

Filtering properties to improve FFT-based methods

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1 – Introduction

The purpose of this communication is to demonstrate how filtering the elastic properties of a considered unit-cell can be an efficient way to improve the precision, or reduce the computation time (for a given precision), of the classical FFT-based method [1], regardless the question of the algorithm (basic scheme, Lagrangian, Accelerated, Conjugate Gradient etc...).

At first, it is shown that the solution provided by the classical FFT-based method, should be regarded as an approximate solution on an approximate microstructure. Then filtering is proposed as a way to optimize this approximate microstructure with respect to the exact microstructure. This filtering of elastic properties is defined by the size (radius) of the filter and the averaging rule (Voigt, Reuss, other). Numerical results on various microstructures are discussed as a function of these two points.

2 – An approximate solution on an approximate microstructure

The (exact) problem to solve is to evaluate the strain (stress and displacement) field(s) within an heterogeneous unit cell Ω described by its stiffness tensor field c and submitted to a macroscopic strain E and periodic boundary conditions. Following Moulinec [1], the exact solution is given by the following continuous equations:

$$\begin{cases} \varepsilon(\mathbf{x}) = -(\Gamma_0 * \tau)(\mathbf{x}) + E & \text{for } \mathbf{x} \in \Omega \\ \tau(\mathbf{x}) = (c(\mathbf{x}) - c_0) : \varepsilon(\mathbf{x}) & \text{for } \mathbf{x} \in \Omega \end{cases}$$

Where Γ_0 is the periodic Green operator for an homogeneous medium of stiffness c_0 . The convolution product can be written in Fourier space:

$$\begin{cases} \hat{\varepsilon}(\mathbf{k}_a) = -\hat{\Gamma}_0(\mathbf{k}_a) : \hat{\tau}(\mathbf{k}_a) & \text{for } \mathbf{a} \in \mathbb{Z}^3 \text{ and } \mathbf{a} \neq \mathbf{0} \\ \hat{\varepsilon}(\mathbf{0}) = E \end{cases}$$

It will be shown that the solution provided by classical FFT-based methods corresponds more to the loading of an approximate microstructure than of the exact microstructure, the approximate microstructure being defined by:

$$\tilde{c}(\mathbf{x}) = \sum_{\mathbf{a} \in J} \hat{c}_{\mathbf{a}} \exp(i\mathbf{k}_{\mathbf{a}} \cdot \mathbf{x}) \cong c(\mathbf{x}) \quad \text{for } \mathbf{x} \in \Omega$$

3 – Filtering to optimize the approximate microstructure

As FFT-based methods provide approximate solutions for an approximate microstructure,

fully defined by the coefficients \widehat{c}_α , now the question is: is it possible to optimize the approximate microstructure (with respect to the exact microstructure) from the choice of \widehat{c}_α ? And consequently, is it a way to improve the precision of the simulation for a given (exact) microstructure?

The classical usage is to deduce \widehat{c}_α from an FFT over \tilde{c}_α , with $\tilde{c}_\alpha = \tilde{c}(\mathbf{x}_\alpha) = c(\mathbf{x}_\alpha)$: at grid points, approximate and exact microstructures coincide. However, for high elastic contrasts, plotting $\tilde{c}(\mathbf{x})$ on a refined grid exhibits strong oscillations in the interfaces neighbourhoods: these oscillations are thought to be at the origin of the spurious oscillations classically observed on stress and strain fields when using this strategy.

Here, the strategy consists to evaluate \tilde{c}_α (and then \widehat{c}_α) from an averaged behaviour evaluated over a sphere (or a disk in two dimensions) of radius r surrounding \mathbf{x}_α :

$$\tilde{c}_\alpha = \overline{\tilde{c}}(\mathbf{x}_\alpha, r)$$

Different questions will be discussed on arbitrary microstructures:

- For a given averaging rule (Reuss, Voigt or other), is there an optimal value for r ?
- For this optimal value, what is the optimal averaging rule?
- Is it possible to determine these optimal parameters just from the microstructure or must they be identified from simulations (on smaller uni-cells or less refined grids)?

Together with these answers, it will be demonstrated that this strategy can be a very efficient way to :

- improve the precision of the simulation for a given resolution,
- or reduce the grid resolution and the computation time (independantly from the FFT-solver) for a given precision,

[1] H. Moulinec and P. Suquet. A fast numerical-method for computing the linear and nonlinear mechanical-properties of composites. *Comptes Rendus De L Academie Des Sciences Serie Ii*, 318(11):1417–1423, June 1994.