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A filter-based computational homogenization method for handling non-separated scales problems

J. Yvonnet¹, A. Tognevi^{1,2}, G. Bonnet¹, M. Guerich²

¹ Université Paris-Est, MSME UMR 8208 CNRS, 5 Bd Descartes 77454 Marne-la-Vallée Cedex 2, France, julien.yvonnet@univ-paris-est.fr

² Département de Mécanique des Systèmes, Ecole Supérieure d'Ingénieurs Léonard de Vinci (ESILV), 92916 Paris la Défense Cedex, France

Résumé — In this work, a computational homogenization framework based on filters is proposed to handle homogenization with arbitrary scale separation. Classical homogenization is extended by using low-pass filters instead of averaging operators, leading to a naturally nonlocal elastic framework, where the kernel function is fully constructed by means of computations on a unit cell describing the microstructure. An associated Finite Element Framework is proposed to deal with heterogeneous structures containing inclusions with characteristic length of the same order than loading fluctuation wavelength.

Mots clés — Homogenization, Non-separated scales, Filter-based homogenization.

1 Introduction

Classical homogenization assumes separation of scales. This assumption is only valid when the characteristic fluctuation wavelength of an applied strain field over a given microstructure is supposed to be large compared with the scale of the microstructure. Otherwise, the scales are considered as *non-separated* and the overall effective behavior at a given point depends on the strain states at other points in the neighborhood, defining a nonlocal effective behavior. Several families of methodologies have been proposed to handle lack of scale separation [1, 2, 3, 4]. The objective of this work is to provide a new computational homogenization method able to handle arbitrary scale separation.

2 Mesoscopic description of mechanical fields by numerical filters

In [5, 6], a framework for homogenization able to handle arbitrary scale separation has been proposed by replacing averaging operators by numerical filters (Gaussian, or least-square-based).

First, we define two scales, one scale associated to fine scale strain and stress fields $\boldsymbol{\varepsilon}(\mathbf{x})$ and $\boldsymbol{\sigma}(\mathbf{x})$, and another (upper) scale called "Mesoscale", associated to strain and stress fields denoted by $\hat{\boldsymbol{\varepsilon}}(\mathbf{x})$ and $\hat{\boldsymbol{\sigma}}(\mathbf{x})$, respectively, and called "Mesoscopic" strain and stress fields. These fields are related to each other through the following relations :

$$\hat{\boldsymbol{\varepsilon}}(\mathbf{x}) = \mathcal{F}(\boldsymbol{\varepsilon}(\mathbf{x})), \quad \hat{\boldsymbol{\sigma}}(\mathbf{x}) = \mathcal{F}(\boldsymbol{\sigma}(\mathbf{x})), \quad (1)$$

where $\mathcal{F}(\cdot)$ is a linear operator, acting as a low-pass filter on the fine scale fluctuations. Associating \mathcal{F} with a characteristic length h related to the fluctuations observation at the mesoscale, the following properties are assumed for \mathcal{F} :

$$\lim_{h \rightarrow 0} \mathcal{F}^h(\boldsymbol{\varepsilon}(\mathbf{x})) = \boldsymbol{\varepsilon}(\mathbf{x}), \quad \lim_{h \rightarrow \infty} \mathcal{F}^h(\boldsymbol{\varepsilon}(\mathbf{x})) = \langle \boldsymbol{\varepsilon}(\mathbf{x}) \rangle. \quad (2)$$

In [6], we introduced a least-square-based filter in the form :

$$\mathcal{F}(\boldsymbol{\varepsilon}_{ij}(\mathbf{x})) = \sum_{p=1}^P M^p(\mathbf{x}) \hat{\boldsymbol{\varepsilon}}_{ij}^p, \quad (3)$$

where $M^p(\mathbf{x})$ are piece-wise polynomial basis functions (e.g. finite element shape functions) and $\hat{\boldsymbol{\varepsilon}}_{ij}^p$ are coefficients, interpreted as the nodal values of the mesoscopic strain field at some nodes of a coarse grid

associated with the mesoscopic mesh (see [6] for more details), for each component ij . These values are assumed associated with a compatible mesoscopic strain field.

Given the fine scale strain field $\varepsilon(\mathbf{x})$ on a discrete fine mesh composed of N nodes \mathbf{x}^m , $m = 1, \dots, N$, the unknown coefficients $\hat{\varepsilon}_{ij}^p$ are found by minimizing the following functional :

$$U = \sum_{m=1}^N \left(\sum_{p=1}^P M^p(\mathbf{x}^m) \hat{\varepsilon}_{ij}^p - \varepsilon_{ij}(\mathbf{x}^m) \right)^2. \quad (4)$$

Following [5], we then introduce the following split of microscopic strain into a filtered (mesoscopic) part and a remaining fluctuation $\tilde{\varepsilon}(\mathbf{x})$:

$$\varepsilon(\mathbf{x}) = \hat{\varepsilon}(\mathbf{x}) + \tilde{\varepsilon}(\mathbf{x}). \quad (5)$$

Let us consider a unit cell characterizing the microstructure defined in a domain $\Omega \in \mathbb{R}^D$, D being the dimension of the space, with boundary $\partial\Omega$. We define the following localization problem on the unit cell for non-separated scales : assuming known an applied (non-constant) mesoscopic strain field $\hat{\varepsilon}(\mathbf{x})$, find $\varepsilon(\mathbf{x})$ satisfying :

$$\nabla \cdot (\boldsymbol{\sigma}(\mathbf{x})) = 0 \quad \text{in } \Omega \quad (6)$$

and

$$\mathcal{F}(\varepsilon(\mathbf{x})) = \hat{\varepsilon}(\mathbf{x}) \quad \text{in } \Omega \quad (7)$$

with

$$\boldsymbol{\sigma}(\mathbf{x}) = \mathbb{C}(\mathbf{x}) : \varepsilon(\mathbf{x}) \quad (8)$$

where $\mathbb{C}(\mathbf{x})$ is a fourth-order elasticity tensor. Condition (7) is an extension of the classical averaging condition of homogenization in the case of separated scales. It can be interpreted as follows : the filtered part of the compatible strain field satisfying (6)-(8) must match $\hat{\varepsilon}(\mathbf{x}) \forall \mathbf{x} \in \Omega$. An iterative scheme has been proposed in [6] to enforce this condition.

3 Mesoscopic homogenized model

In this framework, we have shown in [5] that the constitutive law at the meso scale is given by :

$$\hat{\boldsymbol{\sigma}}(\mathbf{x}) = \int_{\Omega} \hat{\mathbb{C}}(\mathbf{x}, \mathbf{y}) : \hat{\varepsilon}(\mathbf{y}) d\mathbf{y}, \quad \hat{\mathbb{C}}(\mathbf{x}, \mathbf{y}) = \mathcal{F} \{ \mathbb{C}(\mathbf{x}) : \hat{\mathbb{A}}(\mathbf{x}, \mathbf{y}) \}, \quad (9)$$

where $\hat{\mathbb{C}}(\mathbf{x}, \mathbf{y})$ is a nonlocal elastic tensor defined in Ω . Note that the constitutive law (9) is general for linear filter operators satisfying conditions (2), and then remains valid when \mathcal{F} is chosen e.g. as a Gaussian filter. Another remark is that in contrast to classical nonlocal elasticity [1], the present nonlocal elasticity operator *does not have translational invariance*, i.e. $\hat{\mathbb{C}}(\mathbf{x}, \mathbf{y}) \neq \hat{\mathbb{C}}(\mathbf{x} - \mathbf{y})$. This constitutes a key feature of the the model to continuously define mesoscopic constitutive laws for arbitrary scale separation.

A discrete framework can be formulated as follows. Using (3), we define $\hat{\varepsilon}(\mathbf{x})$ in the form

$$\hat{\varepsilon}_{ij}(\mathbf{x}) \simeq \sum_p M^p(\mathbf{x}) \hat{\varepsilon}_{ij}^p \quad (10)$$

where the nodal values $\hat{\varepsilon}_{ij}^p$ are defined on a coarse grid discretizing the structure at the mesoscopic scale and M^p are interpolations functions. Using the filter operator \mathcal{F} defined by (3), we obtain the following relationships :

$$\hat{\boldsymbol{\sigma}}(\mathbf{x}) = \sum_p \hat{\mathbb{C}}^p(\mathbf{x}) : \hat{\varepsilon}^p, \quad \hat{\mathbb{C}}^p(\mathbf{x}) = \mathcal{F} \{ \mathbb{C}(\mathbf{x}) : \hat{\mathbb{A}}^p(\mathbf{x}) \}, \quad (11)$$

and

$$\hat{\mathbb{A}}^p(\mathbf{x}) = M^p(\mathbf{x}) \mathbb{I} + \Psi^p(\mathbf{x}) - \mathcal{F}(\Psi^p(\mathbf{x})), \quad (12)$$

where $\Psi^p(\mathbf{x})$ are transformation tensors associated to each node p of the coarse mesh on the unit cell, defined by :

$$\Psi_{ijkl}^p(\mathbf{x}) = e_{ij}^{p,(kl)}(\mathbf{x}), \quad (13)$$

where $e^{p,(kl)}$ is the strain solution field obtained by solving on the unit cell an elementary problem (see details in [6]) and where $\chi^{p,(kl)}(\mathbf{x})$ is a non-uniform eigenstrain prescribed over the support of $M^p(\mathbf{x})$ and defined as

$$\chi^{p,(kl)}(\mathbf{x}) = \frac{M^p(\mathbf{x})}{2} (\mathbf{v}_k \otimes \mathbf{v}_l + \mathbf{v}_l \otimes \mathbf{v}_k) \quad (14)$$

where \mathbf{v}_i are the base vectors of a Cartesian coordinate system. Then the local strain field can be re-localized by the relationship :

$$\boldsymbol{\varepsilon}(\mathbf{x}) = \sum_p \hat{\mathbb{A}}^p(\mathbf{x}) \hat{\boldsymbol{\varepsilon}}^p. \quad (15)$$

4 Numerical examples

The methodology is illustrated in the following example. A heterogeneous structure, as depicted in Figure 1 (b), is subjected to 4 points bending. The unit cell described in Fig. 1 (a) is used to compute the nonlocal constitutive operators described in section 3. Results in Figures 2 and 3 show that the proposed method allows reproducing both the simplified model (mesoscopic model) computed on a coarse grid, but also provides a good approximation for local fields, which can be obtained by post-treatment through localization rule (15). We also show the limits of classical homogenization methods and extended versions, in such situations when scales cannot be separated.

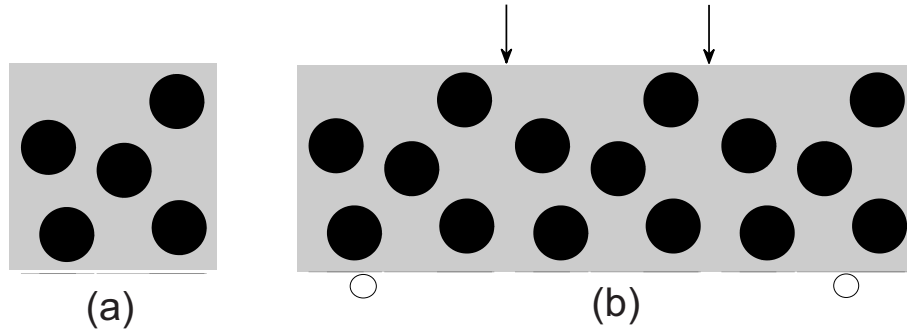


FIGURE 1 – (a) Unit cell ; (b) heterogeneous structure subjected to 4 points bending.

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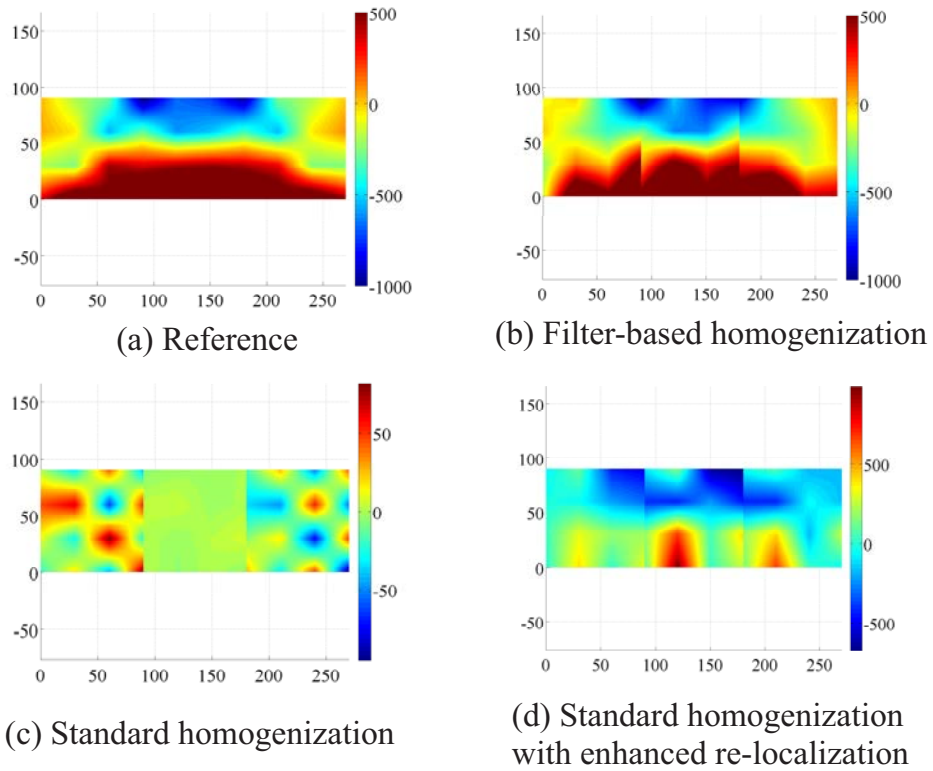


FIGURE 2 – Stress fields obtained at the mesoscopic scale (on the coarse grid) : comparisons between several models.

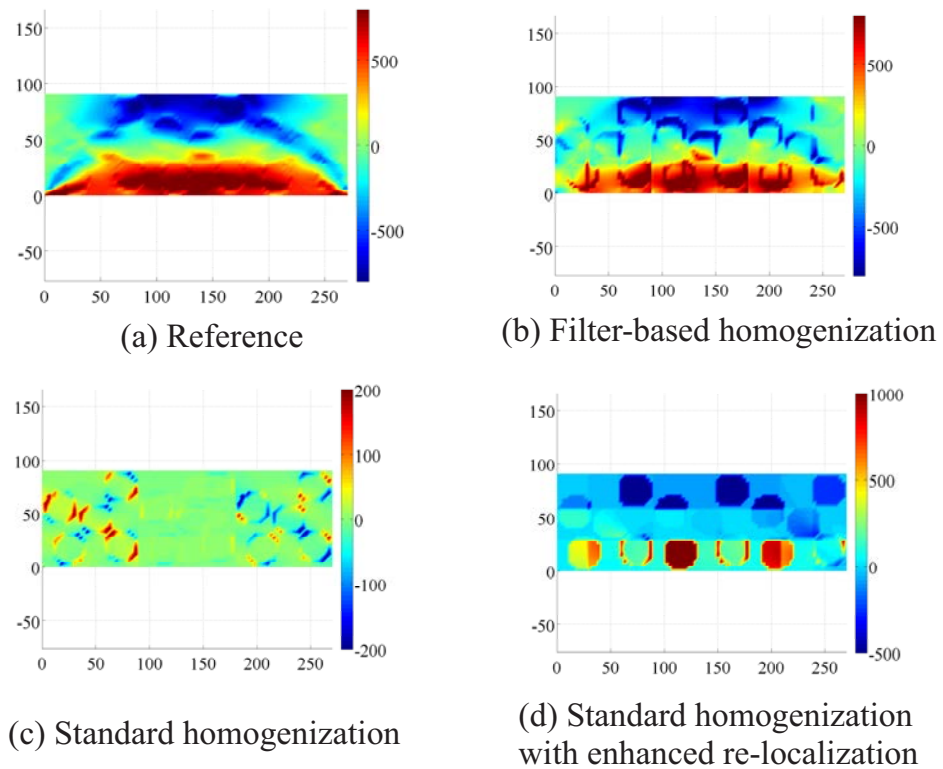


FIGURE 3 – Stress fields obtained at the microscopic scale (on the finest grid) : comparisons between several models.