Stochastic homogenization in the framework of domain decomposition to evaluate effective elastic properties of random composite materials : application to a 2D case of fiber composites

P. Karamian-Surville[1,2,3,a)] and W. Leclerc[1,2,3]

[1]Normandie Univ, France

[2]UNICAEN, LMNO, F-14032 Caen, France

[3]CNRS, UMR 6139, F-14032, Caen France

[a)]Corresponding author: philippe.karamian@unicaen.fr. Presenting author: philippe.karamian@unicaen.fr

ABSTRACT

The paper deals with the setting up of a stochastic homogenization method in the framework of domain decomposition. We focus our investigation on the random fibre composites in the elasticity field. We generate a random representative volume elements (RVE) of the composite and evaluate its elastic properties by the double-scale homogenization. We propose an adaptation of this latter in the domain decomposition framework in order to drastically reduce the calculation cost which is important in this context.

Keywords: Domain decomposition, RVE, Random composites materials,Stochastic homogeneization.

Introduction

Random fibre composites are difficult to model and study. The complexity of their strongly entangled network of fibres leads to technical drawbacks related to the mesh generation. In addition, their study requires the generation of large and numerous RVE during the numerical evaluation of the effective properties. Domain decomposition methods are efficient tools to decrease the calculation time which is important (give a value for example gain of 50% or 30%) in this context. Two adaptations of the homogenization method are proposed in this paper: a modified Schur complement method, and a combination of the FETI-1 method, and the method of Schur complement. In this article, we present both concepts and provide some relevant results demonstrating their ability in the context of random fiber composites. First, a 2D square RVEs with the help of random parameters describing the morphology of the network of fibres is generated. A meshing process, according to voxelisation approach of RVEs is made: the model with an n-order approximate geometry [2, 4, 6]. Then a finite element study is realized in order to estimate elastic properties with the help of the double-scale homogenization [1, 7]. In order to use the double-scale homogenization method we had to make two main adaptations. First, when generating the RVEs we take care of the continuity of fibers between each sub-domains, second we have to eliminate redundant information over the edges. The calculation is performed according to one of two proposed domain decomposition methods. The paper is outlined as follows. First, we present the minimization problem associated to the double-scale homogenization and describe both modified domain decomposition methods. Second, we provide some numerical results in effective properties.

Domain decomposition methods

This section is devoted to the implementation of the homogenization method in order to adapt it to the domain decomposition method. A brief recall of the equations governing a linear elastic boundary value problem is done. Two approaches of domain decomposition are proposed to solve it. The first method is the modified Schur complement method, whereas the second one, is a mixture of FETI-1 method and the Schur complement.

Setting up of the problem

Let Ω be a open bounded set of R^2 or R^3 . Let $\partial\Omega = \partial_1\Omega \cup \partial_2\Omega$ designates the border of Ω. The periodic multi-scale homogenization is a powerful tool to evaluate effective properties [1, 7]. The method consists in expanding some constitutive equations according to several scales of the medium. In the present contribution, we consider the framework of the linear elasticity. Thus,

$$\begin{cases} -div\sigma(\mathbf{u}^\epsilon) = \mathbf{f} \quad \text{a.e in} \quad \Omega \\ \sigma_{ij}(\mathbf{u}^\epsilon) = C^\epsilon_{ijkh} e_{khx}(\mathbf{u}^\epsilon) \\ e_{khx}(\mathbf{u}^\epsilon) = \frac{1}{2}(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}) \\ \sigma_{ij}(\mathbf{u}^\epsilon) n_j|_{\partial_1\Omega} = F_j \\ \mathbf{u}^\epsilon|_{\partial_2\Omega} = \mathbf{O} \end{cases} \tag{1}$$

where σ is the stress tensor, e is the strain-displacement, C^ϵ_{ijkh} is the local stiffness tensor, $\mathbf{f}$ is the loading and $\mathbf{u}^\epsilon$ is the displacement which is expanded according to the ϵ parameter. We suppose a pseudo-periodic medium and consider a two-scale expansion of Equation 1. The first scale called macroscopic is denoted as x, and the second one called microscopic is denoted as y. Variational considerations lead to a new formulation of the equations at the macro-scale which take into account the local disruptions related to the heterogeneities. Hence, we can extract the following formulation of the effective stiffness tensor,

$$\tilde{C}_{ijkl} = \frac{1}{|Y|} \int_Y C_{ijmn} \left[\delta_{mk}\delta_{nl} + e_{mny}\left(\omega^{kl}(y)\right) \right] dy \tag{2}$$

Y denotes the periodic cell and $|Y|$ its volume. C_{ijmn} is the local stiffness tensor which depends on both the medium (heterogeneity or matrix) and the corresponding behaviour law. ω^{kl} is a local solution in the cell with periodic boundary conditions. Thus, the effective tensor turns out to be the sum of the mean of properties and a corrective term related to the local disruption at the microscopic scale.

Partitioning of the RVEs

We generate 2D square RVEs according to a set of random parameters describing the complex microstructure of a random fibre composite. The RVEs are conceived and meshed according to the technique outlined in [4] and with the help of CASTEM we generate properly the RVEs. The basic idea consists in approximating the real geometry according to a grid of quadrangular elements. Such a concept turns out to be suitable in the framework of domain decomposition due to the uniformity of the elements. Thus, we evenly subdivide the RVEs into several square subdomains without remeshing. The similarity between the RVE and each subdomain enables us to denote them as sub-RVEs. Figure 1 illustrates an example of partitioning of a RVE into four sub-RVEs. One can notice that we consider non-overlapping domains, both the periodicity and the continuity of fiber at the interfaces are ensured by taking a special care to maintain the geometrical continuity so that they match together once the sub-domains are together. Γ^i designates the set of inner boundaries, and Γ^e the set of outer boundaries. $\Gamma = \Gamma^i \cap \Gamma^e$ represents the gathering of the both previous sets. Ω_n represents the area of the nth subdomain.

Modified Schur complement method

In a first approach, we adapt the Schur complement method to the calculation of effective properties by the double-scale homogenization. Once Equation 1 is descretized using finite elements, for the considered example (see Figure 1) in which we consider four subdomains, this one leads to a discrete system which reads as follows:

$$\underbrace{\begin{bmatrix} K_{11} & 0 & 0 & 0 & \tilde{K}'_{\Gamma 1} \\ 0 & K_{22} & 0 & 0 & \tilde{K}'_{\Gamma 2} \\ 0 & 0 & K_{33} & 0 & \tilde{K}'_{\Gamma 3} \\ 0 & 0 & 0 & K_{44} & \tilde{K}'_{\Gamma 4} \\ \tilde{K}_{\Gamma 1} & \tilde{K}_{\Gamma 2} & \tilde{K}_{\Gamma 3} & \tilde{K}_{\Gamma 4} & \tilde{K}_{\Gamma\Gamma} \end{bmatrix}}_{\mathbf{K}} \underbrace{\begin{bmatrix} \omega^{kl}_1 \\ \omega^{kl}_2 \\ \omega^{kl}_3 \\ \omega^{kl}_4 \\ \tilde{\omega}^{kl}_\Gamma \end{bmatrix}}_{\mathbf{u}} = \underbrace{\begin{bmatrix} \mathbf{f}^{kl}_1 \\ \mathbf{f}^{kl}_2 \\ \mathbf{f}^{kl}_3 \\ \mathbf{f}^{kl}_4 \\ \tilde{\mathbf{f}}^{kl}_\Gamma \end{bmatrix}}_{\mathbf{f}} \tag{3}$$

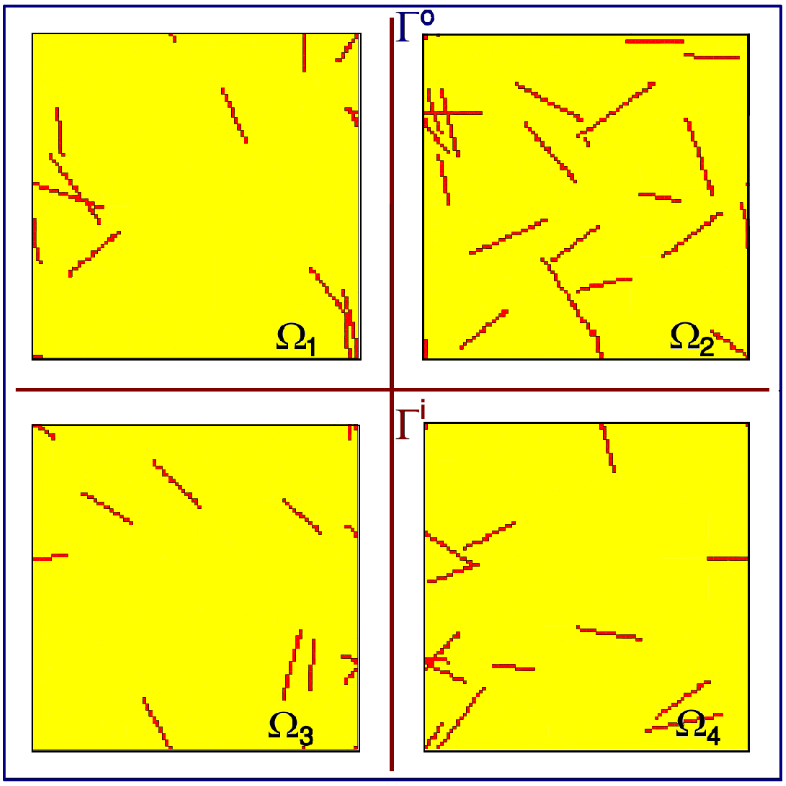

Figure 1: Partitioning of a RVE in 4 subdomains

K_{ii} designates the stiffness tensor of the ith subdomain, ω_i^{kl} is the microscopic displacement and $\mathbf{f}_i^{kl}$ the applied strength which is zero in the present context. $\tilde{K}_{\Gamma i}$ is typically the tensor of the nodes located on the boundary Γ for each subdomain i. $\tilde{\omega}_{\Gamma}^{kl}$ is the vector of solutions in both displacement on the boundary and homogenized coefficients. Generally speaking, the $\tilde{}$ denotes 3 additional terms in 2D (6 in 3D) relative to the assessment of elastic coefficients. Practically, the solving is realized with the help of a new system $S\,\mathbf{u}_\Gamma = \mathbf{b}$ where S is the Schur complement and $\mathbf{b}$ its corresponding second member which is equal to $\tilde{\mathbf{f}}_\Gamma^{kl}$. We have,

$$S = \tilde{K}_{\Gamma\Gamma} - \sum_i \tilde{K}_{\Gamma i} K_{ii}^{-1} \tilde{K}'_{\Gamma i} \tag{4}$$

Mixed FETI-1 and Schur complement method

We propose an adaptation of the FETI method in the framework of the double-scale homogenization. The method is the dual of the Schur complement one in the sense that the interface problem is formulated in Lagrange multipliers and not in displacements. We consider the basic form of the process called FETI-1 [2, 3]. Different modifications have to be performed to adapt the approach to the double-scale homogenization. First, the hypothesis of periodicity leads to practical difficulties related to an excessive number of rigid body modes when taking into account by Lagrange multipliers. A possible way to get round the drawback is to rewrite the problem in another base which leads to the appearance of unsuitable coupling terms between subdomains. Our choice is to consider the periodicity on the outer boundaries Γ^e by the primal Schur complement. Hence, we talk about a mixed FETI-1 and Schur complement method. Second, we must consider additional terms related to the homogenized coefficients. The terms are added to the tensor describing the connections on the outer boundaries and consequently taken into account by the Schur complement as well. Thus, the only connections on the inner boundaries are described by Lagrange multipliers. Under these hypotheses, the matrix-vector system to solve is similar to the previous one,

$$\begin{bmatrix} K_{11} & 0 & 0 & 0 & R'_1 \\ 0 & K_{22} & 0 & 0 & R'_2 \\ 0 & 0 & K_{33} & 0 & R'_3 \\ 0 & 0 & 0 & K_{44} & R'_4 \\ R_1 & R_2 & R_3 & R_4 & K_R \end{bmatrix} \begin{bmatrix} \omega_1^{kl} \\ \omega_2^{kl} \\ \omega_3^{kl} \\ \omega_4^{kl} \\ \Lambda^{kl} \end{bmatrix} = \begin{bmatrix} \mathbf{f}_1^{kl} \\ \mathbf{f}_2^{kl} \\ \mathbf{f}_3^{kl} \\ \mathbf{f}_4^{kl} \\ \mathbf{f}_R^{kl} \end{bmatrix} \tag{5}$$

where R_i and K_R are two tensors describing the connections at the interfaces and, $\mathbf{f}_i^{kl}$ and $\mathbf{f}_R^{kl}$ the second members corresponding to the subdomains and the interfaces respectively. Such a system can not be directly solved by the conjugate gradient method because of the floating subdomains. A classical FETI interface problem has to be performed on the Lagrange multipliers, for which a second level of multipliers are provided by the rigid body modes. The new system is then solved by a preconditioned conjugate gradient and leads us to a direct assessment of the homogenized coefficients.

Numerical results

Algorithms of the two previous methods have been implemented in C++ language. The present section provides some numerical results obtained from the modified Schur complement method. Effective elastic properties are assessed and compared with a direct calculation.

Hypotheses

We consider a set of 2D unit RVEs for which the fibres are randomly oriented and distributed. A special care is carried out to guarantee the periodicity, this treatment is ensured during the generation of the RVE with the help of the n-order approximate geometry to build meshes. The length and the width of each heterogeneity is fixed at 0.2 and 0.01 respectively, and we suppose no curvature. Each RVE is subdivided into 4, 9, 16 and 36 non-overlapping subdomains. We suppose the continuity of the medium as well as the connection of the meshes on the boundaries of each part. Thus, one heterogeneity can be located on several domains and crosses several inner boundaries. The density of fibres is randomly distributed between 0 and 30 fibres per unit cell. The meshes are generated according to the concept of 0-order approximate geometry. In other words, each inclusion is approximated by a grid of quadrangular elements the size of which is equal to the diameter of the heterogeneities. The elastic properties are assessed in two steps. First, we evaluate some coefficients for each RVE with the help of the modified Schur complement method. Second, we take the average of the results obtained from a complete set of representative patterns. The suitable number of realizations is estimated according to statistical considerations. Each fibre is supposed to follow a transverse isotropic behaviour law. The longitudinal and transverse Young's modulus are set at 1050 and 600 GPa respectively. The shear modulus is set at 450 GPa. The matrix is an isotropic polymer resin with Young's and shear moduli set at 4.2 and 1.55 GPa respectively. We deliberately choose a high-contrast of properties to maximise the conditioning of the matrix in the solving which one is realized by a preconditioned conjugate gradient.

Elastic moduli

A sample of 86 RVEs is built according to the previous hypotheses. Figure 2 exhibits the evolution of the effective Young's modulus depending on the density of fibres for different levels of partitioning. A comparison is realized with a usual direct calculation performed on the same sample of representative patterns without partitioning. One must keep in mind that we consider the same grid of quadrangular elements whatever the level of subdivision is such that the degrees of freedom number is constant. Globally the differents curves fit together which highlights the consistency of the method. However, the greater both the number of fibres and subdomains are the more some small discrepancies are observable between the different curves. Thus, the relative error is 3.48% between the calculation realized with 36 subdomains and the direct calculation for a density of fibres set at 30.

"Once the RVEs are split into several subdomains in order to guarantee the continuity of fibres through the interfaces, we have to replace some elements labelled as matrix in fibre. This process ensures the continuity of cross fibres, but modifies the rate of matrix for the global RVES, especially for a high contrast of properties of fibre and a large number of subdomains, what leads an effect on the calculation of the effective mechanical properties and explains why we observe a discrepancies on numerical results between the global RVEs, and RVEs, themselves divided into several subdomains."Figure 2 illustrates

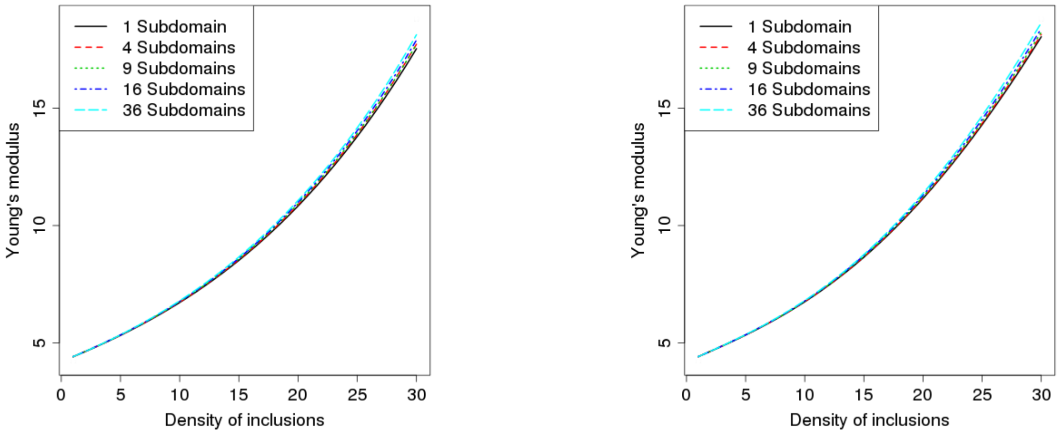

Figure 2: Influence of the density of fibres on the effective Young's modulus in the case of a direct calculation

the same results in the case of a direct calculation of the matrix-vector system of Equation 3 with partitioning. One can observe the same discrepancies as previously seen in the case of a domain decomposition calculation.

Conclusion

Two domain decomposition methods have been adapted and set up to evaluate elastic properties of a random fibre composite with the help of the double-scale homogenization. Both modified Schur complement method and mixed FETI-1 Schur complement method take into account some additional tensors related to both the homogenized coefficients and the hypothesis of periodicity, but are solved as classical ones. Numerical results highlight the consistency of the modified Schur complement method in the framework of a high entanglement of fibres and a high contrast of properties between the matrix and the heterogeneities.

Acknowledgement

The authors wish to thank the High-Performance Computing Centre of Normandie (CRIAAN) for the computing means put at their disposal.

References

[1] A. Bensoussan, J.L. Lions and G.C. Papanicolaou. Asymptotic analysis for periodic structures. Springer, North Holland, Amsterdam edition, 1978.

[2] C. Fahrat and F.X. Roux. A method of finite element tearing and interconnecting and its parallel solution algorithm. International Journal of Numerical Methods in Engineering, 32:1205 – 1227, 1991.

[3] C. Fahrat and F.X. Roux. Implicit parallel processing in structural mechanics. Computational Mechanics Advances, North Holland, 2(1):1 – 124, 1994.

[4] W. Leclerc, P. Karamian and A. Vivet. An efficient stochastic and double-scale model to evaluate the effective elastic properties of 2D overlapping random fibre composites. Computational Science of Materials, 481 – 493, 2013.

[5] W. Leclerc, P. Karamian, A. Vivet and A. Campbell. Numerical evaluation of the effective elastic properties of 2D overlapping random fibre composites. Technische Mechanik, 32:358 – 368, 2012.

[6] L. Mishnaevsky Jr. Automatic voxel-based generation of 3D microstructural FE models and its application to the damage analysis of composites. Material Science and Engineering A, 407(1-2):11 – 23, 2005.

[7] E. Sanchez-Palencia. Non-homogeneous media and vibration theory. Springer, Berlin, 127, 1980.