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Filtering material properties to improve FFT-based methods for numerical homogenization

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ABSTRACT

FFT-based solvers introduced in the 1990s for the numerical homogenization of heterogeneous elastic materials have been extended to a wide range of physical properties. In parallel, alternative algorithms and modified discrete Green operators have been proposed to accelerate the method and/or improve the description of the local fields. In this short note, filtering material properties is proposed as a third complementary way to improve FFT-based methods. It is evidenced from numerical experiments that the grid refinement and consequently the computation time and/or the spurious oscillations observed on local fields can be significantly reduced. In addition, if the two filters based on Voigt or Reuss homogenization rules can improve or deteriorate the method depending on the microstructure, a stiff inclusion within a compliant matrix or the reverse, the proposed '2-layer' filter is efficient in both situations. The study is proposed in the context of linear elasticity but similar results are expected in a different physical context (thermal, electrical...).

1. Introduction

The spectral methods based on the Lippmann–Schwinger equation associated to a discrete Green operator are efficient numerical iterative methods devoted to the evaluation of physical properties of heterogeneous unit cells submitted to periodic boundary conditions. If the method proposed initially [9] suffers from various drawbacks, different propositions have been made to improve it. These propositions can be classified into two categories. The first category [3–6,12] operates on the iterative algorithm to reduce the number of iterations until convergence, without changing the numerical solution, while the second category [1,11] modifies the discrete Green operator to improve both the numerical solution fields and the convergence properties. Actually, spurious oscillations are commonly observed on the numerical solution fields when using the discrete Green operator proposed initially.

The purpose of this short note is to propose the filtering of material properties as a complementary way to improve these methods without any modification of the iterative algorithm or of the discrete Green operator. The idea is inspired by previous works [1,2,10] assigning homogenized properties to heterogeneous finite elements or voxels (i.e. crossed by an interface between two materials), which can be regarded as a mechanical filter whose size is the same as the element size. Here the effect of the filter radius is considered and a new mechanical filter based on a multilayer homogenization rule is proposed in addition to the classical Voigt and Reuss rules. The benefits of this approach, evidenced by a simple numerical experiment, are the improvement of the spatial convergence properties as well as the reduction of spurious oscillations.

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In this example, for a given convergence criterion, the required spatial resolution can be divided by a factor between 2.6 and 7.2, corresponding to a reduction of the problem size by a factor between 6.7 and 51.8 in 2D. Thus, reducing the problem size, filtering materials properties decreases the computation time. Moreover, this does not strongly affect the convergence properties of the iterative algorithm, here the classical fixed-point algorithm [8].

2. Filtering mechanical properties

The exact problem to solve is the evaluation of the strain (stress and displacement) field(s) within a heterogeneous unit cell Ω described by its stiffness tensor field c and submitted to a macroscopic strain E with periodic boundary conditions. The exact solution is given by the following equations from which a fixed-point algorithm can be derived [8]:

$$\varepsilon(x) = -(\Gamma_0 * \tau)(x) + E \quad \text{for } x \in \Omega \tag{1a}$$

$$\tau(x) = \big(c(x) - c_0\big) : \varepsilon(x) \quad \text{for } x \in \Omega \tag{1b}$$

Γ_0 is the periodic Green operator for a homogeneous medium of stiffness c_0. The convolution product $*$ can be written in Fourier space as follows:

$$\begin{cases} \hat{\varepsilon}(k_a) = -\hat{\Gamma_0}(k_a) : \hat{\tau}(k_a) & \text{for } a \in \mathbb{Z}^3 \text{ and } a \neq 0 \\ \hat{\varepsilon}(0) = E \end{cases} \tag{2}$$

Usually, in order to obtain an approximate solution to the problem on a grid of size $N_1 \times, N_2 \times, N_3$, the polarization τ (Eq. (1b)) is simply evaluated at grid points x_α, then a Fast Fourier Transform (FFT) is used to evaluate $\hat{\tau}(k_a)$ for $a \in J$ $(= \prod_{d=1,3}\{-(N_d-1)/2,\ (N_d-1)/2\}$, with N_d being odd), then the Green operator is applied on a truncated Fourier space (Eq. (2) with $a \in J$) and finally the strain at grid points x_α is deduced from an inverse FFT. A new polarization field can be evaluated from this strain field and so on.

However, if using a pointwise evaluation of the stiffness tensor on points x_α to evaluate the polarization ($c(x_\alpha)$ used in Eq. (1b)) is simple and common, it is also questioning: isn't there any better choice especially when a grid point lies close to a material interface? In line with previous works [1,2,10], we propose to work with a locally filtered homogenized behavior $\tilde{c}$ defined by a uniform filter of shape ω centered around x_α, acting on phase indicator functions to define phase volume fractions, and a homogenization rule (HR) accounting for these volume fractions and the corresponding behaviors: $\tilde{c}(x_\alpha) = HR(c, \omega(x_\alpha))$.

When considering sufficiently refined grids, most of the surfaces $\omega(x_\alpha)$ consist of a single phase and $\tilde{c}(x_\alpha) = c(x_\alpha)$. When at least two phases belong to $\omega(x_\alpha)$, their volume fractions $f_i(x_\alpha)$ are evaluated (for example by averaging indicator functions evaluated on a refined grid) and Voigt or Reuss homogenization rules can be used as proposed previously in a slightly different context [2]:

$$\tilde{c}(x_\alpha) = Voigt\big(c, \omega(x_\alpha)\big) = \sum_{i=1}^{N\,phase} f_i(x_\alpha) c_i \tag{3}$$

$$\tilde{c}(x_\alpha) = Reuss\big(c, \omega(x_\alpha)\big) = \left(\sum_{i=1}^{N\,phase} f_i(x_\alpha) c_i^{-1} \right)^{-1} \tag{4}$$

c_i are the stiffness tensors of the phases present within $\omega(x_\alpha)$.

In addition, a new homogenization rule based on the solution of a two-phase multilayered microstructure is proposed when two phases, separated by an interface, belong to $\omega(x_\alpha)$. In that case, in addition to the volume fractions $f_1(x_\alpha)$ and $f_2(x_\alpha)$, a planar approximation of the interface crossing the filter must be evaluated. Using P and OP respectively for the "in-plane" and "out-of-plane" components (with respect to the approximate planar interface) of the stress σ and strain ε tensors, the interface and averaging conditions read:

$$\begin{cases} \sigma_1^{OP} = \sigma_2^{OP} = \sigma^{OP} \\ \varepsilon_1^{P} = \varepsilon_2^{P} = \varepsilon^{P} \end{cases} \tag{5a}$$

$$\begin{cases} f_1 \sigma_1^{P} + f_1 \sigma_2^{P} = \sigma^{P} \\ f_2 \varepsilon_1^{OP} + f_2 \varepsilon_2^{OP} = \varepsilon^{OP} \end{cases} \tag{5b}$$

Solving this set of equations leads to the definition of the "2-layer" homogenized stiffness tensor.

In the following, the three homogenization rules are applied with different filter radii, to a simple 2D microstructure, a disk (radius $\frac{\pi}{15} \sim 0.21$) centered within a square unit cell (size 1×1). Both inclusion and matrix have an elastic isotropic behavior with the same Poisson coefficient, $\nu = 0.3$, and the elastic contrast is given by the Young modulus ratio, $E_{inclusion}/E_{matrix}$. The loading is a uniaxial average strain (1%). The classical fixed-point algorithm described in Section 1 is used with a 10^{-4} stress equilibrium criterion (see definition in [9]). The spatial resolution is defined by the number of pixels per side of the unit cell. The filter radius is defined with respect to the pixel size: a radius of 0.5 corresponds to