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An advanced numerical method for predicting effective elastic properties of heterogeneous composite materials

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ABSTRACT

This paper presents a new numerical methodology for predicting the effective elastic properties of composite materials. The material microstructure was generated in a repeated unit cell, the so-called representative volume elementary (RVE) using a developed microstructure generator. The homogenisation was first performed using the variational asymptotic method for unit cell homogenisation (VAMUCH) and by applying the eXtended Finite Element Method (XFEM) directly. Moreover, we propose a new methodology to introduce the XFEM into the VAMUCH principle. Thus, the obtained new scheme (i.e. the eXtended VAMUCH) uses the Variational Asymptotic Method on nonconforming meshes. All the implemented methods were validated and compared each other using existing benchmarking tests, then more complex microstructures are investigated. The obtained results were globally very well in agreement. The proposed methodology was found efficient to determine accurately the composite properties and showed several advantages.

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1. Introduction

Effective properties of heterogeneous materials can be identified using experimental tests, analytical homogenisation models or numerical homogenisation procedures, see [1–4]. However, an important class of heterogeneous materials have a periodic microstructure where modelling the behaviour requires specific treatment. For instance, the interaction between constituents is not taken into account in mean field based methods. Moreover, it has been proven that the spatial variability in the microstructure influences the overall behaviour of the material. Hence, the choice of the representative volume elementary (RVE) is crucial in the homogenisation procedure. Homogenisation based on Finite Element Method (FEM) that uses the RVE concept is increasing in these last decades. In such methods, the FEM can be introduced directly by considering periodic boundary conditions under some special loadings. Another accurate method that uses the FEM to approximate a virtual displacement is called the variational asymptotic method for unit cell (UC) homogenisation (VAMUCH). The effective properties can be obtained by considering periodic boundary conditions applied to the RVE without any loading. These FEM based methods are very attractive and accurate however they suffer from the FEM drawbacks such as the requirement of the mesh to be aligned to the discontinuities. Another limitation is the distortion of the finite elements under large deformation and the necessity of remeshing when the geometries evolve. To alleviate these drawbacks, the eXtended Finite Element Method (XFEM) is introduced. The XFEM has been successfully applied to different problems such as crack modelling and crack growth in layered composite structures [5–12]. The mesh can be non-conform to the material discontinuities and/or boundaries and no re-meshing is required. Basically, the concept of the XFEM is the enrichment of the shape functions of the elements crossed by the discontinuities or the singularities by special functions using the partition of unity principle. The expression of these functions depends on the nature of the discontinuity (i.e. weak discontinuity, strong discontinuity) and the singularity as well as the nature of the medium (i.e. dense, porous). To perform easily and efficiently the enrichment, XFEM adopts the level set function concept; first to locate discontinuities and in many cases to express the enrichment functions. For instance, the signed distance between nodes and inclusion/matrix interfaces distinguishes inclusions from the matrix boundaries. This is achieved by the change of the level set function sign, consequently the interface is located implicitly by the zero level set.

This paper provides two methodologies to predict the material effective properties; the direct XFEM based homogenisation and the XFEM coupled with VAMUCH, see [13]. Because the two schemes use the RVE concept, we have first developed an algorithm able to generate randomly microstructures. The inclusions shape and volume fraction can be tailored automatically where

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periodicity of the microstructure is respected and the overlapping of inclusions is avoided. Once the microstructure is generated, a level set function is calculated on the mesh nodes (structured quadrilateral mesh in most cases) by which all the inclusion/matrix interfaces are located. XFEM allows the mesh to be not aligned with the interfaces and the jump in deformation caused by the material mismatch is handled by the introduction of the enrichment functions. In our model, this weak discontinuity is enhanced by using the modified absolute function introduced in [7]. After that, the periodic boundary conditions are applied to the RVE in both schemes.

The paper proposes an efficient method for predicting the effective elastic properties of the composite without any tedious tasks linked to the mesh requirements in one hand and capable to take into account complex geometries and interaction between constituents in the other hand. Thus, whatever the degree of complexity of the used RVE, simple regular meshes can be used to perform the homogenisation. This fact makes an enormous difference between the proposed method and FEM based methods. To validate the implemented method, the obtained results are compared with those obtained using linear averaging relations and those reported in the literature.

The paper is arranged as follows: first, the micro-structure generation algorithm is presented, then the concept of XFEM and level set function is briefly reviewed and adapted to the context of composite materials, then the discretization of the governing equations is reported. XFEM and VAMUCH Homogenisation techniques are detailed in the third section. Further, several numerical applications are performed to compare between the two schemes and to discuss the obtained results. Finally, the paper is ended by a brief conclusion.

2. Microstructure generator

Models with periodic boundaries are usually used to simulate bulk material structures. Our developed algorithm is designed to simulate 2D microstructures (it can be extended to 3D case). Knowing the volume fracture of the composite and the inclusions size, the number of inclusions is first calculated using Eq. (1). Within a generated RVE, the inclusions size is kept constant and their shape is assumed to be elliptical in the general case (circular shaped inclusions are special case). The inclusions are generated in a target square using the random sequential addition (RSA). Each inclusion centre $(x_c,\ y_c)$ will be on a random location in the target space (commonly, RVE space of 1×1 area).

$$n_{inc} = v_f\, A/(\pi\, l_s\, l_b). \tag{1}$$

In Eq. (1), n_{inc} is the total number of inclusions, v_f is the inclusions volume fraction, A is the RVE area, $l_s,\ l_b$ are respectively, one-half of the ellipse's major and minor axes. The random location of the ellipse centre leads to situations where part of the inclusion penetrates the sample external boundaries (rigid boundaries). In this case and in order to produce periodic distribution, the inclusion is cut along the concerned edge and the excess part is reproduced in the inner part of the opposite edge. This automatic procedure is activated for every inclusion/edge intersection. Another important condition to be respected when generating the microstructure is the minimal allowed distance d_{min} between inclusions. This condition is necessary to perform an efficient meshing of the domain and avoids overlapping of inclusions. It is found that the optimal minimal allowed distance is given by: $d_{min} = 0.035\ l_s$, see [14]. The main followed steps to build a randomly distributed elliptical inclusions with a given volume fraction is summarised in the flowchart of Fig. 1. Noteworthy, the computational time is proportional to the volume fraction, this is due to the increase of the trial steps number. The minimal allowed distance between inclusions is the main factor undermining the generation process, it imposes severe restrictions on the volume fraction in some cases. In order to reduce the computation cost, this condition is checked between two points from two neighbour inclusions if and only if the distance between the two fictitious enveloping circles is little than the allowed distance, as depicted in Fig. 2. These fictitious circles have the same centre as the elliptic inclusions and have a radius of l_b.

Once the total number of inclusions is reached, the inclusions centre coordinates $(x_{ci},\ y_{ci})$ and the ellipses orientation angles θ_i are saved and the microstructure generation is achieved. In the next step, a level set function is calculated for the XFEM homogenisation requirements and an implicit representation of the obtained RVE can be performed. For comparison purposes, in this work we added an extra task needed for FEM based homogenisation which consists to draw explicitly the obtained microstructure. The final configuration is sent to a *GMSH* meshing software, see [15], where the RVE is meshed by triangular conforming elements which are required for standard VAMUCH homogenisation.

3. Homogenisation procedure

The RVE concept was used to develop analytical homogenisation models for linear elasticity after which many methods have been emerged. However, most of these methods consider RVEs with simple geometries and do not take into account inclusions interaction. Recently, more sophisticated methods are introduced e. g. effective self-consistent scheme (ESCS) or interaction direct derivative (IDD) and showed high performances regarding to their preceding ones, see Zheng and Du 2001, Du and Zheng 2002. Commonly, the FEM is very used to model the mechanical response, but the XFEM is preferred when domains present complex geometries or evolving boundaries, and the fundamentals of the homogenisation scheme remain the same. These so-called unit cell methods can handle easily the complexity of the microstructure and take into account the interaction between inclusions.

3.1. Homogenisation using VAMUCH

VAMUCH micromechanical model was introduced by Yu and Tang [13], it consists to expand the energy functional asymptotically with less assumption regarding to the mathematical homogenisation theory (MHT). VAMUCH has many specific advantages mainly the fact that no external loading is needed to perform the computation and the effective material properties are obtained after only one analysis. The problem formulation consists to minimise the following functional of the total potential energy within the UC, see Yu and Tang [13], and Koutsawa et al. [16] (see Fig. 3).

$$\Pi = \sum_{n=-\infty}^{\infty} \int_{\Omega} \frac{1}{2} C_{ijkl}(x_1, x_2, x_3)\epsilon_{ij}\epsilon_{kl} dV, \tag{2}$$

where n stands for the number of the repeated unit cells that form an imaginary unbounded and unloaded heterogeneous material which has the same micro-structure as the loaded and bounded one, $\mathbf{C}$ is the fourth order elasticity tensor of each UC constituents, ϵ is the strain tensor defined in the local cartesian coordinate system which is centred at the middle of the UC and $\mathbf{x} = (x_1, x_2, x_3)$. During the minimisation, the following constraints should be respected

$$\boldsymbol{\chi}_i\left(x_1 = -\frac{d_1}{2}, x_2, x_3\right) = \boldsymbol{\chi}_i\left(x_1 = +\frac{d_1}{2}, x_2, x_3\right), \tag{3}$$

$$\boldsymbol{\chi}_i\left(x_1, x_2 = -\frac{d_2}{2}, x_3\right) = \boldsymbol{\chi}_i\left(x_1, x_2 = +\frac{d_2}{2}, x_3\right), \tag{4}$$

$$\boldsymbol{\chi}_i\left(x_1, x_2, x_3 = -\frac{d_3}{2}\right) = \boldsymbol{\chi}_i\left(x_1, x_2, x_3 = +\frac{d_3}{2}\right), \tag{5}$$

$$\langle \boldsymbol{\chi}_i \rangle = 0. \tag{6}$$

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