

**EVALUATION OF EFFECTIVE ELASTIC PROPERTIES, OF RANDOMLY DISTRIBUTED
ELLIPTICAL AND CIRCULAR POROUS INCLUSIONS, USING THE NUMERICAL
HOMOGENIZATION TECHNIQUE**

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Abstract

The aim of presenting this paper is to evaluate the effective material properties of multi-phase two-dimensional elastic random heterogeneous material. A numerical homogenization technique based on the finite element method with representative volume element is used to evaluate the effective material properties with various boundary conditions. Finite element simulation is performed in the case of linear elasticity. The effective material properties obtained using the numerical homogenization techniques were compared with different analytical methods. The variance of computed apparent properties of several different realizations for each volume size is used to define the precision of the estimation. A new model is first proposed for the three-phase random heterogeneous elastic materials and extended to the case of multi-phase random heterogeneous elastic material. In the case of multi-phase material, the integral range is introduced in order to relate the error estimation to the representative volume element size. The notion of equivalent material is presented here like a great point in the new approach of studying the random heterogeneous material by the definition of the equivalent two-phase elastic material to the multi-phase heterogeneous elastic material.

Key words: Representative volume element, homogenization, finite element method, random composite, integral range, equivalent morphology.

1. INTRODUCTION

One of important research topics in composite materials is to evaluate their effective mechanical properties, Hashin and Shtrikman (1963); Christensen and Lo (1979); Vinson and Sierakowski (1987); Gibson (1994) and Kanit et al. (2003). To resolve such problems, a number of classical micro-mechanics theories have been developed and published in the literature. Originally introduced to estimate the average constants of polycrystals, the Voigt approximation is one of the simplest models used to evaluate the effective properties of a composite. Voigt assumed that the strain throughout the bulk material is uniform. The inverse assumption to Voigt is the Reuss approximation, which assumes that the stress is uniform throughout the phases. Hashin and Shtrikman (1963) established, using variational principles, bounds on materials that could be considered as “mechanical mixtures of a number of different isotropic and homogeneous elastic phases” and, in bulk, regarded as statistically isotropic and homogeneous. These two point bounds had been improved by the three point bounds, Milton (1982); Milton and Phan-Thien (1982) and Torquato (1991), that incorporate information about the phase arrangement through the statistical correlation parameters.

A different way to solve homogenization problems is to use numerical techniques and simulations on samples of the microstructure. These techniques, used to estimate the effective properties of random heterogeneous materials from the constitutive law and the spatial distribution of their different components, are a main subject in the mechanics of random materials. It is related to the determination of the size of the representative volume element (RVE) which has been recently studied widely with the numerical and statistical tools, Sab (1992); Ostoja-Starzewski (1993); Gusev (1997); Terada et al. (1998); Ostoja-Starzewski (1998a); Ostoja-Starzewski (1998b); Kanit et al. (2003); Sab and Nedjar (2005); Lachihab and Sab (2008).

The aim of this study is the evaluation of two dimensional effective elastic properties, of randomly distributed elliptical and circular porous inclusions, using the numerical homogenization technique cited in Kanit et al. (2003) for different volume fractions of pores $P = 0.1$ and 0.3 with different major/minor radius ratio of ellipse $r = 0.5$ and 1.0 . The variance of computed apparent properties for each volume size is used to define the precision of the estimation. This variance is related by a parameter A said the integral range.

In this study we give the notion of A and its role to estimate the effective elastic properties. The notion of the integral range is applied and explained as a precise morphological parameter. The results of the numerical methods were compared with the analytical estimate : self consistent model (SC) given by Herve and Zaoui (1995) for the effective bulk modulus k^{eff} and by Christensen and Lo (1979) for the effective shear modulus μ^{eff} . The concepts of *equivalent morphology* and the *more heterogeneous material* are also presented.

2. MORPHOLOGICAL DESCRIPTION

In the present work, we have considered a two dimensional (2D) porous material, where the phase 2 (matrix) contains the phase 1 (porous inclusions), with $P_1 = P$ and $P_2 = 1 - P$ are respectively the volume fractions of phase 1 and phase 2. For the morphology of the phase 1, the ellipsoidal and circular forms are used separately in two cases, with a randomly distribution and orientation. We define a and b , respectively, as minor and major radius of ellipsoidal inclusion and $r = a/b$ there ratio.

The physical properties : Young's modulus E , Poisson's ratio ν , bulk k and shear μ modulus of matrix and inclusions, used in the numerical simulations are given in table 1.

	$E [MPa]$	ν	$k [MPa]$	$\mu [MPa]$
Matrix	10^4	0.3	9615	3846
Inclusion	$\simeq 0$	0.49	$\simeq 0$	$\simeq 0$

Table 1: Physical properties of matrix and inclusions.

In this study, a multi-phase element technique is used to generate meshes. An image of microstructure is used to attribute the proper phase property to each integration point of a regular mesh, according to the color of the underlying element. To study two-phase materials, two colors are used. This technique is illustrated by figure 1.

Since, one of the major goals of this study is to estimate the integral range which is purely a morphological parameter, and to preserve the shape of the randomly oriented ellipses, a fine grid of 200 by 200 multiphase elements is used, figure 1(b).

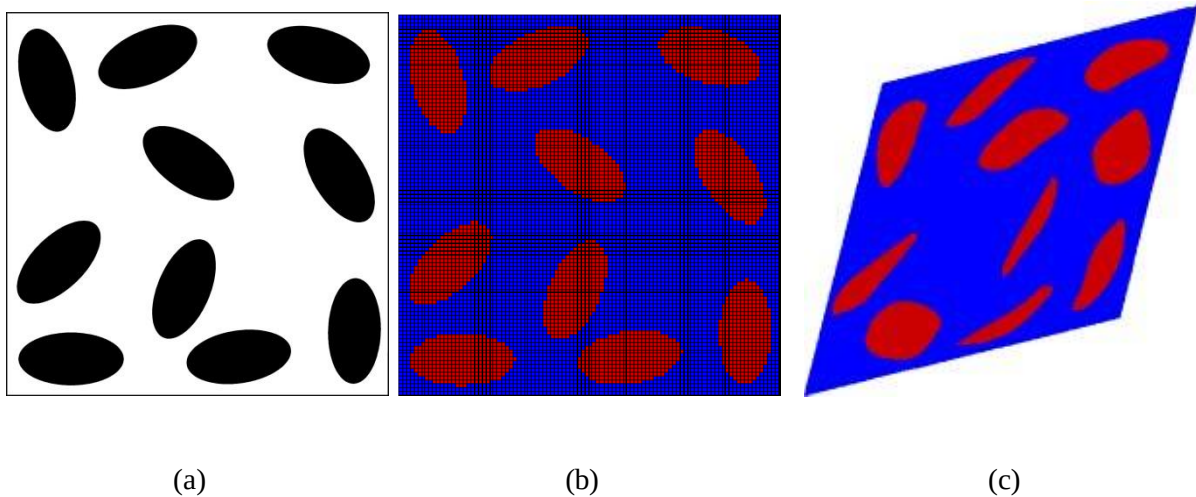


Figure 1: Example of effective shear computation : (a) original microstructure $P = 0.3$; (b) meshed microstructure, (c) deformed microstructure in shear computation example.

3. ESTIMATION OF APPARENT ELASTIC MODULI

The elements and notations of homogenization theory necessary for the numerical determination of effective properties are carried out in this section for linear elasticity. A special attention is focused on boundary conditions to be prescribed on volume elements and to the definition of effective and apparent properties. Three types of boundary conditions are usually used, for this kind of problems, to estimate effective properties of heterogeneous material. Let's denote S the surface made of heterogeneous materials:

- *Kinematic uniform boundary conditions (KUBC)* : the displacement u is imposed at point x belonging to the boundary ∂S of surface S such that :

$$u_i = E_{ij} \cdot x_j \quad \forall \underline{x} \in \partial S \quad (1)$$

E_{ij} are the cartesian components of a given symmetrical second rank tensor that does not depend on $\underline{x}$. This implies that :

$$\langle \varepsilon_{ij} \rangle = \frac{1}{S} \int_S \varepsilon_{ij} dS = E_{ij} \quad (2)$$

The macroscopic stress tensor $\sum_{ij}$ is then defined by the spatial average :

$$\sum_{ij} \square \langle \sigma_{ij} \rangle = \frac{1}{S} \int_S \sigma_{ij} dS \quad (3)$$

The symbol $\square$ means equals by definition to.

• *Static uniform boundary conditions (SUBC)* : the traction vector is prescribed at the boundary :

$$\sigma_{ij} \cdot n_j = \sum_{ij} \cdot n_j \quad \forall \underline{x} \in \partial S \quad (4)$$

$\sum_{ij}$ is a given symmetrical second-rank tensor independent of $\underline{x}$. The vector normal to ∂S at $\underline{x}$ is denoted by $\underline{n}$. This implies that:

$$\langle \sigma_{ij} \rangle = \frac{1}{S} \int_S \sigma_{ij} dS = \sum_{ij} \quad (5)$$

The macroscopic strain tensor is then defined as the spatial average :

$$E_{ij} \square \langle \varepsilon_{ij} \rangle = \frac{1}{S} \int_S \varepsilon_{ij} dS \quad (6)$$

• *Periodicity boundary conditions (PBC)* : the displacement field over the entire surface S takes the form :

$$u_i = E_{ij} x_j + v_i \quad \forall \underline{x} \in S \quad (7)$$

Where the fluctuation v_i is periodic. It takes the same value at two homologous points on opposite faces of S . The traction vector $\sigma_{ij} n_j$ takes opposite values at two homologous points on opposite faces of S .

Specific boundary value problems are defined in this subsection that will be used for the determination of isotropic effective elastic properties. These are special cases of the previous KUBC and PERIODIC boundary conditions, for which specific values of E are chosen. In the case of KUBC and PERIODIC conditions prescribed to a given surface S , one takes :

$$E_k = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix} \quad (8)$$

And

$$E_\mu = \begin{bmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{bmatrix} \quad (9)$$

An "apparent bulk modulus" k^{app} and an "apparent shear modulus" μ^{app} can be defined as :

$$k^{app} = \langle \sigma \rangle : E_k = \frac{1}{2} \text{trace}[\langle \sigma \rangle] = \frac{1}{2} (\langle \sigma_{11} + \sigma_{22} \rangle) \quad (10)$$

$$\mu^{app} = \langle \sigma \rangle : E_\mu = \langle \sigma_{12} \rangle \quad (11)$$

where $\langle \sigma \rangle$ is the average value of σ .

For 2D isotropic problems, in the case of two phases, the plane bulk moduli k and the plane shear moduli μ are expressed as function of the Young's modulus and Poisson's ratios of the matrix and inclusions by :

$$k = \frac{E}{2(1+\nu)(1-2\nu)} \quad , \quad \mu = \frac{E}{2(1+\nu)} \quad (12)$$

For 2D problems, Herve and Zaoui (1995) proposed an expression of the effective plane bulk modulus k^{eff} of two phase composite as :

$$k^{eff} = \frac{k_2(\mu_2 + k_1) + \mu_2 P(k_1 - k_2)}{(\mu_2 + k_1) + P(k_2 - k_1)} \quad (13)$$

and the shear modulus μ^{eff} one by Christensen and Lo (1979) :

$$\mu^{eff} = \mu_2 \left(1 + \frac{P}{\frac{\mu_2}{\mu_1 - \mu_2} + \frac{k_2 + \frac{7}{3}\mu_2}{2k_2 + \frac{8}{3}\mu_2}(1-P)} \right) \quad (14)$$

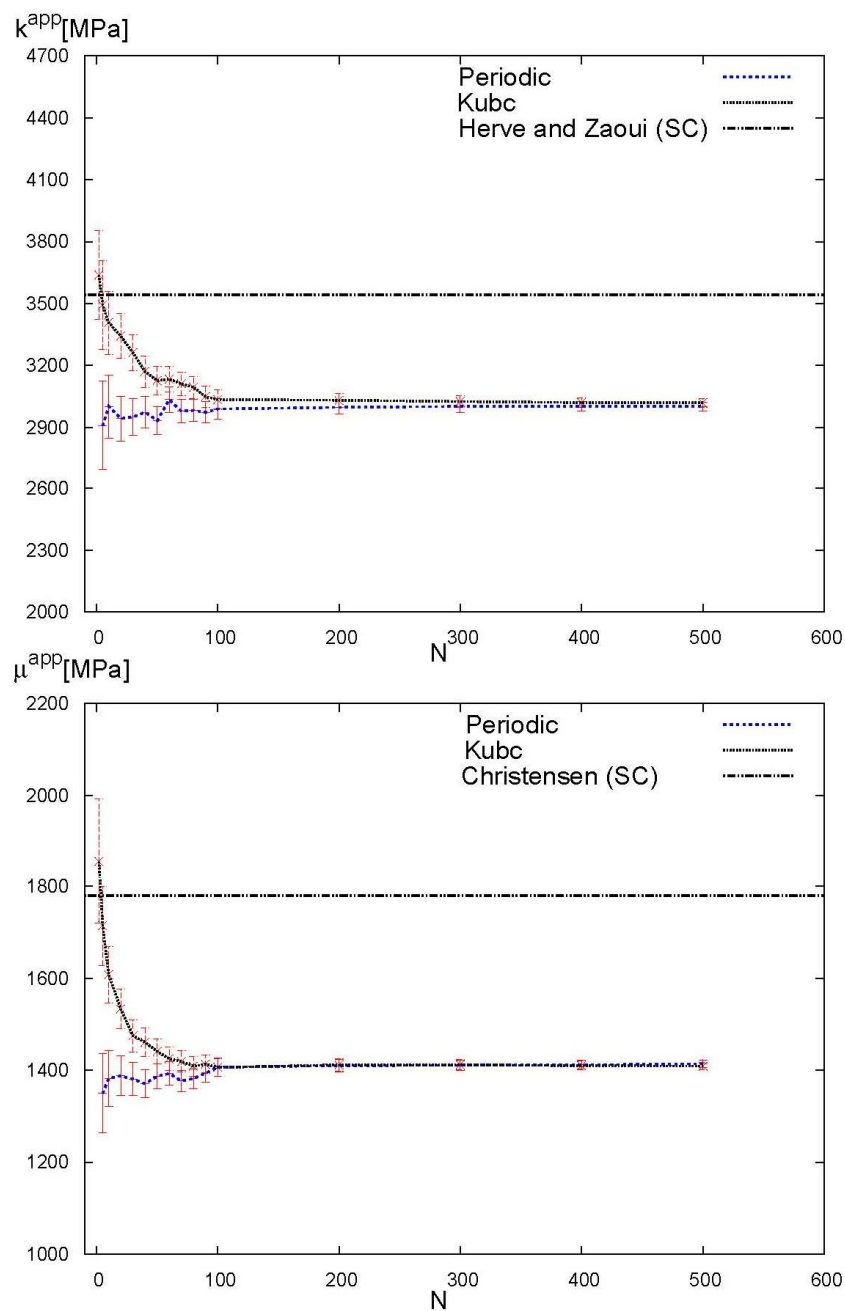


Figure 2: Mechanical properties k^{app} and μ^{app} in terms of the number of inclusions $P = 0.3$ and $r = 0.5$

Our numerical simulations are compared with this model. In this study, two volume fractions of inclusion phase are used: $P = 0.1$ and 0.3 . To see the effect of morphology on the effective properties, two values of major/minor radius ratio of the ellipsoidal inclusions: $r = 0.5$ and 1.0 are considered ($r = 1.0$ present the case of circular inclusion). The numerical simulations based on the finite element method are carried out for two different boundary conditions: kinematic uniform boundary conditions (KUBC) and the periodic condition (PBC). We present, in figure 2, the obtained values of the mechanical properties (the bulk modulus k^{app} and shear modulus μ^{app}) in terms of the volume size (or equivalently the number N of inclusions) for the case $P = 0.3$ with $r = 0.5$. In this case, the approximative value of RVE is $N = 100$ inclusions for the two properties, see figure 2.

The values of k^{eff} and μ^{eff} found for large volume sizes, for all studied cases, are reported in table 2 and compared to the Voigt, Hashin-Shtrikman HS^+ bounds and the self-consistent model (SC). Since we consider a porous material, the two null bounds, Reuss and Hashin-Shtrikman HS^- , are not represented.

Shape	Volume fraction	Property	Voigt	HS^+	SC	Error %	Simulation
$r = 0.5$	$P = 0.1$	k	8653	7287	6923	8	6405
		μ	3461	3180	2956	4	2815
$r = 0.5$	$P = 0.3$	k	6730	4307	3846	22	3002
		μ	2692	2127	1780	20	1412
$r = 1.0$	$P = 0.3$	k	6730	4307	3846	4	3700
		μ	2692	2127	1780	14	1512

Table 2: Values of numerical results, Voigt bound, Hashin-Shtrikman's bound HS^+ , Self-Consistent estimate (SC) for the studied cases and the relative error between simulation values and SC model.

4. FLUCTUATION OF APPARENT PROPERTIES AND DETERMINATION OF INTEGRAL RANGES

The effective properties are defined as spatial averages of fields $Z(x)$ over a surface S . We will have to consider now fluctuations of the average values over different realizations of the random composite material inside the surface S . In geostatics, it is well known that for an ergodic stationary random function, one can compute the variance $D_Z^2(S)$ of its average $\bar{Z}(S)$ value over the surface S , Matheron (1989) and Lantuéjoul (1991):

$$D_Z^2(S) = D_Z^{*2} \left(\frac{A}{S} \right) \quad (15)$$

Where D_Z^{*2} is the point variance of $Z(x)$ and A is the integral range of the random function $Z(x)$. The integral range gives information on the domain size of the structure for which the parameters measured have a good statistical representativity, Matheron (1971, 1975, 1989); Lantuéjoul (1991); Caillaud et al. (1994) and Jeulin (2001). It is useful to predict the variability of properties of a material as a function of the geometry of parts. Caillaud et al. (1994) proposed in the case of a two-

phase material with elastic property Z_1 for phase 1 and Z_2 for phase 2, the point variance D_Z^{*2} of the random variable Z as :

$$D_Z^{*2} = P(1-P)(Z_1 - Z_2)^2 \quad (16)$$

The relation (15) becomes:

$$D_Z^2 = P(1-P)(Z_1 - Z_2)^2 \left(\frac{A}{S} \right) \quad (17)$$

Our numerical simulations were fitted according to the relation (17) to estimate the integral range which named A_{fit} .

In the theory of samples, the absolute error ε_{abs} on the mean value of studied property Z , obtained with n independent (different) realizations of surface S , is given as a function of the variance $2D_Z(S)$ by :

$$\varepsilon_{abs} = \frac{2D_Z(S)}{\sqrt{n}} \quad (18)$$

which gives the relative error ε_{rela} by :

$$\varepsilon_{rela} = \frac{\varepsilon_{abs}}{Z} = \frac{2D_Z(S)}{Z\sqrt{n}} \quad (19)$$

The minimal number of different realizations n necessary and sufficient for the estimation of the effective property Z_{eff} with a given absolute error ε_{abs} on a surface S is:

$$n(S) = \frac{4}{\varepsilon_{rela}^2 * Z^2} D_Z^{*2} \left(\frac{A}{S} \right) \quad (20)$$

where the deterministic RVE corresponds to $n = 1$.

4.1. Integral range :

The integral range A is a standard tool for measuring the size of a RVE of a stationary and ergodic random structure, and to predict the variability of the volume fraction according to the scale of observation. In the 3D space, volume V consists of V/A volume elements, see Kanit et al. (2003).

Therefore, the specimen V is statistically equivalent to $N = V/A$. In the 2D case this equation becomes $N = S/A$, where S is the surface of inclusion.

To calculate the theoretical integral range, we must determine approximatively the number of inclusions N corresponding to the deterministic RVE, for this we compare the results between numerical computation of periodic boundary conditions (PBC) and kinematic uniform boundary conditions (KUBC) until the error between two calculations is less than 2%.

The comparison is done only for a large volume, because Kanit et al. (2003) show that PBC and KUBC converge for large volumes.

The proposed theoretical expression of the integral range, noted A_{th} , is :

$$A_{th} \cong \frac{P}{N_{RVE}} \quad (21)$$

where N_{RVE} is the number of inclusions in the deterministic RVE. Table (3) gives the different values of A for each property and for each studied case. It is clear from this table the good agreement between A_{th} and A_{fit} . Which means, that, in this type of microstructure, the integral range is simply the surface of one inclusion in a volume equal to the deterministic RVE. So we can determine and plot the variations of variance as a function of number of inclusions.

Figures (3), (4) and (5) represent the obtained values and variances of apparent moduli k^{app} and μ^{app} in terms of number of inclusions. Since the porous material presents a high contrast, see table (2), and for a better representation of the curves, we limit their comparison to the SC model.

Shape	Volume fraction	Property	A_{th}	A_{fit}	N_{RVE}
$r = 0.5$	$P = 0.1$	k	0.01	0.00979	10
		μ	0.01	0.0117	10
$r = 0.5$	$P = 0.3$	k	0.003	0.00275	100
		μ	0.003	0.00283	100
$r = 1.0$	$P = 0.3$	k	0.0033	0.00354	90
		μ	0.0033	0.00348	90

Table 3: Values of A for different volume fractions, for different cases computed with PBC.

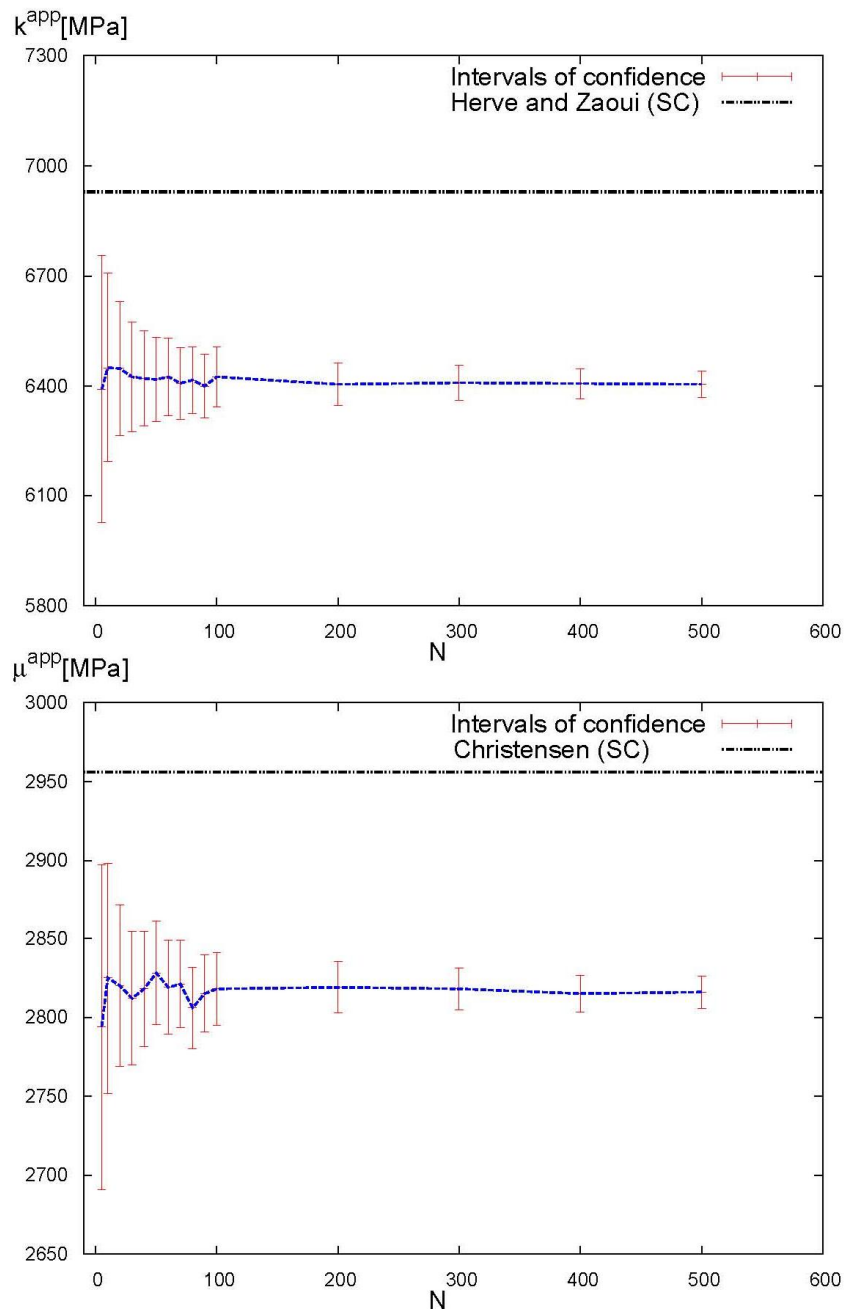


Figure 3: Dispersion and mean values of the apparent elastic properties k and μ in terms of the number of inclusions for volume fraction $P = 0.1$ and $r = 0.5$

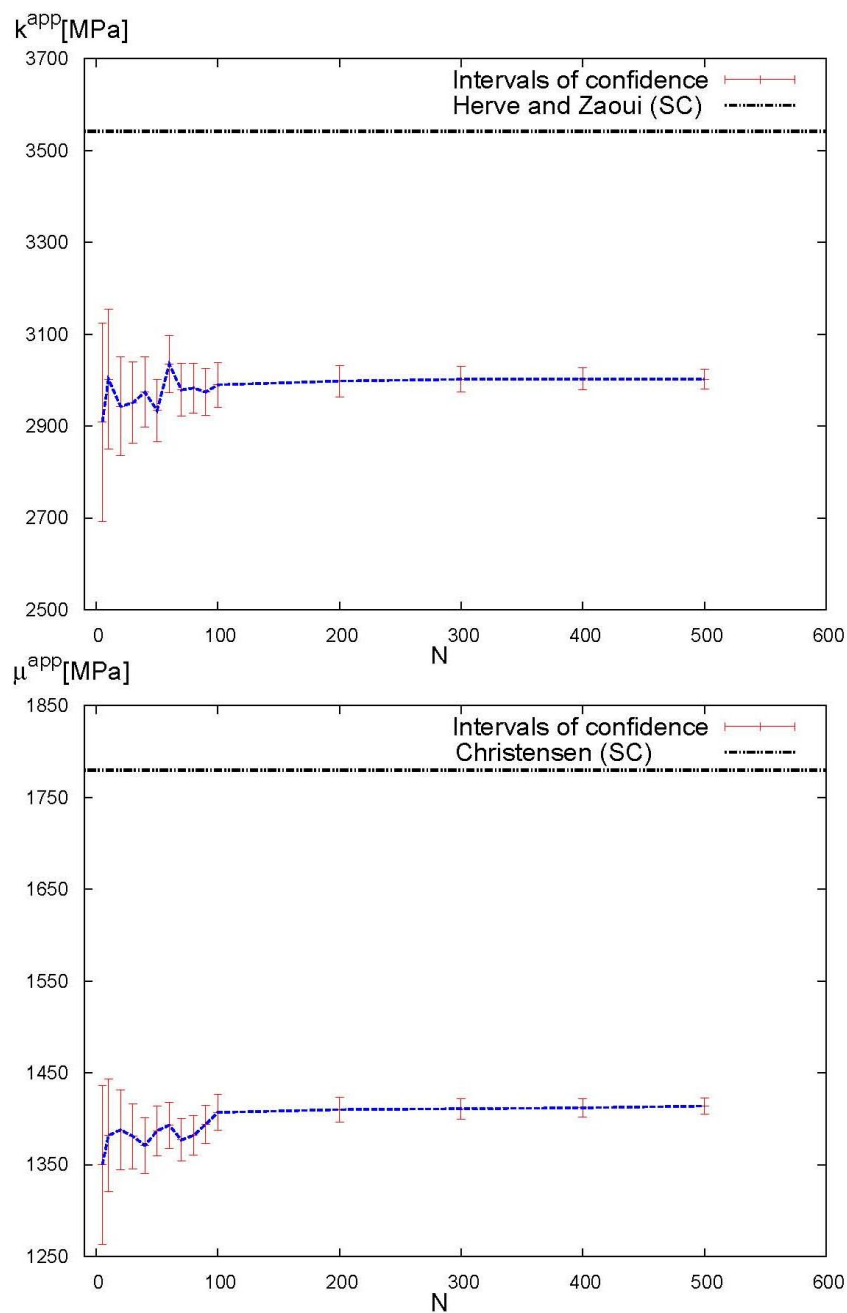


Figure 4: Dispersion and mean values of the apparent elastic properties k and μ in terms of the number of inclusions for volume fraction $P = 0.3$ and $r = 0.5$

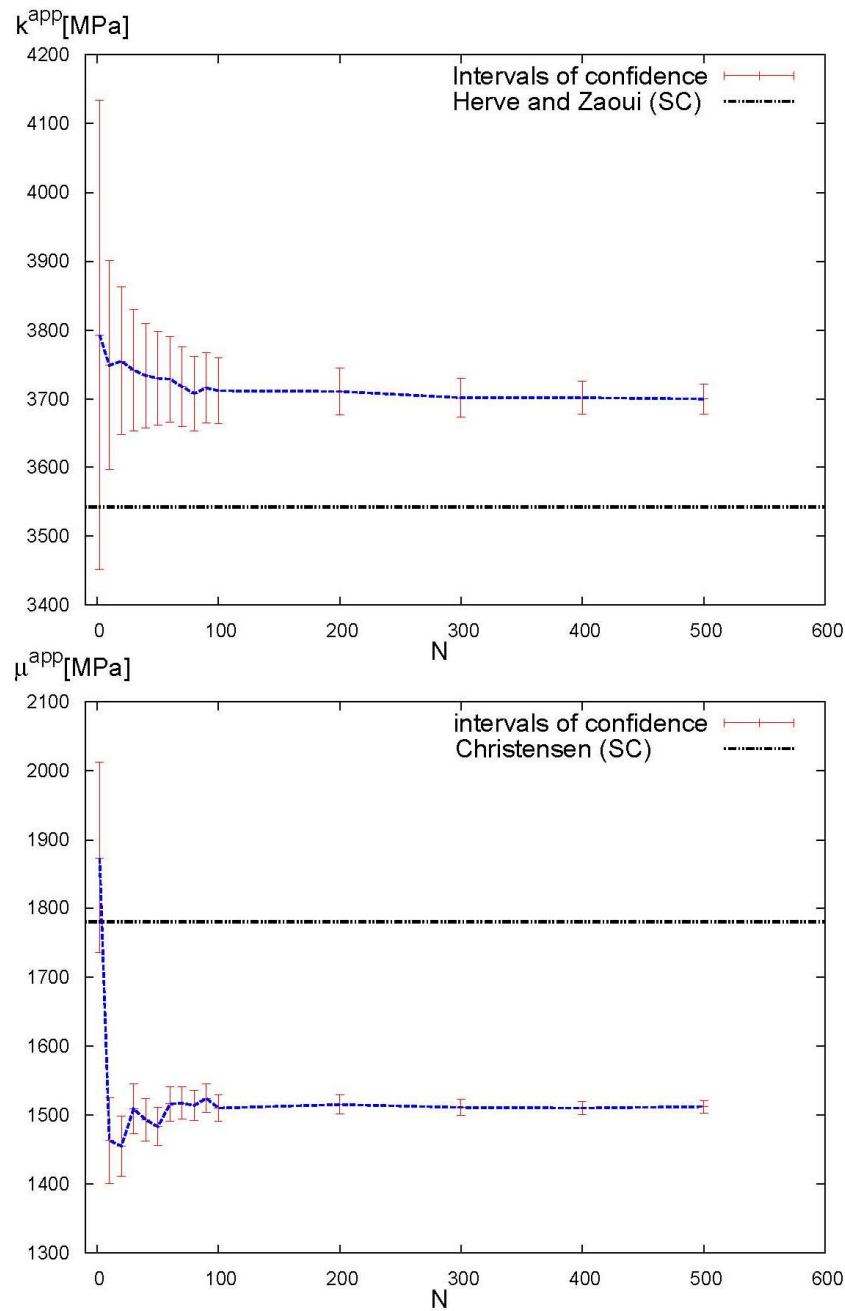


Figure 5: Dispersion and mean values of the apparent elastic properties k and μ in terms of the number of inclusions for volume fraction $P = 0.3$ and $r = 1.0$

4.2. Equivalent morphology concept

The notion of equivalent morphology is new in the modeling of random heterogeneous microstructures, it states, after the results given by table 3, that:

The integral range A is the surface of one inclusion in the deterministic RVE domain. So A is a purely morphological parameter depending on the surface of the inclusion, not on the mechanical properties neither on the shape of the inclusion.

Since the circular inclusion is the more isotropic shape so any shape of inclusion (ellipse, triangle, square, rectangle) can be replaced by the circular one where the surface and the number of circle must be equal to that of the inclusion set. Figure 6 summarizes this concept of equivalent morphology.

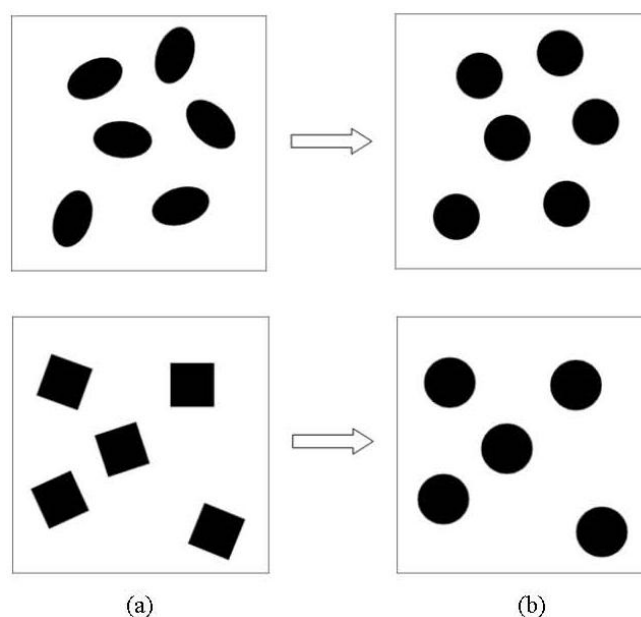


Figure 6: Concept of equivalent morphology : (a) original morphology, (b) equivalent morphology with a same size of inclusions

4.3. Notion of the more heterogeneous material:

The aim of this section is the determination of the volume fraction P^* corresponding to the more heterogeneous properties of a material. Let's note that a more heterogeneous material is one which possesses the most different effective properties from those of its constituents (matrix, inclusion) and which gives the largest size of the RVE. According to equation (17) that allows us evaluate the point variance and knowing that the value of the variance is very small for the RVE, we can take for example: $D_Z(S) = 1$ for $N = N_{RVE}$. By inserting these values in equation (17) and taking into consideration the proposed equation (21) of the integral range, the equation (17) becomes:

$$P(1-P)(Z_1 - Z_2)^2 \left(\frac{P}{N_{RVE}^2} \right) = 1 \quad (22)$$

We can express now the RVE in term of the volume fraction P by :

$$N_{RVE} = P\sqrt{(1-P)}(Z_1 - Z_2) \quad (23)$$

If we set $c = (Z_1 - Z_2)$, the equation (23) becomes :

$$N_{RVE} = c P\sqrt{(1-P)} \quad (24)$$

The extremum of the function (24) is given for $P^* = 2/3$, figure 7. From these results we can conclude that the most heterogeneous case of two-phase material (matrix, inclusion) are obtained for a volume fraction $P^* = 2/3$. This is due essentially to the difference in the morphology of the two constituents of the microstructure. In our case, the first phase (inclusion) with a particular form is embedded in the second phase (matrix). Therefore, the equilibrium behavior of these two phases will be located at a point $P \neq 0.5$, which is confirmed by the results found.

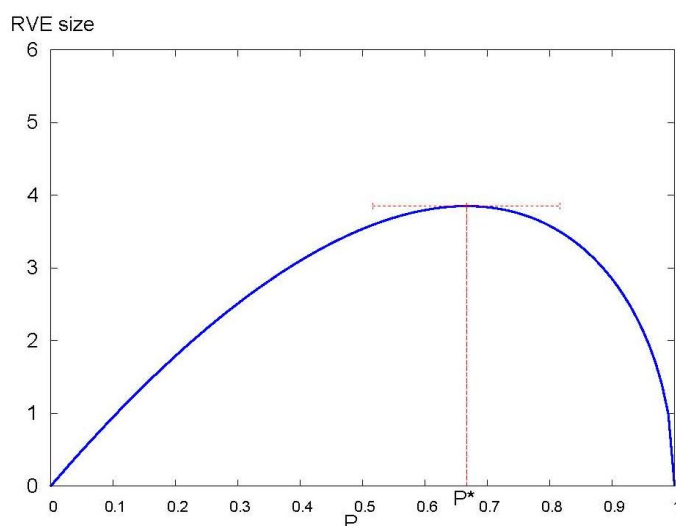


Figure 7: Variation of the RVE in terms of volume fraction and volume fraction P^* for the more heterogeneous material.

5. CONCLUSIONS

An enlarged definition of representative volume element was proposed by Kanit et al. (2003) which apply that the effective linear properties of random composites can be determined not only by numerical simulations on large volume elements of heterogeneous material, but also as mean values of apparent properties of a rather small volumes. For determination of its sizes for any microstructure, a statistical and numerical approach was proposed by Kanit et al. (2003).

This approach has been adopted in this work for determining the mechanical properties of the studied microstructure, and this taking into account the effect of the physical property, the surface fractions of

components, the relative precision for the estimation of the effective property and the number of realizations of the microstructure.

A difference is observed between the results of the literature and those obtained by simulation. This allows to assert that the SC model is less effective to give accurate results for such problems. The integral range A , which plays a central role in the statistical method, is simply related to the variance and domain size and does not depend on the effective property itself but only on the morphology, see Kanit et al. (2003). In this work a model for this integral range was proposed and identified. We concluded that A is a purely morphological parameter depending on the surface of the inclusion, not on the mechanical properties neither on shape of the inclusion. So any shape of inclusion can be replaced by the circular one where the surface and the number of circle must be equal to that of the inclusion set.

Finally, Basing on the proposed model, the volume fraction P^* corresponding to the more heterogeneous properties of two-phase material (matrix, inclusion) is obtained.

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