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Fourier-based schemes for computing the mechanical response of composites with accurate local fields

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ABSTRACT

We modify the Green operator involved in Fourier-based computational schemes in elasticity, in 2D and 3D. The new operator is derived by expressing continuum mechanics in terms of centered differences on a rotated grid. Using the modified Green operator leads, in all systems investigated, to more accurate strain and stress fields than using the discretizations proposed by Moulinec and Suquet (1994) [1] or Willot and Pellegrini (2008) [2]. Moreover, we compared the convergence rates of the "direct" and "accelerated" FFT schemes with the different discretizations. The discretization method proposed in this work allows for much faster FFT schemes with respect to two criteria: stress equilibrium and effective elastic moduli.

1. Introduction

Fourier-based algorithms, or "FFT" methods for short, are an efficient approach for computing the mechanical response of composites. Initially restricted to linear-elastic media, FFT tools are nowadays employed to treat more involved problems, ranging from viscoplasticity [3] to crack propagation [4]. In FFT methods, the microstructure is defined by 2D or 3D images and the local stress and strain tensors are computed along each pixel or "voxel" in the image. Coupled with automatic or semi-automatic image segmentation techniques [5], this allows for the computation of the mechanical response of a material directly from experimental acquisitions, like focused ion beam or 3D microtomography techniques [6]. The latter often deliver images containing billions of voxels, for which FFT methods are efficient [7,8]. This allows one to take into account representative volume elements of materials which are multiscale by nature such as concrete or mortar [9]. From a practical viewpoint, the simplicity of FFT methods is attractive to researchers and engineers who need not be experts in the underlying numerical methods to use them. Nowadays, FFT tools are available not only as academic or free softwares [10,11] but also as commercial ones [12].

In the past years, progress has been made in the understanding of FFT algorithms. Vondřejc and co-workers have recently shown that the original method of Moulinec and Suquet [1] corresponds, under one technical assumption, to a particular choice of approximation space and optimization method [13] (see also [14]). This property allows one to derive other FFT schemes that use standard optimization algorithms, such as the conjugate gradient method. In this regard, making use of variational formulations, efficient numerical methods have been proposed that combine FFTs with an underlying gradient descent algorithm [15,16].

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Different approximation spaces or discretization methods have also been proposed, where, contrary to the original scheme, the fields are not trigonometric polynomials anymore. Brisard and Dormieux introduced "energy-based" FFT schemes that rely on Galerkin approximations of Hashin and Shtrikman's variational principle [16,14] and derived modified Green operators consistent with the new formulation. They obtained improved convergence properties and local fields devoid of the spurious oscillations observed in the original FFT scheme [14,17]. In the context of conductivity, accurate local fields and improved convergence rates have also been obtained from modified Green operators based on finite-differences [18]. These results follow earlier works where continuum mechanics are expressed by centered [19,20] or "forward and backward" finite differences [2].

This work focuses on the effect of discretization in FFT methods. It is organized as follows. We first recall the equations of elasticity in the continuum (Section 2). We give the Lippmann–Schwinger equations and the "direct" and "accelerated" FFT schemes in Section 3. In Section 4, a general formulation of the Green operator is derived that incorporates methods in [2], and a new discretization scheme is proposed. The accuracy of the local stress and strain fields are examined in Section 5 whereas the convergence rates of the various FFT methods are investigated in Section 6. We conclude in Section 7.

2. Microstructure and material elastic response

We are concerned with solving the equations of linear elasticity in a square or cubic domain $\Omega = [-1/2; 1/2]^d$ in dimension d ($d = 2$ or 3):

$$\sigma_{ij}(\boldsymbol{x}) = C_{ij,kl}(\boldsymbol{x})\varepsilon(\boldsymbol{x}), \qquad \partial_i\sigma_{ij}(\boldsymbol{x}) \equiv 0, \qquad \varepsilon_{ij}(\boldsymbol{x}) = (1/2)\big[\partial_i u_j(\boldsymbol{x}) + \partial_j u_i(\boldsymbol{x})\big] \tag{1}$$

where $\boldsymbol{\varepsilon}(\boldsymbol{x})$ is the strain field, $\boldsymbol{\sigma}(\boldsymbol{x})$ the stress field, $\boldsymbol{u}(\boldsymbol{x})$ the displacement vector field, $\mathbb{C}(\boldsymbol{x})$ the local elasticity tensor and $\boldsymbol{x}$ is a point in Ω. Tensorial components refer to a system of Cartesian coordinates $(\mathbf{e}_1; \mathbf{e}_2)$ in 2D and $(\mathbf{e}_1; \mathbf{e}_2; \mathbf{e}_3)$ in 3D. The material has an isotropic local elastic response that reads:

$$C_{ij,kl}(\boldsymbol{x}) = \lambda(\boldsymbol{x})\delta_{ij}\delta_{kl} + \mu(\boldsymbol{x})(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \tag{2}$$

where δ is the Kronecker symbol and $\lambda(\boldsymbol{x})$ and $\mu(\boldsymbol{x})$ are constant-per-phase Lamé's first and second coefficients. The local bulk modulus $\kappa = \lambda + (2/d)\mu$ and the elastic moduli take on values:

$$\lambda(\boldsymbol{x}) = \lambda^\alpha, \qquad \kappa(\boldsymbol{x}) = \kappa^\alpha, \qquad \mu(\boldsymbol{x}) = \mu^\alpha$$

in phase α. For simplicity, we restrict ourselves to binary media and, by convention, $\alpha = 1$ is the matrix and $\alpha = 2$ the inclusions. Hereafter, we fix Poisson's ratios in each phase to $\nu^1 = \nu^2 = 0.25$ so that, in 3D and 2D [21], we have $\mu^\alpha/\kappa^\alpha = 0.6$. The contrast of properties χ reads:

$$\chi = \frac{\kappa^2}{\kappa^1} = \frac{\mu^2}{\mu^1} = \frac{\lambda^2}{\lambda^1} \tag{3}$$

where $0 \le \chi \le \infty$. In the matrix, we also fix $\kappa^1 = 1$ ($d = 2$ or 3), $\mu^1 = 0.6$ ($d = 2$ or 3), $\lambda^1 = 0.4$ ($d = 2$), $\lambda^1 = 0.6$ ($d = 3$), so that the local properties of the material are parametrized by one unique variable, the contrast of properties χ. In 3D, the Young modulus is $E^1 = 3/2$ in the matrix and $E^2 = 3\chi/2$ in the inclusion. The medium is porous when $\chi = 0$ and rigidly-reinforced when $\chi = \infty$.

Periodic boundary conditions are applied with the material subjected to an overall strain loading $\overline{\boldsymbol{\varepsilon}}$:

$$\sigma_{ij}(\boldsymbol{x})n_j(\boldsymbol{x}) - \# \quad (\boldsymbol{x} \in \partial\Omega), \qquad \big\langle\varepsilon_{kl}(\boldsymbol{x})\big\rangle = \overline{\varepsilon_{kl}} \tag{4}$$

where $\boldsymbol{n}$ is the normal at the boundary $\partial\Omega$ of the domain Ω, oriented outward, $-\#$ denotes anti-periodicity and $\langle\cdot\rangle$ denotes the spatial mean over Ω. The resulting effective elastic tensor $\widetilde{\mathbb{C}}$ is computed from:

$$\big\langle\sigma_{ij}(\boldsymbol{x})\big\rangle = \widetilde{C}_{ij,kl}\overline{\varepsilon_{kl}} \tag{5}$$

3. Lippmann–Schwinger equation and FFT methods

Fourier methods are by principle based on the Lippmann–Schwinger equations. The latter follow from (1) and (4) as [22]:

$$\tau_{ij}(\boldsymbol{x}) = \sigma_{ij}(\boldsymbol{x}) - C^0_{ij,kl}\varepsilon_{kl}(\boldsymbol{x}), \qquad \varepsilon_{ij}(\boldsymbol{x}) = \overline{\varepsilon_{ij}} - \int_{\boldsymbol{x}'} \mathrm{d}^d\boldsymbol{x}' G_{ij,kl}\big(\boldsymbol{x}' - \boldsymbol{x}\big)\tau_{kl}\big(\boldsymbol{x}'\big) \tag{6}$$

where we have introduced a homogeneous "reference" elasticity tensor $\mathbb{C}^0$ and its associated polarization field $\boldsymbol{\tau}$ and Green operator $\mathbb{G}$. In the above we assume $\langle\mathbb{G}\rangle = 0$ so that $\overline{\boldsymbol{\varepsilon}} = \langle\boldsymbol{\varepsilon}(\boldsymbol{x})\rangle$ holds. The Green operator has, in the Fourier domain, the closed form [23]:

$$G_{ij,kl}(\boldsymbol{q}) = \big\{q_i\big[q_m C^0_{mj,kn} q_n\big]^{-1} q_l\big\}_{\mathrm{sym}} \tag{7}$$