame $(\underline{e}_i)_{i=1,2,3}$ so that introducing the notion of tensor variance is useless here. The following presentation relies on the prior knowledge of the definition of tensors as multilinear operators and the classical isomorphism between the euclidean space and its dual through the scalar product

$$\begin{aligned} \phi : E &\longrightarrow E^* \\ \underline{v} &\longmapsto \underline{v} \cdot \bullet \end{aligned} \tag{A.1}$$

which allows to identify vectors and linear forms.

Consider two tensors $\mathcal{T}$ and $\mathcal{T}'$ of respective orders p and q. The tensor product $\mathcal{T} \otimes \mathcal{T}'$ is the $(p+q)$ order tensor decomposed as

$$\mathcal{T} \otimes \mathcal{T}' = \mathcal{T}_{i_1,\dots,i_p} \mathcal{T}'_{i_{p+1},\dots,i_{p+q}} \underline{e}_{i_1} \otimes \dots \otimes \underline{e}_{i_{p+q}} \tag{A.2}$$

where Einstein convention of immplicit summation over repeated indices is adopted and $\underline{e}_{i_1} \otimes \dots \otimes \underline{e}_{i_{p+q}}$ is the multilinear form such that[1]

$$(\underline{e}_{i_1} \otimes \dots \otimes \underline{e}_{i_{p+q}})(\underline{e}_{j_1}, \dots, \underline{e}_{j_{p+q}}) = \delta_{i_1,j_1} \dots \delta_{i_{p+q},j_{p+q}} \tag{A.3}$$

The notation $\mathcal{T} \overset{s}{\otimes} \mathcal{T}'$ indicates a tensor product followed by a symmetrization over the last index of $\mathcal{T}$ and the first of $\mathcal{T}'$, i.e.

$$\mathcal{T} \overset{s}{\otimes} \mathcal{T}' = \frac{\mathcal{T}_{i_1,\dots,i_p} \mathcal{T}'_{i_{p+1},\dots,i_{p+q}} + \mathcal{T}_{i_1,\dots,i_{p+1}} \mathcal{T}'_{i_p,\dots,i_{p+q}}}{2} \underline{e}_{i_1} \otimes \dots \otimes \underline{e}_{i_{p+q}} \tag{A.4}$$

It follows that

$$\underline{u} \overset{s}{\otimes} \underline{v} = \frac{\underline{u} \otimes \underline{v} + \underline{v} \otimes \underline{u}}{2} \tag{A.5}$$

and an example of generalization involving a second-order tensor a and vectors $\underline{u}$ and $\underline{v}$

$$\underline{u} \overset{s}{\otimes} \mathrm{a} \overset{s}{\otimes} \underline{v} = \frac{u_i\, a_{jk}\, v_l + u_i\, a_{jl}\, v_k + u_j\, a_{ik}\, v_l + u_j\, a_{il}\, v_k}{4} \underline{e}_i \otimes \underline{e}_j \otimes \underline{e}_k \otimes \underline{e}_l \tag{A.6}$$

[1] $\delta_{ij} = 1$ if $i = j$ and 0 if $i \neq j$ (Kronecker symbol)

The simple dot product or contracted product between $\mathcal{T}$ and $\mathcal{T}'$ involves by convention a contraction between the last index of $\mathcal{T}$ and the first of $\mathcal{T}'$, which leads to the $(p+q-2)$ order tensor

$$\mathcal{T} \cdot \mathcal{T}' = \mathcal{T}_{i_1,\dots,i_{p-1},k}\, \mathcal{T}'_{k,i_p,\dots,i_{p+q-2}}\, \underline{e}_{i_1} \otimes \dots \otimes \underline{e}_{i_{p+q-2}} \tag{A.7}$$

As regards the double dot product, the classical convention consists in consuming the indices going up from the extremities, which means that a first contraction acts as in the simple dot product then a second contraction is performed between the penultimate index of $\mathcal{T}$ and the second one of $\mathcal{T}'$. However and alternate convention adopted here is proposed in (Brisard, 2014)[2], which somehow consists in considering that the double contraction operates over the two last indices of $\mathcal{T}$ as a pair and the two first indices of $\mathcal{T}'$ as the corresponding pair. In other words, this operation is such that if a and b are two second-order tensors and $\mathbb{T}$ is a fourth-order tensor

$$\mathrm{a} : \mathrm{b} = a_{ij} b_{ij} \quad \text{and} \quad \mathbb{T} : \mathrm{a} = T_{ijkl}\, a_{kl}\, \underline{e}_i \otimes \underline{e}_j \tag{A.8}$$

and the transpose tensor ${}^t\mathbb{T}$ is consistently defined by

$${}^t\mathbb{T} : \mathrm{a} = \mathrm{a} : \mathbb{T} \quad \Leftrightarrow \quad \left({}^t\mathbb{T}\right)_{ijkl} = \left(\mathbb{T}\right)_{klij} \tag{A.9}$$

Another useful operator introduced in (Brisard, 2014) is the modified tensor product denoted by $\boxtimes$. The fourth-order tensor $\mathrm{a} \boxtimes \mathrm{b}$ (where a and b are two second-order tensors) is defined by its operation over any second-order tensor p and by its components

$$\begin{aligned} (\mathrm{a} \boxtimes \mathrm{b}) : \mathrm{p} &= \mathrm{a} \cdot \mathrm{p} \cdot {}^t\mathrm{b} = a_{ik}\, p_{kl}\, b_{jl}\, \underline{e}_i \otimes \underline{e}_j \\ (\mathrm{a} \boxtimes \mathrm{b})_{ijkl} &= a_{ik}\, b_{jl} \end{aligned} \tag{A.10}$$

A symmetrized version of $\boxtimes$ denoted by $\overset{s}{\boxtimes}$ can also be introduced. It operates as

$$\begin{aligned} (\mathrm{a} \overset{s}{\boxtimes} \mathrm{b}) : \mathrm{p} &= (\mathrm{a} \boxtimes \mathrm{b}) : \left(\frac{\mathrm{p} + {}^t\mathrm{p}}{2}\right) = \mathrm{a} \cdot \left(\frac{\mathrm{p} + {}^t\mathrm{p}}{2}\right) \cdot {}^t\mathrm{b} \\ (\mathrm{a} \overset{s}{\boxtimes} \mathrm{b})_{ijkl} &= \frac{a_{ik}\, b_{jl} + a_{il}\, b_{jk}}{2} \end{aligned} \tag{A.11}$$

It follows from these definitions that the fourth-order identity, as an operator over second-order tensors, writes $\mathbb{1} = 1 \boxtimes 1$ where 1 is the second-order identity. The fourth-order operator allowing to extract the symmetric part of a second-order tensor writes $\mathbb{I} = 1 \overset{s}{\boxtimes} 1$. The latter tensor, which obviously complies with the conditions of minor symmetries, is classically used to play the role of fourth-order identity operating over symmetric second-order tensors.

[2] see https://sbrisard.github.io/posts/20140219-on_the_double_dot_product.html

Some remarkable relationships result from the previous definitions

$$
\begin{aligned}
&(\mathrm{a} \boxtimes \mathrm{b}) : (\underline{u} \otimes \underline{v}) = (\mathrm{a} \cdot \underline{u}) \otimes (\mathrm{b} \cdot \underline{v}) && (a)\\
&(\mathrm{a} \boxtimes \mathrm{b}) : (\mathrm{c} \boxtimes \mathrm{d}) = (\mathrm{a} \cdot \mathrm{c}) \boxtimes (\mathrm{b} \cdot \mathrm{d}) && (b)\\
&(\mathrm{a} \overset{s}{\boxtimes} \mathrm{b}) : (\mathrm{c} \overset{s}{\boxtimes} \mathrm{d}) = \frac{(\mathrm{a} \cdot \mathrm{c}) \overset{s}{\boxtimes} (\mathrm{b} \cdot \mathrm{d}) + (\mathrm{a} \cdot \mathrm{d}) \overset{s}{\boxtimes} (\mathrm{b} \cdot \mathrm{c})}{2} && (c)\\
&(\mathrm{a} \overset{s}{\boxtimes} \mathrm{a}) : (\mathrm{b} \overset{s}{\boxtimes} \mathrm{b}) = (\mathrm{a} \cdot \mathrm{b}) \overset{s}{\boxtimes} (\mathrm{a} \cdot \mathrm{b}) && (d)\\
&{}^t(\mathrm{a} \boxtimes \mathrm{b}) = {}^t\mathrm{a} \boxtimes {}^t\mathrm{b} && (e)\\
&{}^t(\mathrm{a} \overset{s}{\boxtimes} \mathrm{a}) = {}^t\mathrm{a} \overset{s}{\boxtimes} {}^t\mathrm{a} \;\text{ but }\; {}^t(\mathrm{a} \overset{s}{\boxtimes} \mathrm{b}) \neq {}^t\mathrm{a} \overset{s}{\boxtimes} {}^t\mathrm{b} && (f)\\
&(\mathrm{a} \boxtimes \mathrm{b})^{-1} = \mathrm{a}^{-1} \boxtimes \mathrm{b}^{-1} && (g)\\
&(\mathrm{a} \overset{s}{\boxtimes} \mathrm{a})^{-1} : \mathrm{p} = (\mathrm{a}^{-1} \overset{s}{\boxtimes} \mathrm{a}^{-1}) : \mathrm{p} \;\text{ if }\; {}^t\mathrm{p} = \mathrm{p} \;\text{ but }\; (\mathrm{a} \overset{s}{\boxtimes} \mathrm{b})^{-1} \neq \mathrm{a}^{-1} \overset{s}{\boxtimes} \mathrm{b}^{-1} && (h)
\end{aligned}
\tag{A.12}
$$

A.2 Kelvin-Mandel convention

The Kelvin-Mandel convention allows to write the matrix of a symmetric second-order tensor in a given orthonormal frame $(\underline{e}_i)_{i=1,2,3}$ under the form of a vector of $\mathbb{R}^6$

$$
\mathrm{Mat}(\varepsilon, (\underline{e}_i)) = \begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{31} \\ \varepsilon_{12} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{23} & \varepsilon_{33} \end{pmatrix} \mapsto \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \sqrt{2}\,\varepsilon_{23} \\ \sqrt{2}\,\varepsilon_{31} \\ \sqrt{2}\,\varepsilon_{12} \end{pmatrix} \tag{A.13}
$$

The vector of $\mathbb{R}^6$ in (A.13) corresponds to the components of the second-order tensor ε in the basis ordered as

$$
\mathcal{B} = \left(\underline{e}_1 \otimes \underline{e}_1, \underline{e}_2 \otimes \underline{e}_2, \underline{e}_3 \otimes \underline{e}_3, \sqrt{2}\,\underline{e}_2 \otimes \underline{e}_3, \sqrt{2}\,\underline{e}_3 \otimes \underline{e}_1, \sqrt{2}\,\underline{e}_1 \otimes \underline{e}_2\right) \tag{A.14}
$$

The tensors of the basis (A.14) form an orthonormal frame spanning the space of symmetric second-order tensors equipped with the double contraction ":" as scalar product. It follows that the double contraction between symmetric second-order tensors is no other than the classical scalar product of the corresponding vectors of $\mathbb{R}^6$ written according to the convention (A.13).

Moreover a fourth-order tensor with minor symetries ($C_{ijkl} = C_{jikl} = C_{ijlk}$), which can be seen as a linear operator acting over symmetric second-order tensors by double contraction, writes in the same convention under the form of a 6×6 square matrix (the solid lines separate blocks affected by different factors whereas the colored components highlight a central block playing a major role in the sequel)

$$
\mathrm{Mat}(\mathbb{C},\mathcal{B}) = \left(\begin{array}{ccc|ccc}
C_{1111} & C_{1122} & C_{1133} & \sqrt{2}\,C_{1123} & \sqrt{2}\,C_{1131} & \sqrt{2}\,C_{1112} \\
C_{2211} & C_{2222} & C_{2233} & \sqrt{2}\,C_{2223} & \sqrt{2}\,C_{2231} & \sqrt{2}\,C_{2212} \\
C_{3311} & C_{3322} & \color{red}{C_{3333}} & \color{red}{\sqrt{2}\,C_{3323}} & \color{red}{\sqrt{2}\,C_{3331}} & \sqrt{2}\,C_{3312} \\
\hline
\sqrt{2}\,C_{2311} & \sqrt{2}\,C_{2322} & \color{red}{\sqrt{2}\,C_{2333}} & \color{red}{2\,C_{2323}} & \color{red}{2\,C_{2331}} & 2\,C_{2312} \\
\sqrt{2}\,C_{3111} & \sqrt{2}\,C_{3122} & \color{red}{\sqrt{2}\,C_{3133}} & \color{red}{2\,C_{3123}} & \color{red}{2\,C_{3131}} & 2\,C_{3112} \\
\sqrt{2}\,C_{1211} & \sqrt{2}\,C_{1222} & \sqrt{2}\,C_{1233} & 2\,C_{1223} & 2\,C_{1231} & 2\,C_{1212}
\end{array}\right) \tag{A.15}
$$

The result of $\mathbb{C} : \varepsilon$ writes as a classical matrix-vector product of (A.15) by (A.13).

However another way of ordering the tensors of (A.14) which proves useful for the calculation of crack compliance is based on a gathering of one set of three in-plane and another one of three out-of-plane tensors (the latter involving $\underline{n} = \underline{e}_3$ assumed to be the normal of the crack and the former not)

$$
\mathcal{B}^* = \Bigg(\underbrace{\underline{e}_1 \otimes \underline{e}_1, \underline{e}_2 \otimes \underline{e}_2, \sqrt{2}\,\underline{e}_1 \overset{s}{\otimes} \underline{e}_2,}_{\text{in-plane}} \quad \underbrace{\underline{e}_3 \otimes \underline{e}_3, \sqrt{2}\,\underline{e}_2 \overset{s}{\otimes} \underline{e}_3, \sqrt{2}\,\underline{e}_3 \overset{s}{\otimes} \underline{e}_1}_{\text{out-of-plane}} \Bigg) \tag{A.16}
$$

such that the matrix of $\mathbb{C}$ in $\mathcal{B}^*$ is now obtained by permutations of lines and columns of (A.15) to give

$$
\mathrm{Mat}(\mathbb{C},\mathcal{B}^*) = \left(\begin{array}{ccc|ccc}
C_{1111} & C_{1122} & \sqrt{2}\,C_{1112} & C_{1133} & \sqrt{2}\,C_{1123} & \sqrt{2}\,C_{1131} \\
C_{2211} & C_{2222} & \sqrt{2}\,C_{2212} & C_{2233} & \sqrt{2}\,C_{2223} & \sqrt{2}\,C_{2231} \\
\sqrt{2}\,C_{1211} & \sqrt{2}\,C_{1222} & 2\,C_{1212} & \sqrt{2}\,C_{1233} & 2\,C_{1223} & 2\,C_{1231} \\
\hline
C_{3311} & C_{3322} & \sqrt{2}\,C_{3312} & C_{3333} & \sqrt{2}\,C_{3323} & \sqrt{2}\,C_{3331} \\
\sqrt{2}\,C_{2311} & \sqrt{2}\,C_{2322} & 2\,C_{2312} & \sqrt{2}\,C_{2333} & 2\,C_{2323} & 2\,C_{2331} \\
\sqrt{2}\,C_{3111} & \sqrt{2}\,C_{3122} & 2\,C_{3112} & \sqrt{2}\,C_{3133} & 2\,C_{3123} & 2\,C_{3131}
\end{array}\right) \tag{A.17}
$$

One may notice that the bottom right 3×3 block of (A.17) exactly corresponds to the colored block in (A.15).

A.3 Walpole basis

The Walpole basis (Walpole, 1984) allowing to write any fourth-order transversely isotropic relatively to a an axis oriented by the unit vector $\underline{n}$ is composed of the six following tensors built from $1_n = \underline{n} \otimes \underline{n}$ and $1_T = 1 - 1_n$

$$
\begin{aligned}
&\mathbb{E}_1 = 1_n \otimes 1_n \quad ; \quad \mathbb{E}_2 = \frac{1_T \otimes 1_T}{2} \quad ; \mathbb{E}_3 = \frac{1_n \otimes 1_T}{\sqrt{2}} \quad ; \quad \mathbb{E}_4 = \frac{1_T \otimes 1_n}{\sqrt{2}} \quad (a) \\
&\mathbb{E}_5 = 1_T \overset{s}{\boxtimes} 1_T - \frac{1_T \otimes 1_T}{2} \qquad\qquad ; \mathbb{E}_6 = 1_T \overset{s}{\boxtimes} 1_n + 1_n \overset{s}{\boxtimes} 1_T \qquad\qquad (b)
\end{aligned} \tag{A.18}
$$

Any transversely isotropic fourth-order tensor can be decomposed as

$$\mathbb{L} = \ell_1\,\mathbb{E}_1 + \ell_2\,\mathbb{E}_2 + \ell_3\,\mathbb{E}_3 + \ell_4\,\mathbb{E}_4 + \ell_5\,\mathbb{E}_5 + \ell_6\,\mathbb{E}_6 \tag{A.19}$$

The six parameters can be conveniently gathered in a triplet composed of a 2×2 matrix containing the four first parameters ℓ_i $(1 \leq i \leq 4)$ and the two last parameters ℓ_5 and ℓ_6

$$\mathbb{L} \equiv (L, \ell_5, \ell_6)\,, \quad L = \begin{pmatrix} \ell_1 & \ell_3 \\ \ell_4 & \ell_2 \end{pmatrix} \tag{A.20}$$

Such a synthetic notation allows simple calculations of products and inverses which consist in classical matrix or scalar products and inverses

$$\begin{aligned} &\mathbb{L} : \mathbb{M} \equiv (LM, \ell_5 m_5, \ell_6 m_6) && (a) \\ &\mathbb{L}^{-1} \equiv \left(L^{-1}, \frac{1}{\ell_5}, \frac{1}{\ell_6}\right) && (b) \end{aligned} \tag{A.21}$$

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 (B.3) in (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 (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 (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 (B.1) can be written here

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

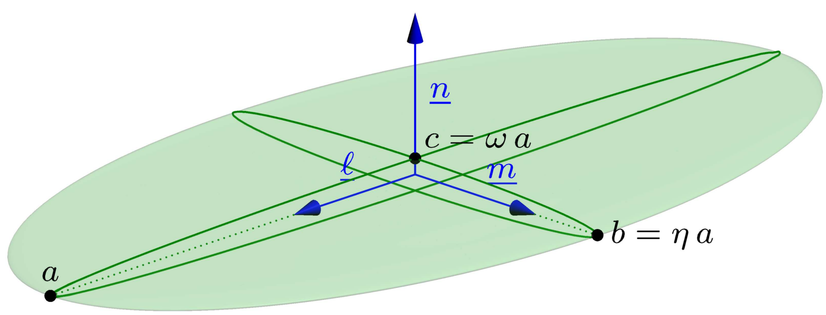

Figure B.1: Ellipsoidal crack

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 arbitrarly anisotropic matrix, an algorithm allowing to estimate the limit (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)

```python
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

```python
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()
```

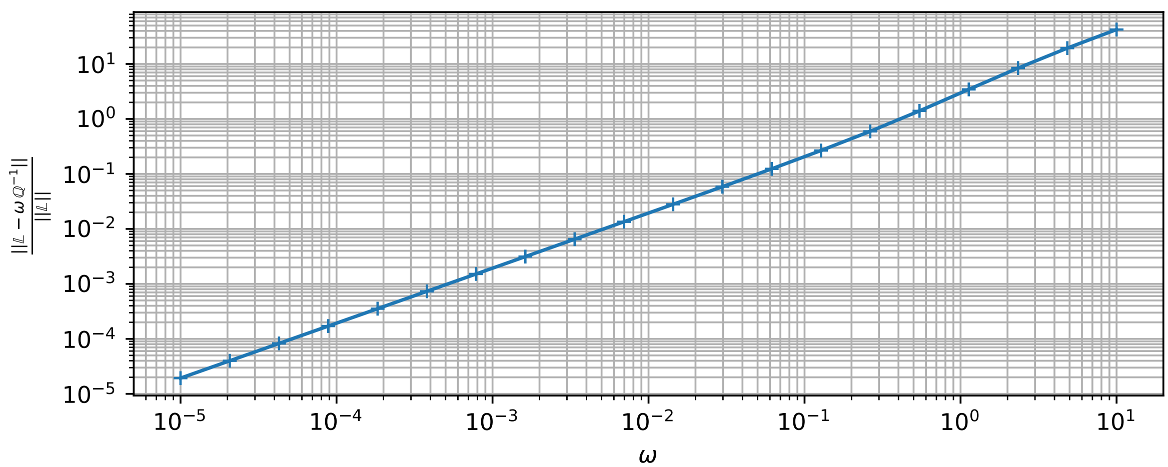

Figure B.2: Influence of the aspect ratio on the contribution tensor

C Hill polarization tensor in conductivity