COMPUTATION OF BOUNDS ELASTIC PROPERTIES OF POLYCRYSTALS BASED ON FAST FOURIER TRANSFORM METHOD

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Abstract
The present paper derives numerical bounds of the elastic properties of polycrystals. The homogenized elastic coefficients are computed from Voronoi-type unit cells. The main result of the article determines the upper and lower bounds for a case of polycrystals made up of cubic single crystals by using the fast Fourier transform method (FFT) based on the shape function. Our method guarantees the exact solutions in comparison to the Moulinec and Suquet’s method within some uncontrolled approximations. The proposed method could be extended to account for other material symmetries such as hexagonal or tetragonal crystals.

Keywords: Elastic coefficients; numerical bounds; shape functions; polycrystals; Voronoi; fast Fourier transform.

1. Introduction
An alternative approach to Finite Element Method (FEM) has been proposed in the middle of the nineties by Moulinec and Suquet [1] for the computation of the effective properties of linear elastic periodic composites. The unit cell problem is solved by means of an iterative scheme which uses the periodic Green’s tensor for the strain and could be directly applied to digital images which come from microstructure. The main advantages of this approach over the FEM is that it does not require the introduction of a “high dimension” stiffness matrix. The FFT methods only need the storage of tables whose dimensions are the number of DoF (the FEM requires the storage of the rigidity matrix whose dimension is the square of the DoF). The memory needed for solving the unit cell problem with FFT methods is then significantly reduced. The FFT method allows to expand the solution of the Lippmann-Schwinger equation into Neumann series, along the lines of a method which was first introduced for composite conductors by Brown [2] and later by Kroner [3]. The convergence of the method has been largely studied in the literature particularly for the problems with high contrasts between the phase elastic properties. Other formulation has been then provided to improve the convergence: the (dual) stress based formulation in [4, 5] and the accelerated schemes in [6, 7, 8]. Accelerated schemes are not considered in the present study since the contrast in

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polycrystal is sufficiently low to use the basic strain and stress based iterative schemes. An alternative approach based on the shape functions has been developed by Bonnet [5] to improve the FFT solutions. The close-form expressions of the shape functions are available for inclusions having ellipsoidal shapes in the book of Nemat-Nasser [9], for instance. Later, in [10], it has been proved that the use of the shape functions in the FFT-based iterative schemes provides rigorous bounds of the effective elastic properties of the composites. More precisely, the strain and stress based FFT solutions deliver an upper and lower bound respectively. The lower and upper bounds of the homogenized elastic coefficients are computed by means of the FFT method combined with the use of the shape functions. The microstructure of the polycrystal is generated by Voronoi tessellations. The polycrystal is constituted of single crystal which are polygons (for 2D problems) and polyhedrons (for 3D ones). The shape functions of the polygons and polyhedrons have been recently provided in [11].

2. Derivation of bounds with FFT schemes

2.1. The cell problem for linear elastic composites with prescribed macroscopic strain or stress

We consider a heterogeneous elastic material defined by a parallelepipedic unit cell and three (two for plane strain or plane stress problems) vectors of translation invariance. The unit cell is made up of M phases whose elastic tensor (resp. compliance) is denoted by $\mathbb{C}_\alpha$ (resp. $\mathbb{S}_\alpha = (\mathbb{C}_\alpha)^{-1}$) for $\alpha = 1\ldots M$. At local scale, the compatibility equations, linear elastic constitutive equations, equilibrium and periodic conditions at the boundary of the idealized unit cell can be summered as follows:

$$
\begin{align}
\varepsilon(x) &= \frac{1}{2} (\nabla u(x) + \nabla^t u(x)), \forall x \in V \\
\sigma(x) &= \mathbb{C}(x) : \varepsilon(x), \forall x \in V \\
div(\sigma(x)) &= 0, \forall x \in V \\
u(x) - E\hat{x} &\quad \text{periodic} \\
\sigma(x).\hat{n} &\quad \text{antiperiodic}
\end{align}
$$

in which the stiffness tensor $\mathbb{C}(x)$ (resp. the compliance) of the heterogeneous medium is given by:

$$
\mathbb{C}(x) = \sum_{\alpha} I^\alpha(x) \mathbb{C}^\alpha, \quad \mathbb{S}(x) = \sum_{\alpha} I^\alpha(x) \mathbb{S}^\alpha
$$

with

$$
I^\alpha(x) = \begin{cases} 
1 & \text{if } x \in V^\alpha \\
0 & \text{if } x \in V - V^\alpha
\end{cases}
$$
\( I^\alpha(x) \) for \( \alpha = 1 \ldots M \) are the characteristic functions describing volumes \( V^\alpha \) which comply with \( \sum_\alpha I^\alpha(x) = 1 \). Prescribed macroscopic strain \( E = \langle \varepsilon \rangle_V \) or macroscopic stress \( \Sigma = \langle \sigma \rangle_V \) are classically considered (the brackets denote the volume average over \( V \)). Variational principles based on the macroscopic elastic energy are now considered to determine a lower and an upper bound for the effective elastic coefficients of the composites. Let us introduce the strain elastic energy \( U(\varepsilon(u)) \) and the complementary elastic potential \( W(\sigma) \) by:

\[
U(\varepsilon(u)) = \frac{1}{2} \langle \varepsilon(u) : C : \varepsilon(u) \rangle_V, \quad W(\sigma) = \frac{1}{2} \langle \sigma : S : \sigma \rangle_V
\]

(3)

Since the elastic tensors \( C \) and \( S \) are positive definite, the following energy minimization principles hold for any kinematically admissible displacement \( u^* \) and statically admissible stress field \( \sigma^* \) (see for instance [12]):

\[
\frac{1}{2} E : \mathbb{C}^{\text{hom}} : E \leq U(\varepsilon(u^*)) \tag{4}
\]

\[
\frac{1}{2} \Sigma : \mathbb{S}^{\text{hom}} : \Sigma \leq W(\sigma^*) \tag{5}
\]

2.2. Discretization with Fourier series

Due to the periodicity, the strain and stress fields are expanded into Fourier series. The expansion in Fourier series of any real quantity \( f \) is denoted by:

\[
f(x) = \sum_{n=-N}^{n=N-1} \hat{f}(\xi_n) \exp(i \xi_n \cdot x), \quad \hat{f}(\xi) = \langle f(x) \exp(-i \xi \cdot x) \rangle_V
\]

(6)

where \( \xi_n \) denotes the discrete wave vectors given by:

\[
\xi_n = 2\pi n \zeta, \quad n = -N \ldots N - 1, \quad \zeta = \frac{1}{L_i}
\]

(7)

and \( L_1, L_2, L_3 \) are the half of the cell along the three space directions \( x_1, x_2, \) and \( x_3 \). Obviously, the problem is discretized along each space direction, this would involve the use of two indexes \( n_1 \) and \( n_2 \) for 2-D problems and three for 3-D ones. For simplicity, we shall use the notation \( \hat{f}_n \), the Fourier transform of \( f \) associated with the wave vector \( \xi_n \). Particularly, the Fourier component corresponding to \( n = 0 \) of the quantity \( \hat{f} \) represents its average over the volume of the cell, \( \hat{f}_0 = \langle f(x) \rangle_V \). Then, the
quantity $\hat{\varepsilon}_n = E$ is known when the macroscopic strain $E$ is prescribed to the unit cell. In this case, the macroscopic stress is $\Sigma = \hat{\sigma}_n$ that is determined by the resolution of the unit cell problem. The homogenized elasticity tensor is determined such that $\Sigma = C^{\text{hom}} : E$. Alternatively, when the macroscopic stress is applied, the macroscopic strain has to be determined.

In the next section, classic variational principles are considered to obtain elementary bounds for the macroscopic elastic energy. These variational principles are based on the consideration of admissible subsets made up of compatible fields for the strain, and equilibrated fields for the stress. These admissibility conditions can be formulated by mean of two suitable projection operators $P_n$ and $Q_n$, defined for every $\xi_n \neq 0$ by:

$$Q_n = E_1(\xi_n) + E_3(\xi_n), \quad P_n = E_2(\xi_n) + E_4(\xi_n)$$

in which the $E_i(\xi_n)$ for $i = 1...4$ are the first four tensors of the Walpole basis [14]. Let us recall the six tensors of this basis: $E$

$$
\begin{align*}
E_1(\xi) &= \frac{1}{3} Q(\xi) \otimes Q(\xi), \\
E_2(\xi) &= P(\xi) \otimes P(\xi) \\
E_3(\xi) &= Q(\xi) \bar{Q}(\xi) - E_1(\xi), \\
E_4(\xi) &= Q(\xi) \bar{P}(\xi) + P(\xi) \bar{Q}(\xi) \\
E_5(\xi) &= P(\xi) \otimes Q(\xi), \\
E_6(\xi) &= Q(\xi) \otimes P(\xi)
\end{align*}
$$

where $P$ and $Q$ are given by:

$$P(\xi) = \frac{1}{|\xi|^2} \xi \otimes \xi, \quad Q(\xi) = I - P(\xi)$$

and $I$ is the second order identity tensor. As already shown in [8], the strain field is compatible if its Fourier coefficients $\hat{\varepsilon}_n$ comply with

$$\forall n \neq 0, \quad Q_n : \hat{\varepsilon}_n = 0$$

Alternatively, the equilibrium for the stress field leads to the following condition for its Fourier coefficients $\hat{\sigma}_n$:

$$\forall n \neq 0, \quad P_n : \hat{\sigma}_n = 0$$

With these notations, the subset of kinematical and statical admissible fields, denoted $E_N$ and $S_N$ respectively, are defined by:
Using the variational principles (4) and (5), two estimates for the effective elastic properties can be deduced from:

\[ \frac{1}{2} E : C^{\text{hom}} : E \leq \frac{1}{2} E : C_N^\varepsilon : E = \min_{\varepsilon \in \mathcal{E}} U(\varepsilon) \] \[ \frac{1}{2} \Sigma : S^{\text{hom}} : \Sigma \leq \frac{1}{2} \Sigma : S_N^\sigma : \Sigma = \min_{\sigma \in \mathcal{S}} W(\sigma) \]  

\( C_N^\varepsilon \) and \( S_N^\sigma \) are two estimates of the homogenized elastic tensor in which the index \( N \) refers to the dimension of the subset of admissible fields for the strain and the stress.

From the second equation in (13) we see that: \( (S_N^\sigma)^{-1} \leq (S_N^{\text{hom}})^{-1} \)

Classically, the following inequality is deduced for the elasticity tensors:

\[ C_N^\sigma \leq (S_N^{\text{hom}})^{-1} = C_N^{\text{hom}} \leq C_N^\varepsilon \]  

with the notation \( C_N^\sigma = (S_N^\sigma)^{-1} \).

2.3. Derivation of bounds elastic properties with FFT

The stationary point of \( U \) with respect to \( \hat{\varepsilon}_n \) can be determined by means of a FFT based iterative scheme which uses the shape functions. The terminology “shape function” will be more explained in the next section. The details of the minimization procedure can be found in [10]. The following recurrence relation is then used to compute the Fourier components of the strain field:

\[ (\hat{\varepsilon}_n)^{i+1} = (\hat{\varepsilon}_n)^i - \Gamma_n^0 : \left[ \sum_{\alpha=1}^{\alpha=p} C^\alpha : (\hat{\varepsilon}_n^\alpha)^i \right] \]  

which starts with \( \hat{\varepsilon}_n = 0 \) for \( n \neq 0 \) and \( \hat{\varepsilon}_0 = E \). In Eq. (15), \( \Gamma_n^0 \) are the Fourier coefficients of the Green tensor associated to the reference material of rigidity \( C^0 \). The fourth order tensor \( \Gamma^0 \) is the Green operator for the strain. Its components depend on the wave vectors and the elastic coefficients of a reference material \( C^0 \). The reference material is chosen in order to provide the better rate of convergence of the iterative scheme. The method for its determination has been well documented in the literature.
and is not detailed here (the reader could refer to [7, 12, 8] for more details on these issues). Considering an isotropic elastic reference material, the Green operator can be decomposed along the Walpole basis:

\[
\forall n \neq 0, \hat{\Gamma}_n^0 = \frac{1}{\lambda_0 + 2\mu_0} \mathbb{E}_2 \left( \xi_n \right) + \frac{1}{2\mu_0} \mathbb{E}_4 \left( \xi_n \right) \quad (16)
\]

and \( \hat{\Gamma}_n^0 = 0 \) for \( n = 0 \). In Eq. (16), \( \lambda_0 \) and \( \mu_0 \) are the Lamé coefficients of the reference medium. In Eq. (15), \( \varepsilon_\alpha \) represents the product between the strain and the characteristic function \( I^\alpha (x) \) of the phase \( V^\alpha \):

\[
\varepsilon_\alpha (x) = I^\alpha (x) \varepsilon(x) \quad (17)
\]

and \( \hat{\varepsilon}_n^\alpha \) are its Fourier coefficient. The exact expressions of \( \hat{\varepsilon}_n^\alpha \) for \( \alpha = 1…M \) is then computed by the discrete convolution product between the Fourier components of the strain and the Fourier components of the characteristic functions \( I^\alpha (x) \):

\[
\hat{\varepsilon}_n^\alpha = \sum_{m=-N}^{m=N-1} \hat{I}^\alpha (\xi_n - \xi_m) \hat{\varepsilon}_m \quad \hat{\sigma}_n^\alpha = \sum_{m=-N}^{m=N-1} \hat{I}^\alpha (\xi_n - \xi_m) \hat{\sigma}_m \quad (18)
\]

Since \( n \) and \( m \) vary from \(-N\) to \(-1\), \( n - m \) vary from \(-2N\) to \(2N - 2\). It follows that in Eq. (18), \( \hat{I}^\alpha_n (\xi_n - \xi_m) \) must be computed on a double grid (dimension is \( 4N \times 4N \)) while the coefficients \( \hat{\varepsilon}_m \) are computed on the simple grid (dimension is \( 2N \times 2N \)). The components \( \hat{I}^\alpha_n (\xi_n) \) must be computed before the iteration process and stored. The procedure is computationally more expensive than in [1] because the convolution product is made on the double grid while the former method uses a representation of the elasticity tensor on the simple grid. However, the representation on the double grid is necessary to compute exactly the discrete convolution product and then to ensure the bound character of the solutions. Moreover, the method accounts for the real geometry of the cell when exact Fourier coefficients of the characteristic function are used while the product between the elastic tensor with the strain is made with the approximation:

\[
\hat{\varepsilon}_n^\alpha \approx FFT \left[ I^\alpha (x_n) FFT^{-1} (\hat{\varepsilon}_n) \right] \quad (19)
\]

in which \( I^\alpha (x_n) \) are the values of \( I^\alpha (x) \) computed at the nodes of a regular grid in the real space. The shape functions account for the real geometry of the unit cell when the exact expressions of these functions could be derived. The lower bound for the elastic tensor is computed with the stress based iterative scheme. This scheme has been formulated by using [4, 5]:
\[
(\hat{\sigma}_n)^{i+1} = (\hat{\sigma}_n)^i - \Delta_n^0 : \left[ \sum_{\alpha=1}^{a=p} S^\alpha : (\hat{\sigma}_n)^i \right]
\]  
(20)

which is initialized with \( \hat{\sigma}_n = 0 \) for any \( n \neq 0 \) and \( \hat{\sigma}_0 = \Sigma \). In Eq. (20), \( \hat{\lambda}_n^0 \) are the Fourier coefficients of the Green tensor for the stress, defined by:

\[
\hat{\lambda}_n^0 = \mathbb{C}^0 - \mathbb{C}^0 : \hat{\mathbf{f}}_n : \mathbb{C}^0 = \frac{2 \mu_0(3\lambda_0 + 2\mu_0)}{\lambda_0 + 2\mu_0} \mathbb{E}_0 (\hat{\xi}_n) + 2\mu_0 \mathbb{E}_0 (\hat{\xi}_n)
\]  
(21)

for \( n \neq 0 \) and \( \hat{\lambda}_n^0 = 0 \) for \( n = 0 \).

At each step of the stress based iterative scheme, we need to compute \( \hat{\sigma}_n^\alpha \) obtained as the convolution product between the shape functions and the stress. \( \hat{\sigma}_n^\alpha \) is computed from Eq. (18) in which the strain \( \varepsilon \) is replaced by the stress \( \sigma \) at both sides of the equality. The convergence test used for the strain based iterative scheme is based on the equilibrium for stress. The dual scheme uses a convergence condition based on the compatibility of the strain:

\[
\text{strain-scheme: } \| \mathbf{P}_n : \left[ \sum_{\alpha=1}^{a=p} \mathbb{C}^0 : (\hat{\sigma}_n^\alpha) \right] \| < \varepsilon, \text{stress-scheme: } \| \mathbf{Q}_n : \left[ \sum_{\alpha=1}^{a=p} \mathbb{S}^\alpha : (\hat{\sigma}_n^\alpha) \right] \| < \varepsilon
\]  
(22)

Typically, the precision in the interval \([10^{-4}, 10^{-3}]\) can guarantee the convergence condition of this scheme (see [8]). Where the precision \( \varepsilon = 10^{-4} \) is considered in the applications. It is worth noted that the iterative schemes (15) and (20) are formally equivalent to those introduced in [1, 13] and [4, 5].

3. Application to 2D-polycrystals

3.1. Local elastic law

We consider a 2D-polycrystal made up of \( M \) single cubic-crystals. The elastic tensor of the crystal \( \alpha \) is denoted by \( \mathbb{C}_\alpha \) with the components \( C^\alpha_{ijkl} (i, j, k, l = 1, 2) \). For convenience, it is more suitable to read the local elasticity rule with a matrice representation. For instance, in the 2D case, the elastic law written in the basis \( B_\alpha \) oriented along the axis of the crystal is:

\[
\begin{bmatrix}
\sigma_1 \\
\sigma_2 \\
\sigma_6
\end{bmatrix}_{B_\alpha} = \begin{bmatrix}
C^\alpha_{11} & C^\alpha_{12} & C^\alpha_{16} \\
C^\alpha_{12} & C^\alpha_{22} & C^\alpha_{26} \\
C^\alpha_{16} & C^\alpha_{26} & C^\alpha_{66}
\end{bmatrix}_{B_\alpha} \begin{bmatrix}
\varepsilon_1 \\
\varepsilon_2 \\
\varepsilon_6
\end{bmatrix}_{B_\alpha}
\]  
(23)

where the following notation has been used for the components of the strain and the stress:
and the components $C_{ij}^\alpha$ are related to those of $C_{ijkl}^\alpha$ by:

\[

c_{11} c_{12} c_{16} \quad c_{12} c_{22} c_{26} \quad c_{16} c_{26} c_{66,\alpha} = \begin{bmatrix}
C_{1111}^\alpha & C_{1122}^\alpha & \sqrt{2}C_{1112}^\alpha \\
C_{1222}^\alpha & C_{2222}^\alpha & \sqrt{2}C_{2212}^\alpha \\
\sqrt{2}C_{1112}^\alpha & \sqrt{2}C_{2212}^\alpha & \sqrt{2}C_{1212}^\alpha
\end{bmatrix}_{B_{\alpha}}.
\]

The elasticity law in the crystal is assumed to be cubic. As a consequence the material has three independent elastic coefficients $\lambda$, $\mu_1$, $\mu_2$, and:

\[

c_{11} c_{12} c_{16} \quad c_{12} c_{22} c_{26} \quad c_{16} c_{26} c_{66,\alpha} = \begin{bmatrix}
\lambda + 2\mu_1 & \lambda & 0 \\
\lambda & \lambda + 2\mu_1 & 0 \\
0 & 0 & 2\mu_2
\end{bmatrix}_{B_{\alpha}}.
\]

In the FFT method, the strain and the stress are computed in a global frame $B$. The components of the elastic tensor must be computed in this global frame. Let author denote by $\varepsilon'_{ij}$ and $\sigma'_{ij}$ the components of the strain and stress written in the global frame. The orientation of the crystal in the global frame is given by the angle $\theta$.

The base change relations giving the components of the strain $\varepsilon'_{ij}$ as function of $\varepsilon_{ij}$ are:

\[
\varepsilon'_{1} = c^2 \varepsilon_1 + s^2 \varepsilon_2 - \sqrt{2}cs \varepsilon_6 \quad (27)
\]

\[
\varepsilon'_{2} = s^2 \varepsilon_1 + c^2 \varepsilon_2 + \sqrt{2}cs \varepsilon_6 \quad (28)
\]

\[
\varepsilon'_{6} = \sqrt{2}cs(\varepsilon_2 - \varepsilon_1) + (c^2 - s^2) \varepsilon_6 \quad (29)
\]

in which $c = \cos(\theta)$ and $s = \sin(\theta)$. The relations giving the components $\sigma'_{ij}$ as function of $\sigma_{ij}$: 80
\[ \sigma'_1 = c^2 \sigma_1 + s^2 \sigma_2 + \sqrt{2}cs \sigma_6 \]  
(30)

\[ \sigma'_2 = s^2 \sigma_1 + c^2 \sigma_2 - \sqrt{2}cs \sigma_6 \]  
(31)

\[ \sigma'_6 = \sqrt{2}cs (\sigma_2 - \sigma_1) + (c^2 - s^2) \sigma_6 \]  
(32)

Introducing Eq. (27) to Eq. (32) in relation (33) with (26) leads to:

\[
\begin{bmatrix}
\sigma'_1 \\
\sigma'_2 \\
\sigma'_6
\end{bmatrix} =
\begin{bmatrix}
C^{a'}_{11} & C^{a'}_{12} & C^{a'}_{16} \\
C^{a'}_{12} & C^{a'}_{22} & C^{a'}_{26} \\
C^{a'}_{16} & C^{a'}_{26} & C^{a'}_{66}
\end{bmatrix}
\begin{bmatrix}
\varepsilon'_1 \\
\varepsilon'_2 \\
\varepsilon'_6
\end{bmatrix}_{B}
\]  
(33)

in which the components \( C^{a'}_{ij} \) are given by:

\[ C^{a'}_{11} = C^{a'}_{22} = \lambda + 2 \mu_1 + 4(\mu_2 - \mu_1)c^2 s^2 \]

\[ C^{a'}_{12} = \lambda + 4(\mu_1 - \mu_2)c^2 s^2 \]

\[ C^{a'}_{16} = -C^{a'}_{26} = 2\sqrt{2}(\mu_1 - \mu_2)cs(s^2 - c^2) \]

\[ C^{a'}_{66} = 2\mu_2 + 8(\mu_1 - \mu_2)c^2 s^2 \]  
(34)

It is readily observed that the components of \( C^{a'}_{ij} \) are the same those \( C^{a}_{ij} \) as soon as \( \mu_1 = \mu_2 \). This corresponds to the particular case of an isotropic elastic medium.

3.2. The shape function of a polygon

The representative cell of the polycrystal is generated by Voronoi tessellations. Each single crystal is then represented by a polygon. The number of edges of the polygon is arbitrary. In a given microstructure, the polygons must contain 3, 4, 5,... edges. Consider a polygon and let us denote the positions of the corners by \( r_1, r_2, r_3, ..., r_i \), the corners being numbered in counter-clockwise direction. The shape function \( I_\alpha \) and the area \( S_\alpha \) of the \( \alpha \)-polygon are given by the expressions in [16]:

\[
\hat{I}^\alpha(\xi) = -i \frac{e_3 \wedge \xi}{S |\xi|^2} \sum_{j=1}^{j} (r_j - r_{j-1}) \sin c \left[ \frac{\xi (r_j - r_{j-1})}{2} \right] \exp \left[ -i \xi \frac{r_j + r_{j-1}}{2} \right] \]  
(35)

\[
S^\alpha = \frac{1}{2} e_3 \sum_{j=1}^{j} r_j \wedge r_{j-1} \]  
(36)

with the convention \( r_0 = r_j \), \( |\xi| \) is the norm of \( \xi \), \( e_3 \) is the normal unit vector to the working plane \((e_1, e_2)\). In the above equation \( S = L_1 L_2 \) is the area of the squared unit cell. It is noted that this expression is preferred over another equivalent expression.
existing in literature for the regularity of the sinc function. In the latter analytical expression, the denominator can vanish at some values of the wave vectors, requiring attention when implementing these formulas. Indeed, sinc\((x)\) tends to zero when \(x\) also tends to zero, but numerically, when \(x = 0\), sinc\((x)\) leads to singularity. The limit must be correctly computed when the term \(\xi \left( r_j - r_{j-1} \right) \) is null.

3.3. Illustration

![Figure 2: Unit cell of the Voronoi periodic structure 2D](image)

A representative cell of the polycrystal is obtained with Voronoi tessellation and is represented in Fig. 2. The orientation of each crystal, defined by the angle \(\theta\), is randomly chosen in the interval \([0, \pi]\). The elastic moduli of the cubic crystal are \(\mu_1 = 1\), \(\mu_2 = 2\) and \(\lambda = 1\). The calculations are performed on 40 reconstructed unit cells. The average value of the effective elastic moduli are \(\lambda^{\text{hom}}\) and \(\mu^{\text{hom}}\).

![Figure 3: Variation of the effective elastic shear modulus \(\mu^{\text{hom}}\) as function of the resolution](image)
The variations of the homogenized elastic shear modulus with the number of wave vectors are provided in Fig. 3. Three solutions are provided in this figure, the strain and the stress based FFT bounds computed with the shape functions, the solution obtained with the original FFT iterative scheme of Moulinec and Suquet [1] without using the shape function. It is observed that the bounds have a uniform convergence and the solution of obtained with the original scheme of Moulinec and Suquet is comprised between the two bounds.

4. Extension to 3D-polycrystals

In this section, we propose to extend the method based on the shape function to the case of 3D polycrystals.

4.1. The shape function of a polyhedron

Each crystal of the 3D-polycrystal is represented by a polyhedron. It is defined by its $K$ faces denoted $\Gamma_k$ for $k = 1..K$. Each face $\Gamma_k$ is a $J_k$-polygon given by the simple polygonal vertex chain $r_{k,1} \ldots r_{k,J_k}$ and by the normal unit vector $\hat{n}_k$ pointing towards the outside of the polyhedron. The shape function of the $\alpha$-polyhedron is $\forall \xi \neq 0$

$$I^\alpha(\xi) = \frac{i}{V} \sum_{k=1}^{K} \frac{\xi \cdot \hat{n}_k}{|\xi|^2} \chi_k(\xi)$$

where $V$ denotes the volume of the unit cell and

$$\chi_k(\xi) = -i \hat{n}_k \wedge \frac{\xi}{|\xi|} \sum_{j=1}^{J_k} (r_{k,j} - r_{k,j-1}) \sin c \left[ \frac{\xi \cdot (r_{k,j} - r_{k,j-1})}{2} \right] \exp \left( -i \xi \cdot \frac{r_{k,j} + r_{k,j-1}}{2} \right)$$

where the convention $r_{k,0} = r_{k,J_k}$ must be used. The two order tensor $q_k$ is the projector onto the plane normal to the unit vector $\hat{n}_k$:

$$q_k = I - \hat{n}_k \otimes \hat{n}_k$$

Note that $\chi_k(\xi)$ is the 2D-shape function of the polygon $k$ without the area $S$ of the 2D unit cell. Indeed, when the polygon if embedded in a squared unit cell, the shape function is $\chi_k(\xi)/S$ where $S$ denotes the area of the unit cell. The volume of a polyhedron can be conveniently computed from:

$$V^\alpha = \frac{i}{6} \sum_{k=1}^{K} \sum_{j=1}^{J_k} (\hat{n}_k \cdot (r_{k,j} \wedge r_{k,j-1}))(\hat{n}_k \cdot r_{k,j-1})$$

4.2. Numerical Analysis

The homogenized elastic coefficients of the polycrystal are now computed with the method based on the shape functions. A unit cell of the polycrystal is shown in Fig. 4.
The cell contains 60 single cubic crystals. The orientation of each crystal is given by the three Euler angles $\theta_1$, $\theta_2$ and $\theta_3$ randomly chosen in the interval $[0, \pi]$.

Fig. 4. Unit cell of the 3D-polycrystal (60 single crystals)

The effective shear modulus and effective compressibility with the number of wave vectors are presented in Fig. 5 and Tab. 1. The result shows that the Moulinec and Suquet solution is again between the two bounds.

Tab. 1. Average values of the effective shear modulus and effective compressibility computed for the 3D-polycrystal as function of the resolution. Comparison between the lower bound (LB) and the upper bound (UB) and the solutions obtained with the original scheme of Moulinec and Suquet (M&S)

<table>
<thead>
<tr>
<th>Resolution</th>
<th>$\mu_{\text{hom}}$</th>
<th>$k_{\text{hom}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>UB</td>
<td>LB</td>
</tr>
<tr>
<td>4x4x4</td>
<td>1.5202</td>
<td>1.4705</td>
</tr>
<tr>
<td>8x8x8</td>
<td>1.5092</td>
<td>1.4877</td>
</tr>
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<td>1.4904</td>
</tr>
<tr>
<td>32x32x32</td>
<td>1.5016</td>
<td>1.4913</td>
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<td>64x64x64</td>
<td>1.5001</td>
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<td>96x96x96</td>
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<td>128x128x128</td>
<td>1.4983</td>
<td>1.4927</td>
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<tr>
<td>256x256x256</td>
<td>1.4975</td>
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5. Conclusion

In this paper we provide rigorous bounds for 2D and 3D elastic polycrystals. The effective elastic coefficients are computed from reconstructed unit cell using standard methods based on Voronoi tessellations. In each single crystal, the elastic law is assumed to be cubic. The effective elastic coefficients are computed by using the FFT methods combined with the use of the shape functions. The method has been introduced by [5] for composites with ellipsoidal inclusions. The present approach has been extended to the case of polycrystal by taking advantages of the exact expressions of the shape function of polygon and polyhedron recently provided in [11].

References

TÍNH TOÁN BIÊN GIỚI HẠN THUỘC TÍNH ĐÀN HỘI CỦA ĐA TINH THỂ TRÊN CƠ SỞ PHƯƠNG PHÁP BIẾN ĐỘI NHANH FOURIER


Từ khóa: Hệ số đàn hồi; giới hạn biên số; hàm dạng; kết cấu đa tính thể; Voronoi; biến đội nhanh Fourier.

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