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Domain decomposition methods to evaluate effective elastic properties of random fibre composites in the framework of the double-scale homogenization



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ABSTRACT

The paper deals with the evaluation of the effective elastic properties in the framework of domain decomposition. The field of random fibre composites, for which the network of heterogeneities is complex and leads to several numerical shortcomings, is considered. 2D representative volume elements (RVEs) of the composite are generated and some elastic properties are estimated with the help of the double-scale homogenization. Such methodology is reliable but turns out to be potentially inefficient due to the required size of RVEs. Two adaptations of domain decomposition methods in the framework of double-scale homogenization are proposed to drastically reduce the calculation costs: a Schur complement method, and a mixed Schur complement and FETI-1 method. Several numerical tests are performed which highlight reliability and efficiency of the first one in the present context.

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1. Introduction

Fibre composites could lead to interesting applications in the industrial field. Their lightness associated to a high stiffness, a good electrical conductivity and a low cost of production are major assets which arouse a great interest in the engineering community. Random fibre composites are composed of randomly distributed and oriented fibres. Experimental measurements are sometimes difficult to set up when, for example, we consider very small scales as in nanocomposites field. In the present paper, the framework of a numerical simulation of random fibre composites is considered in the prospect of the assessment of effective elastic properties. Such a kind of process requires the generation of representative volume elements (RVEs). An RVE can be defined as a volume V large enough to take into account enough informations on the microstructure of the medium (Hill, 1963; Hashin, 1983) and sufficiently small to limit the calculation cost and respect a minimum scale ratio with the macroscopic material (Kanit et al., 2003). Consequently, a key issue is related to the assessment of the dimensions of the RVE which strongly impact the validity of the numerical evaluation. Two methodologies are possible (1) One can construct a large RVE which includes a large number of heterogeneities, inclusions, voids, grains, fibres, ... (2) One can generate

a sampling of small RVEs for which effective properties are obtained from averaging the scope of results (Kanit et al., 2003; Pelissou et al., 2009). The second approach is known as being the most efficient (Leclerc et al., 2012; Leclerc et al., 2013) since large RVEs cannot be handled. However, a great care must be taken when choosing the dimensions of the small cells. Indeed an RVE has to be large enough to avoid a bias introduced by the boundary conditions (Sab, 1992; Ostoja-Starzewski, 1998) and ensure the accuracy of the macroscopic response (Drugan and Willis, 1996).

In the present work, our choice is to consider the second approach for which the size of the RVE is assessed according to the methodology of Kanit et al. (2003). A random draw of a complete set of morphological parameters, namely the length, diameter, orientation and spatial distribution of fibres, is set up to generate one RVE. In addition, intersections between two or more fibres are allowed which leads to a strongly entangled network of heterogeneities. Such a geometrical complexity requires a pixel-based finite element simulation to get round the tricky step of the mesh generation (Mishnaevsky, 2005). We consider the model with an n -order approximate geometry which was studied in this context and exhibited interesting results in calculation time (Leclerc et al., 2012; Leclerc et al., 2013). The basic idea consists in conceiving the mesh according to a structured grid of quadrangular elements the size of which is equal to the effective diameter of fibres. Thus, the critical shortcoming related to the complex geometry of the network of heterogeneities is a priori solved.

However, the required size of simulation grids are sometimes really important. For example, when the spatial distribution is

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inhomogeneous which leads to consider a large representative pattern to efficiently take into account the microstructure of the network of fibres (Jeulin and, 2005; Jeulin and Moreaud, 2006; Jeulin and Moreaud, 2006). The efficiency of the method is then drastically reduced causing the explosion of the calculation cost. One obvious solution in the current context of the fast development of multi-core computations is to use parallel strategies. Domain decomposition provides a solid mathematical framework which is modified to suit such a kind of process. Non-overlapping domain decomposition methods such as Schur complement (Agoshkov and Lebedev, 1985) and FETI-1 methods (Fahrat and Roux, 1227; Fahrat and Roux, 1994) have been extensively studied in this purpose during the last two decades. Thus, their robustness and scalability have been demonstrated and have led to numerous practical applications. Their great advantage is to reduce a global problem to an interface problem for which the degrees of freedom number is widely less important and the conditioning is improved. The Schur complement method is based on the displacements while the FETI-1 focuses on the Lagrange multipliers. Each concept has its own advantages and drawbacks.

The aim of the paper is to adapt the Schur complement and FETI-1 methods in the framework of the periodic double-scale homogenization (Bensoussan et al., 1978; Sanchez-Palencia, 1980). This latter is a powerful tool to assess effective elastic properties, particularly in the fibre composites field. Both domain decomposition methods are modified in such a manner that they directly provide mechanical coefficients such as Young's and shear moduli ones. Some numerical tests are performed on a set of 100 RVEs which are randomly generated depending on a complete set of morphological parameters. Each square representative pattern is subdivided into several similar subdomains for which the continuity on the inner interfaces and the periodicity on the outer ones are ensured. First the reliability of both methods is sequentially investigated. Results highlight their suitability in the context of high contrast heterogeneous media. Second C++ parallel algorithms are set up with the help of MPI libraries. Both issues of efficiency and ideal number of subdivisions are discussed. The paper is outlined as follows, (1) a reminder of both the theoretical framework of the double-scale homogenization and the associated optimization problem are done (2) A description of both modified domain decomposition methods is performed (3) Numerical results are provided to evaluate their reliability and efficiency in the framework of random fibre composites with a high contrast of properties.

2. Double-scale homogenization

This section is devoted to a reminder of the theoretical framework of the double-scale homogenization. We describe both the asymptotic principle which the method is based on and provide the associated variational formulation. Expression of homogenized elastic properties is provided in the context of domain decomposition.

2.1. Setting up

The variational formulation presented and proposed in this section is a generalization of the technique for the calculation of homogenized coefficients (Débordes, 1986) in an asymptotic framework (Bensoussan et al., 1978; Sanchez-Palencia, 1980). The basic idea consists in introducing an additional fictitious variable in test functions, which leads to a symmetric bilinear form taking into account two unknowns related to (1) the macroscopic strain field E (2) the microscopic strain field $e_{kl}(\mathbf{u})$. The artifice allows one to directly evaluate homogenized coefficients, but also

amounts to introducing a field representing the macroscopic stress one Σ . Therefore, this term becomes a changeable data for the variational problem and has to be imposed in such a clever way so that this one leads directly to homogenized coefficients. The choice of the variational formulation is related to the fact that, as we will show thereafter, this one is well adapted to the domain decomposition technique. This remains true providing that great care is taken in the treatment of periodic boundary conditions and internal nodes common to different subdomains.

In the general context of periodic homogenization, strain e and stress σ fields are supposed Y -periodic where Y is a unit cell (Bornert et al., 2001; Magoaric et al., 1675). The strain field $e_{kl}(\mathbf{u})$ is then described as the sum of E regardless to local fluctuations, and a Y -periodic displacement \mathbf{u}^{per} as follows,

$$e_{kl}(\mathbf{u}) = E + e_{kl}(\mathbf{u}^{per}) \quad (1)$$

where the average value of $e_{kl}(\mathbf{u}^{per})$ over Y is equal to zero.

In the context of linear elasticity and a periodic multi-scale approach, a localization problem for which E is given, leads to the following equation,

$$\begin{cases} -\operatorname{div} \sigma(\mathbf{u}^\varepsilon) = \mathbf{f} & \text{in } Y \text{ (+periodic b.c. on } \partial Y) \\ \sigma_{ij}(\mathbf{u}^\varepsilon) = C_{ijkl}^\varepsilon e_{kh}(\mathbf{u}^\varepsilon) \end{cases} \quad (2)$$

where C_{ijkl}^ε is the local stiffness tensor, \mathbf{f} is the loading and b.c. stands for boundary conditions. ∂Y represents the boundary of Y . From a theoretical point of view, ε is a positive real parameter which is supposed to tend to zero. Practically, this one is a very small parameter ($\varepsilon < 10^{-3}$) which is the ratio between a first scale called macroscopic and denoted as x , and a second one called microscopic and denoted as y . The displacement is denoted as \mathbf{u}^ε expanded according to the ε parameter. We seek for an asymptotic expansion as the form,

$$\mathbf{u}^\varepsilon(x, y) = \mathbf{u}^0(x) + \varepsilon \mathbf{u}^1(x, y) + \varepsilon^2 \mathbf{u}^2(x, y) + o(\varepsilon^2) \quad (3)$$

Hence, after expanding and reordering, we deduce the following expression of the strain tensor,

$$\begin{aligned} e_{kl}(\mathbf{u}^\varepsilon) &= e_{klx}(\mathbf{u}^\varepsilon) + \frac{1}{\varepsilon} e_{kly}(\mathbf{u}^\varepsilon) \\ &= \underbrace{(e_{klx}(\mathbf{u}^0) + e_{kly}(\mathbf{u}^1))}_{e_{kl}^0} + \varepsilon \underbrace{(e_{klx}(\mathbf{u}^1) + e_{kly}(\mathbf{u}^2))}_{e_{kl}^1} + o(\varepsilon) \end{aligned} \quad (4)$$

with,

$$e_{klx}(\mathbf{u}^h(x)) = \frac{1}{2} \left[\frac{\partial u_k^h}{\partial x_l} + \frac{\partial u_l^h}{\partial x_k} \right], \quad e_{kly}(\mathbf{u}^h(x)) = \frac{1}{2} \left[\frac{\partial u_k^h}{\partial y_l} + \frac{\partial u_l^h}{\partial y_k} \right] \quad (5)$$

where h denotes the h -th component of the asymptotic expansion of \mathbf{u}^ε . In addition,

$$\sigma_{ij}(\mathbf{u}^\varepsilon) = \underbrace{C_{ijkl}^\varepsilon (e_{klx}(\mathbf{u}^0) + e_{kly}(\mathbf{u}^1))}_{\sigma_{ij}^0} + \varepsilon \underbrace{C_{ijkl}^\varepsilon (e_{klx}(\mathbf{u}^1) + e_{kly}(\mathbf{u}^2))}_{\sigma_{ij}^1} + o(\varepsilon) \quad (6)$$

thus,

$$e_{kl}^h = e_{klx}(\mathbf{u}^h) + e_{kly}(\mathbf{u}^{h+1}) \quad \forall h \in \mathbb{N} \quad (7)$$

$$\sigma_{ij}^h = C_{ijkl}^\varepsilon (e_{klx}(\mathbf{u}^h) + e_{kly}(\mathbf{u}^{h+1})) \quad \forall h \in \mathbb{N} \quad (8)$$

Let us remark that e_{kl}^0 is then strongly analogous to the formulation of $e_{kl}(\mathbf{u})$ described in Eq. (1). Indeed, one can see $e_{klx}(\mathbf{u}^0)$ as the macroscopic strain field E and $e_{kly}(\mathbf{u}^1)$ as the microscopic periodic strain field the average over Y of which is equal to 0. In other words, the first order of the asymptotic expansion of $e_{kl}(\mathbf{u}^\varepsilon)$ leads to the classical formulation of the strain field in periodic homogenization theory.

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