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Computational micromechanics: a variational derivation of FFT-based schemes

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It is a well-established result in the theory of linear composites that the local fields in such materials satisfy an integral equation which can be written symbolically as (Kröner, 1972; Willis, 1981; Milton, 2002; Jeulin, 2005)

$$(\mathbf{I} + \mathbf{\Gamma}^0 \delta \mathbf{L}) \boldsymbol{\varepsilon} = \mathbf{E}, \quad (1)$$

where $\boldsymbol{\varepsilon}$ is the local field under investigation, \mathbf{E} is its average, $\mathbf{\Gamma}^0$ is the Green's operator associated with a homogeneous reference medium \mathbf{L}^0 and $\delta \mathbf{L} = \mathbf{L} - \mathbf{L}^0$ is the deviation of the actual material properties of the composite from the homogeneous reference medium. As recognized by Kröner, this integral equation has the same form as the Lippmann-Schwinger (LS) equation in scattering theory.

The resolution of (1) requires the inverse of $\mathbf{I} + \mathbf{\Gamma}^0 \delta \mathbf{L}$. One of the earlier method to perform this inversion iteratively is based on a fixed point method:

$$\boldsymbol{\varepsilon}^{(k+1)} = -\mathbf{\Gamma}^0 \delta \mathbf{L} \boldsymbol{\varepsilon}^{(k)} + \mathbf{E}, \text{ i.e. } \boldsymbol{\varepsilon}^{(k)} = \sum_{j=0}^k (-\mathbf{\Gamma}^0 \delta \mathbf{L})^j \mathbf{E}. \quad (2)$$

This scheme with one of the phases as reference medium has been used by Brown (1955) to study the first few terms of the series and Moulinec and Suquet (1994) used an optimized reference medium, together with the discrete Fourier transform to turn the formal expansion (2) into an iterative computational scheme. Although the simple fixed point technique is quite efficient for composites with moderate contrast, it is sensitive to the choice of the reference medium and its convergence can be slow for materials with high contrast. Accelerated iterative methods have been proposed, and some of them have been used by D. Jeulin and his coworkers (Escoda et al., 2011). According to Mishra et al. (2016) conjugate gradient methods (see in particular Zeman et al., 2010; Gélébart and Mondon-Cancel, 2013) are among the most efficient existing techniques. However, as noted by these authors, the operator $\mathbf{I} + \mathbf{\Gamma}^0 \delta \mathbf{L}$ is not a self-adjoint operator (the corresponding matrix for the discrete problem is not symmetric) since the operators $\mathbf{\Gamma}^0$ and $\delta \mathbf{L}$ do not commute. So the use of biconjugate gradient methods is in principle required to solve (1).

The starting point of this study is the following question: *can the Lippmann-Schwinger operator be made self-adjoint by some magic?* The answer is "yes" (Schneider, 2017), the proof is elementary and relies on a simple change of scalar product (similar, but different from that used in Jeulin, 2005 p189).

The variational property of the LS equation opens new avenues for computational schemes. Its extension to constituents governed by one non-quadratic potential is straightforward. The extension to materials governed by two potentials relies on incremental variational principles (Mialon, 1986; Ortiz and Stainier, 1999; Bourdin et al., 2008; Michel and Suquet, 2016). Assume that the constitutive laws for each constituents can be written as:

$$\boldsymbol{\sigma} = \frac{\partial w}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}), \quad \frac{\partial w}{\partial \boldsymbol{\alpha}}(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) + \frac{\partial \varphi}{\partial \dot{\boldsymbol{\alpha}}}(\dot{\boldsymbol{\alpha}}) = 0, \quad (3)$$

where $\boldsymbol{\alpha}$ denote a set of internal variables. Then, after time-discretization with an implicit scheme (backward Euler), the fields (strain and internal variables) solution of the local problem (expressing equilibrium of the stress field, compatibility of the strain field with appropriate boundary) at time t_{n+1} has the variational property :

$$(\boldsymbol{\varepsilon}_{n+1}, \boldsymbol{\alpha}_{n+1}) = \underset{\langle \boldsymbol{\varepsilon} \rangle = \bar{\boldsymbol{\varepsilon}}}{\text{Argmin}} \underset{\boldsymbol{\alpha}}{\text{Argmin}} \langle w(\boldsymbol{\varepsilon}, \boldsymbol{\alpha}) + \Delta t \varphi \left(\frac{\boldsymbol{\alpha} - \boldsymbol{\alpha}_n}{\Delta t} \right) \rangle. \quad (4)$$

This variational property is used to derive computational schemes for the class of composites described by (3) which are significantly faster than the usual schemes.

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