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An iterative analytical model for heterogeneous materials homogenization

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ABSTRACT

The purpose of this study was to establish a method based on an iterative scheme to approximate the numerical solution obtained from finite elements analysis for an RVE in two and three dimensions based on the homogenization concept for the assessment of the effective properties. The bounds of Hashin–Shtrikman and Voigt–Reuss were considered in the iterative process based on an updating of the constitutive relations of these models respectively. In this study, by assumption, we took the particular case of the heterogeneous materials with several elastic isotopic phases. The output variables considered using the iterative process are the bulk, shear modulus and the thermal conductivity. We have found a fast convergence of the iterative solution to the numerical result with a suitable concordance between the two solutions at the final step.

1. Introduction

In the last decades, the computational material science received a great interest from many researchers. Many theories and methods based generally on finite elements analysis were developed successfully in order to study the behavior of homogeneous materials. Many sophisticated models were established to get the optimal solution of the materials behavior taking into account many parameters. These methods are limited when we consider the microscopic aspect of the materials related to the complexity of their behavior and the different phases of their microstructure. The traditional constitutive models fail to give a realistic solution for this category of materials. In recent years, the homogenization method is increasingly used to study the behavior of heterogeneous materials, this concept is considered to be the best solution to set a bridge between the micro and the macro scales. Big progress has been made since the pioneering works of Hill [1] on the concept of the RVE (Representative Volume Element) which contains a sufficient number of heterogeneities to be representative for the whole microstructure. A deeper definition is given later by Sab [2] stating that the RVE is representative only if the solution obtained is independent of the boundary conditions. Recently, many works were published on the numerical homogenization for different types of materials such as elastic–plastic composite materials from the behavior point of view [3,4] and to study the reinforcement of composites effect on the overall response [5–8], the thermal conductivity, the microstructure type effects [9], porous materials response in terms of thermal conductivity [10] and the void shape effect when a porous media is considered [11]. The other homogenization method known as the 'analytical' method which consists on using boundary models based on upper and lower bounds to establish an interval which contains the exact solution. Among the various analytical methods available, we can name the first mathematical theories of the homogenization which use asymptotic developments of the mechanical properties [12–14]. There are also, many bounds widely used in mechanical science and physics of solids to frame the properties of heterogeneous material. There are many kinds of bounds which are differentiated by the accuracy of the description of the micro structure. The lower and upper bounds are nearer when the knowledge of the microstructure is better. The most used bounds are the upper and lower bounds of Voigt–Reuss [15,16] and those of Hashin–Shtrikman [17]. Finally, theoretical estimations allow, with some assumptions, the assessment of effective properties of heterogeneous materials. They present the advantage of approaching with more accuracy the effective properties of heterogeneous materials in comparison to the bounds. An estimation can be obtained from a micromechanical approach like the self–consistent model [18], or from variational principles [19]. In this work we proposed a new approach based on the upper and lower bounds of different orders for the heterogeneous materials including an iterative process to approach the numerical solution obtained from finite element analysis in order to obtain the overall mechanical and thermal properties of heterogeneous materials efficiently and rapidly.

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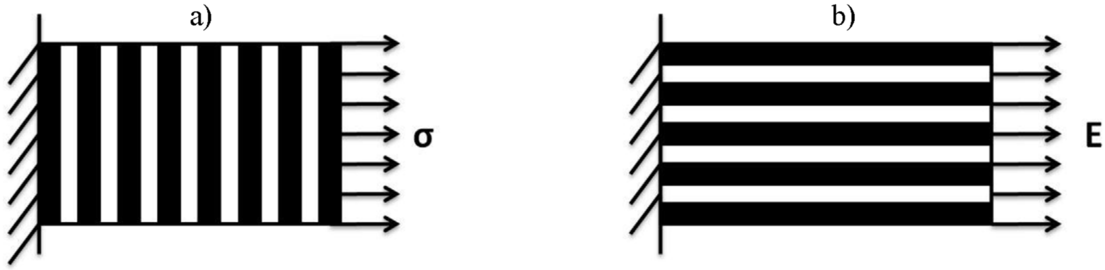

Fig. 1. Geometric interpretations of the first order bounds a) Voigt, b) Reuss.

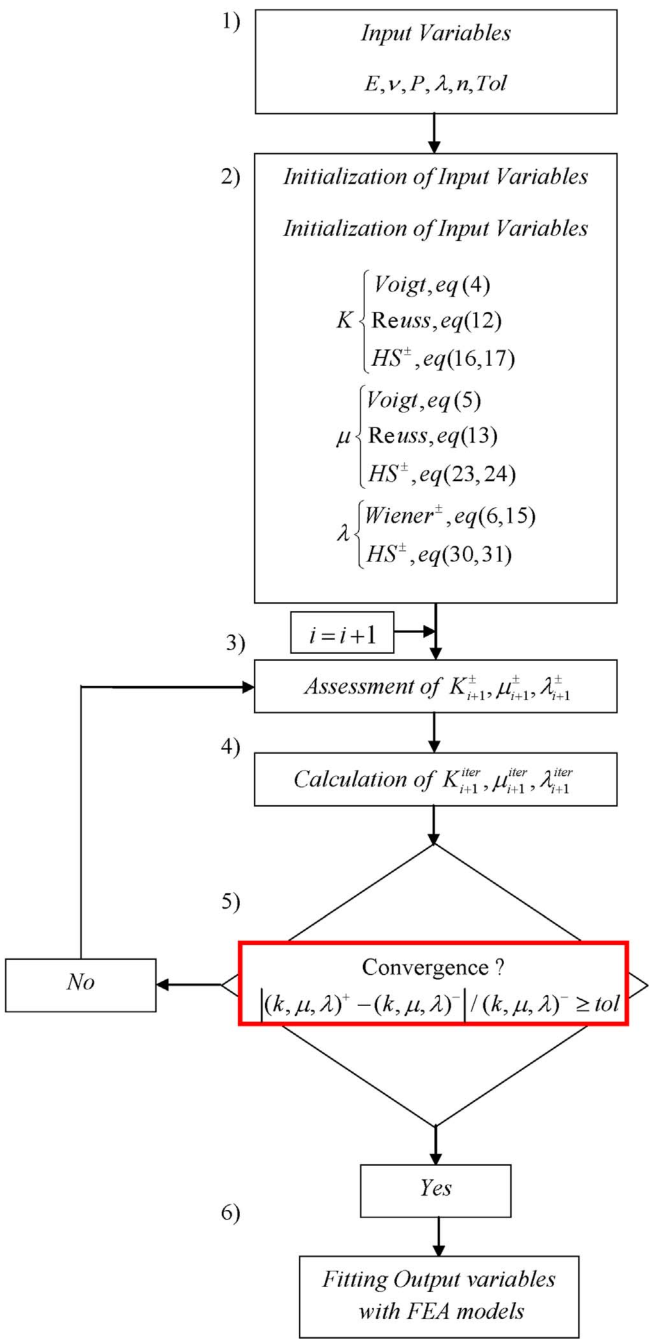

Fig. 2. The iterative scheme resolution flowchart.

2. Homogenization analytical models

2.1. First order bounds

Voigt [15] and Reuss [16] proposed simple approximations for the determination of effective elastic properties of heterogeneous materials, their assumptions have a physical significance as illustrated in Fig. 1. The Voigt approach is suitable for different materials connected in parallel to the applied load when the Reuss model is suitable for the materials connected in series.

2.1.1. The lower bound of Voigt

2.1.1.1. Elastic properties. The Voigt bound matches the assumption that the strain tensor of both the inclusion and matrix are equal to the applied mean strain E_{ij}:

$$\langle \varepsilon_{ij} \rangle = E_{ij} \tag{1}$$

The strain localization tensor is reduced everywhere to the unit tensor:

$$A_{ij}(x) = I_{ij} \tag{2}$$

The expression of equivalent stiffness tensor which leads to the expression of the upper bound of Voigt is as follows:

$$C_{ijkl}^{Voigt} = \sum_{ph=1}^{N} P_{ph}(c_{ijkl})_{ph} \tag{3}$$

For isotropic elasticity, the Voigt bound corresponds to the relations of the bulk and shear modulus is:

$$k^{voigt} = \sum_{ph=1}^{N} P_{ph} k_{ph} \tag{4}$$

$$\mu^{voigt} = \sum_{ph=1}^{N} P_{ph} \mu_{ph} \tag{5}$$

2.1.1.2. Thermal conductivity. In thermal conductivity, the Weiner bound [21] corresponds to the relation of the conductivity modulus as:

$$\lambda^{Wiener+} = \sum_{ph=1}^{N} P_{ph} \lambda_{ph} \tag{6}$$

2.1.2. The lower bound of Reuss

2.1.2.1. Elastic properties. The Reuss bound [16] is the inverse assumption which consider this bound as constant in all phases and equal to the macroscopic imposed stress σ_{ij} as:

$$\langle \sigma_{ij} \rangle = \Sigma_{ij} \tag{7}$$

Stress localization tensor is reduced everywhere to the unit tensor:

$$B_{ijkl}(x) = I_{ijkl} \tag{8}$$

The expression that leads to the flexibility equivalent tensor is: