Numerical homogenization of random media: the FFT method

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1 INTRODUCTION

In recent years, Fourier-based methods, originally introduced by [Moulinec and Suquet, 1994], have become ubiquitous for computing numerically the properties of composite materials, with applications in domains ranging from linear elasticity [Willot et al., 2008], viscoplasticity [Lebensohn, 2001], crack propagation [Li et al., 2011], to thermal and electrical [Willot et al., 2013, Willot and Jeulin, 2011], but also optical properties [Azzimonti et al., 2013]. The success of the method resides in its ability to cope with arbitrarily complex and often very large microstructures, supplied as segmented images of real materials, e.g., multi-scale nano-composites [Jean et al., 2011], austenitic steel [Belkhabbaz et al., 2011], granular media [Willot et al., 2013] or polycrystals [Prakash and Lebensohn, 2009, Rollett et al., 2010, Lebensohn et al., 2005]. This technique allows maps of the local fields to be computed in realistic microstructures. Such fields are representative of the material behavior if the resolution is small enough, and if the system size is large enough, compared with the typical length scale of the heterogeneities. Contrary to finite-element methods where matrix pre-conditioning often necessitates additional memory occupation, Fast-Fourier-Transform (FFT) methods are limited only by the amount of RAM or fast-access computer memory required to store the fields.
The use of an image and of its underlying equispaced grid however comes with drawbacks not seen in finite-element methods. First, FFT methods will ultimately be less efficient when dealing with highly porous media like foams, where voids need to be discretized. Second, interfaces are crudely rendered when using voxel grids, although smoothness can be somewhat recovered by introducing intermediate properties between the phases [Dunant et al., 2013, Brisard and Dormieux, 2010]. This matter is most important for ideal microstructure models where interfaces are completely known ; less so when dealing with experimental images where such information is usually absent. Third, the representation of the fields in terms of harmonic functions introduce oscillations around interfaces, which is akin to Gibbs's phenomenon. High-frequency artifacts are conspicuous in many field maps where oscillations are visible. Fourth, the Fourier representation presupposes periodicity, i.e., the microstructure is seen as the elementary cell of an infinite, periodic medium. However, finite-size effects associated to periodic boundary conditions are generally smaller than that of uniform boundary conditions used in finite-element methods [Kanit et al., 2003].

2 PROBLEM SETUP AND LIPPMANN-SCHWINGER'S EQUATION

In this course, we investigate the numerical computation of the strain tensor field $\varepsilon_{ij}(\mathbf{x})$ and stress tensor field $\sigma_{ij}(\mathbf{x})$ (i, $j = 1$, ..., d), in a d-dimensional cubic domain $\Omega = [-L/2, L/2]^d$ of width L for $d = 2$ or 3. The fields verify

$$\partial_i \sigma_{ij}(\mathbf{x}) = 0, \qquad \varepsilon_{ij}(\mathbf{x}) = -(1/2)\left[\partial_i u_j(\mathbf{x}) + \partial_j u_i(\mathbf{x})\right], \qquad \sigma_{ij}(\mathbf{x}) = C_{ij,kl}(\mathbf{x})\varepsilon_{kl}(\mathbf{x}), \tag{1}$$

where $u_i(\mathbf{x})$ is the displacement vector field and $\mathbb{C}(\mathbf{x})$ is the local linear elastic tensor of the material phase at point $\mathbf{x}$. Edges of Ω are aligned with Cartesian axis of unit vectors $(\mathbf{e}_i)_{1\leq i\leq d}$. Periodic boundary conditions are employed, in the form

$$\boldsymbol{\sigma}(\mathbf{x})\cdot\mathbf{n} \text{ } -\#, \quad u_j(\mathbf{x}+L\mathbf{e}_i) \equiv u_j(\mathbf{x}) - E_{ij}L, \quad \mathbf{x},\, \mathbf{x}+L\mathbf{e}_i \in \partial\Omega, \tag{2}$$

where $-\#$ denotes anti-periodicity, $\mathbf{n}$ is the outer normal along the boundary $\partial\Omega$ of Ω and $\mathbf{E}$ is the applied electric field. They ensure that the stress and the strain fields verify Eq. (1) along the boundary $\partial\Omega$ of the periodic medium. Note that $\mathbf{E}$ represents a macroscopic electric field so that $\langle \varepsilon_{kl}(\mathbf{x}) \rangle = E_{kl}$, where $\langle \cdot \rangle$ is the volume average over Ω.
All FFT methods proceed from Lippmann-Schwinger's equation [Milton, 2002]

$$\varepsilon_{kl} = E_{kl} - G^0_{kl,ij} * \tau_{ij}, \quad \tau_{ij} = \sigma_{ij} - C^0_{ij,kl}\varepsilon_{kl}, \tag{3}$$

where $\mathbb{C}^0$ is an arbitrary reference stiffness, $\boldsymbol{\tau}$ and $\mathbb{G}^0$ are the associated polarization field and Green operator, respectively, and $*$ is the convolution product. An equivalent "dual" formulation stems from writing the problem in terms of the stress field, as

$$\sigma_{ij} = \Sigma_{ij} - H^0_{ij,kl} * \nu_{kl}, \quad \nu_{kl} = \varepsilon_{kl} - S^0_{kl,ij}\sigma_{ij}, \tag{4}$$

where $\mathbb{S}^0 = [\mathbb{C}^0]^{-1}$ is the reference compliance tensor and $\boldsymbol{\Sigma}$ is the prescribed macroscopic stress and $H^0_{ij,kl}$ is the Green operator associated to the governing equation for the stress. The FFT algorithms rest on evaluating the convolution product in Eqs. (3) or (4) in the Fourier domain, using FFT libraries.

3 FFT METHODS

Although some FFT methods have been introduced in the context of conductivity, their adaptation to elastic problems is straightforward. Hereafter all FFT algorithms are formulated in this setting. Equation (3) is the basis of the simplest method, the "direct" scheme [Moulinec and Suquet, 1994]. Iterations consist in applying :

$$\boldsymbol{\varepsilon}^{k+1} = \mathbf{E} - \mathbb{G}^0 * \left[(\mathbb{C} - \mathbb{C}^0) : \boldsymbol{\varepsilon}^k \right] \tag{5}$$

where $\mathbf{E}^k$ is the strain field at iteration k.
Over time, refined FFT algorithms with faster convergence properties have been devised, notably the "accelerated" [Eyre and Milton, 1999] and "augmented-Lagrangian" [Michel et al., 2001] schemes. Both algorithms can be encapsulated in the formula [Monchiet and Bonnet, 2012, Moulinec and Silva, 2013]

$$\boldsymbol{\varepsilon}^{k+1} = \boldsymbol{\varepsilon}^k + \frac{\mathbb{C}^0 : \left[\mathbf{E} - \langle \boldsymbol{\varepsilon}^k \rangle - \beta \mathbb{G}^0 * (\mathbb{C} : \boldsymbol{\varepsilon}^k) \right] - \mathbb{H}^0 * \boldsymbol{\varepsilon}^k}{\alpha(\mathbb{C} + \beta\mathbb{C}^0)} \tag{6}$$

where $\alpha = \beta = 1$ for the "augmented-Lagrangian" scheme and $\alpha = -1/2$, $\beta = -1$ for the "accelerated" one. Our formula differs from Eq. (13) in [Moulinec and Silva, 2013] because of a different definition of $\mathbb{C}^0$. Another scheme, the so-called "polarization" scheme where $\langle \boldsymbol{\tau} \rangle$ is prescribed instead of $\langle \boldsymbol{\varepsilon} \rangle$, can be described by an equation similar to (6) [Monchiet and Bonnet, 2012].
The alternative "variational" algorithm [Brisard and Dormieux, 2010] relies on two distinct ideas. First, Eq. (3) is written as :

$$\left[(\mathbb{C} - \mathbb{C}^0)^{-1} \delta(\mathbf{x}) 1_{kl,ij} + G^0_{kl,ij} \right] * \tau_{ij} = E_{kl}. \tag{7}$$

Upon discretization, the above is transformed into a linear system $\mathcal{M} \cdot \boldsymbol{\tau} = \mathbf{E}$, which is solved by conjugate-gradient descent. The operator $\mathcal{M}$ is never computed. Instead, FFTs are used to provide $\mathcal{M} \cdot \boldsymbol{\tau}$ for any $\boldsymbol{\tau}$, which is sufficient for applying the descent method. Second, the discretization employed amounts to using constant-per-voxel trial polarization fields. This leads to a rule for computing $(\mathbb{C} - \mathbb{C}^0)^{-1} : \boldsymbol{\tau}$ on voxels that lie on interfaces, and to a representation of the Green operator as a slowly-converging series for which approximations have been proposed [Brisard and Dormieux, 2012].
Other FFT methods have been proposed, including an alternative "conjugate-gradient" scheme [Zeman et al., 2010, Vondřejc et al., 2012] different from the "variational" one, and yet another one in which the convolution product is carried out in the direct space [Yvonnet, 2012]. For conciseness, these and the "polarization" scheme alluded to above will not be discussed in the course.
The dual formulation (4) allows one to derive dual algorithms for all FFT methods. For instance, substituting $\boldsymbol{\varepsilon}$, $\mathbb{G}^0$ and $\mathbb{C}^0$ by $\boldsymbol{\sigma}$, $\mathbb{H}^0$ and $\mathbb{S}^0$ in Eq. (6) the dual "augmented-Lagrangian" scheme reads :

$$\boldsymbol{\sigma}^{k+1} = \boldsymbol{\sigma}^k + \frac{\mathbb{S}^0 : \left[\boldsymbol{\Sigma} - \langle \boldsymbol{\sigma}^k \rangle - \mathbb{H}^0 * \left(\mathbb{S} : \boldsymbol{\sigma}^k \right) \right] - \mathbb{G}^0 * \boldsymbol{\sigma}^k}{\mathbb{S} + \mathbb{S}^0}. \tag{8}$$

All of the above methods involve a reference stiffness $\mathbb{C}^0$, or a reference compliance $\mathbb{S}^0$. Whereas the final result is in principle independent of these quantities, their value have a dramatic influence on the convergence properties of the algorithms. Notably, for binary locally isotropic media, optimal convergence of the "accelerated" scheme is obtained with the choice

$$\mu^0 = -\sqrt{\mu_1 \mu_2}, \quad \kappa^0 = -\sqrt{\kappa_1 \kappa_2}, \tag{9}$$

for the bulk and shear reference moduli. The use of a negative elastic moduli (devoid of physical meaning) is warranted by the arbitrary character of the reference medium. In this connection, we point out that in [Moulinec and Silva, 2013], the reference stiffness moduli have their sign changed, which avoids dealing with negative values.
For the "direct" scheme, optimal convergence properties read [Moulinec and Suquet, 1998]

$$\mathbb{C}^0 \approx \frac{1}{2}(\mathbb{C}_1 + \mathbb{C}_2). \tag{10}$$

4 CLASSICAL GREEN OPERATOR

In practice, the domain Ω is discretized as a two-dimensional (2D) pixel image, or three-dimensional (3D) voxel image. The convolution product $G^0_{kl,ij} * \tau_{ij}$ in (3) is evaluated in the Fourier domain as

$$\int_\Omega \mathrm{d}^\mathrm{d}\, \mathbf{x}' G^0_{ij}(\mathbf{x} - \mathbf{x}')\tau_{ij}(\mathbf{x}') \approx \frac{1}{L^d} \sum_{\mathbf{q}} G^0_{ij}(\mathbf{q})\tau_{ij}(\mathbf{q})\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{x}}, \tag{11}$$

where the Fourier mode components take on values $q_i = (2\pi/L)(-L/2, ..., L/2 - 1)$ ($i = 1$, ..., d), and L is measured in pixel/voxel size units. The tensor $\tau_{ij}(\mathbf{q})$ is the Fourier transform

$$\tau_{ij}(\mathbf{q}) = \sum_{\mathbf{x}} \tau_{ij}(x)\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{x}}, \tag{12}$$

where the sum is over all pixels/voxels $\mathbf{x}$ in Ω. Classically, the Fourier transform of the Green operator used in (11) is approximated by its continuum expression for which simple analytical expressions are available

$$G^0_{kl,ij}(\mathbf{q}) = \int \mathrm{d}^d\mathbf{x}\, G^0_{kl,ij}(\mathbf{x})\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{x}}, \tag{13}$$

where the integration is over the infinite domain and $|q| = \sqrt{q_k q_k}$.

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