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Improvement of the estimation of the domain of convergence of FFT-based homogenisation methods with information on the microstructure

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The so-called FFT-based homogenisation methods, introduced in the mid 90's ([1]), meet a still growing interest in the micromechanics community. These methods are all built upon the resolution of the Lippmann-Schwinger equation, which reads in the case of an inhomogeneous elastic material with a stiffness modulus $\boldsymbol{c}$ as

$$\left(\mathbf{I} \ + \boldsymbol{\Gamma}^0 \boldsymbol{\delta c}\right)\boldsymbol{\varepsilon} = \boldsymbol{E} \ , \tag{1}$$

(where $\boldsymbol{c}^0$ is the stiffness of a reference homogeneous material, where $\boldsymbol{\delta c} = \boldsymbol{c} - \boldsymbol{c}^0$, and where $\boldsymbol{\Gamma^0}$ is the Green's operator associated with $\boldsymbol{c}^0$). The overall strain $\boldsymbol{E}$ is prescribed and the strain field $\boldsymbol{\varepsilon}$ is the unknown of the equation.

Equation (1) can be expanded in power series as

$$\boldsymbol{\varepsilon} = \sum_{k=0}^{\infty} \left(-\boldsymbol{\Gamma}^0 \boldsymbol{\delta c}\right)^k \boldsymbol{E} \ . \tag{2}$$

The fixed-point scheme proposed in [1] can be interestingly considered as an iterative process for each step i of which, the approximation $\boldsymbol{\varepsilon}^{(i)}$ of the solution $\boldsymbol{\varepsilon}$ is given by the series (2) truncated at order i, i.e.

$$\boldsymbol{\varepsilon}^{(i)} = \sum_{k=0}^{i} \left(-\boldsymbol{\Gamma}^0 \boldsymbol{\delta c}\right)^k \boldsymbol{E} \ . \tag{3}$$

More concisely, the strain field at iteration i and the corresponding approximation $\tilde{\boldsymbol{c}}^{(i)}$ of the effective modulus can be written as

$$\boldsymbol{\varepsilon}^{(i)} = \sum_{k=0}^{i} \left(-\boldsymbol{\Gamma}^1 \boldsymbol{Z}\right)^k \boldsymbol{E}, \qquad \boldsymbol{c}^{0^{-1}} \tilde{\boldsymbol{c}}^{(i)} = \mathbf{I} + \sum_{k=0}^{i} \left\langle \boldsymbol{Z} \left(-\boldsymbol{\Gamma}^1 \boldsymbol{Z}\right)^k \right\rangle \tag{4}$$

with $\boldsymbol{\Gamma}^1 = \boldsymbol{\Gamma}^0 \boldsymbol{c}^0$ and $\boldsymbol{Z} = \boldsymbol{c}^{0^{-1}} \boldsymbol{\delta c}$

In a similar manner, the scheme proposed by Eyre and Milton ([2]) can be presented as

$$\boldsymbol{\varepsilon}^{(i)} = 2(\boldsymbol{c} + \boldsymbol{c}^0)^{-1} \boldsymbol{c}^0 \sum_{k=0}^{i} (-\boldsymbol{H}^1 \boldsymbol{W})^k \boldsymbol{E}, \qquad \boldsymbol{c}^{0^{-1}} \tilde{\boldsymbol{c}}^{(i)} = \mathbf{I} + 2 \sum_{k=0}^{i} \left\langle \boldsymbol{W} \left(-\boldsymbol{H}^1 \boldsymbol{W}\right)^k \right\rangle \tag{5}$$

with $\boldsymbol{H}^1 = 2\boldsymbol{\Gamma^0}\boldsymbol{c^0} - \mathbf{I}$ and $\boldsymbol{W} = \left(\boldsymbol{c} + \boldsymbol{c}^0\right)^{-1}\boldsymbol{\delta c}$.

The convergence of the schemes (4)) and (5) are driven by the norm of the operators $\boldsymbol{\Gamma}^1\boldsymbol{Z}$ and $\boldsymbol{H}^1\boldsymbol{W}$, respectively. When no information is available on the microstructure of the heterogeneous material under consideration, an upper bound of the rate of convergence can be exhibited, considering that

$$\left|\left|\boldsymbol{\Gamma}^1\boldsymbol{Z}\right|\right| \leq \left|\left|\boldsymbol{Z}\right|\right|, \tag{6}$$

in the case of the fixed-point scheme, and that

$$\left|\left|\boldsymbol{H}^1\boldsymbol{W}\right|\right| \leq \left|\left|\boldsymbol{W}\right|\right|, \tag{7}$$

for the Eyre-Milton scheme. Several studies using this approach have been carried out to estimate the conditions of convergence of the iterative schemes.

It is possible to account explicitly for the microstructure by incorporating it in the operators entering the decomposition of $\boldsymbol{\Gamma}^1\boldsymbol{Z}$ and in $\boldsymbol{H}^1\boldsymbol{W}$. One can write

$$\boldsymbol{\Gamma}^1\boldsymbol{Z} = \sum_{r=1}^{N}\boldsymbol{\Gamma}^1\chi^{(r)}\boldsymbol{Z}^{(r)}, \quad \boldsymbol{Z}^{(r)} = \boldsymbol{c}^{0^{-1}}\boldsymbol{\delta c}^{(r)}, \tag{8}$$

and

$$\boldsymbol{H}^1\boldsymbol{W} = \sum_{r=1}^{N}\boldsymbol{H}^1\chi^{(r)}\boldsymbol{W}^{(r)}, \quad \boldsymbol{W}^{(r)} = (\boldsymbol{c}^{(r)} + \boldsymbol{c}^0)^{-1}\boldsymbol{\delta c}^{(r)}. \tag{9}$$

where $\chi^{(r)}$ is the characteristic function and $\boldsymbol{c}^{(r)}$ the elastic modulus of phase r.

Analytic properties of the effective moduli $\tilde{\mathbf{c}}$ as a function of the contrast between the phases can be used to extend the domain of convergence of the power series.

In the case of the conductivity of a two-phase composite, when it is known that the singularities of $\tilde{\mathbf{c}}$ lie in a interval $[-\beta, -\frac{1}{\beta}]$ more precise estimates of the convergence rates can be exhibited and the efficiency of the different iterative schemes can be compared according to the phase contrast and the value of β.

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