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Abstract:

The Representative Volume Element (RVE) plays a central role in the homogenization of random heterogeneous microstructures, especially for composite and porous materials, with a view to predicting their effective properties. A quantitative evaluation of its size is proposed in this work in linear elasticity and linear thermal conductivity of random heterogeneous materials. A RVE can be associated with different physical and statistical properties of microstructures. The methodology is applied to specific two–phase microstructure–based random sets. Statistical parameters are introduced to study the variation in the RVE size versus volume fractions of components and the contrast in their properties. The key notion of the integral range is introduced to determine these variations. For a given desired precision, we can provide a minimal volume size for the computation of effective mechanical and thermal properties. Numerical simulations are performed to demonstrate that a volume exists which is statistically representative of random microstructures. This finding is an important component for homogenization–based multiscale modeling of materials.

Keywords: Representative volume element; Numerical Homogenization; Microstructures; Composite Materials; Effective properties ; Statistical characterization.

1. Introduction

One important goal of the physics of heterogeneous materials is to derive their effective properties from knowledge of the constitutive laws and the spatial distribution of their components. The homogenization methods used for this purpose have reached a high level of sophistication and efficiency, especially in the case of mechanical properties and the thermal conductivity. They can be found in reference extended papers and textbooks by such authors as Buryachenko (2007), Zimmerman (1989) and Ostoja-Starzewski *et al.* (2016). Numerical homogenization for the macroscopic effective properties is also available. They include the well–known finite element methods or fast Fourier transform. Homogenization refers to the process of considering a statistically homogeneous representation of a heterogeneous material, called Representative Volume Element RVE.

In the last years, the determination of the RVE size has been a topic of extensive research as proposed by Kanit et al. (2003), Gitman et al. (2007) and Phu–Nguyen et al. (2010). The RVE size is very much dependent on the physics constitutive response and random geometry involved. Thus, the results of Drugan and Willis (1996) are of historical rather than practical interest as they do not apply to the entire range of the volume fractions and have actually been calculated using a sine (i.e., periodic) function for the dependence of spatial fields; there exists also yet another problem with their derivation. The results of Kanit et al. (2003) are only applicable to linear elasticity of composites. Despite that, there is still no a single or exact definition of the RVE. For this reason, some of the definitions used by scientists are listed below.

- **Hill (1963):** The RVE is a sample that is structurally entirely typical of the whole mixture on average and contains a sufficient number of inclusions for the apparent overall moduli to be effectively independent of the surface values of traction and displacement, as long as these values are macroscopically uniform.
- **Hashin (1983):** The RVE is a model of the material to be used to determine the corresponding effective properties for the homogenized macroscopic model. The RVE should be large enough to contain sufficient information about the microstructure in order to be representative, however it should be much smaller than the macroscopic body.

- **Drugan and Willis (1996):** The RVE must be chosen sufficiently large compared to the microstructural size for the approach to be valid, and it is the smallest material volume element of the composite for which the usual spatially constant overall modulus macroscopic constitutive representation is a sufficiently accurate model to represent the mean constitutive response. This work gives the minimum RVE size of an elastic composite composed of a random dispersion of non–overlapping identical spheres. Gusev (1997) investigated the same problem but by using the numerical technique.
- **Trusov and Keller (1997):** An RVE is the minimal material volume, which contains statistically enough mechanisms of deformation processes. The increase in this volume should not lead to changes of evolution equations for field–values, describing these mechanisms.
- **Evesque (2000):** The size of the RVE should be large enough with respect to the individual grain size to define overall quantities such as stress and strain, but this size should also be small enough in order not to hide macroscopic heterogeneity.
- **Ostoja–Starzewski (2002):** The RVE is very clearly defined in two situations only : i. unit cell in a periodic microstructure and ii. volume containing a very large mathematically infinite set of microscale elements, possessing statistically homogeneous and ergodic properties.
- **Ostoja–Starzewski (2006):** The RVE is defined by three conditions: i. statistical homogeneity stationarity and ergodicity, ii. Hill condition leading to admissible boundary conditions, iii. variational principle.
- **Trias et al. (2006)**: The criteria used to define the minimal required size for a RVE was proposed. This work establishes the size of RVE for a typical carbon fiber reinforced polymer. It is concluded that the minimum size is L/R=50, where L is the volume length and R the fiber radius.

A more practical RVE definition is found in the framework of homogenization in which a numerical RVE is defined as the smallest volume element that has the same target property / behavior as the full scale material. Numerous attempts have been made in order to quantify the size of RVE on the basis of both statistical and numerical methods, Grufman and Ellyin (2007).

Stroeven *et al*. (2004) have quantified the size of the RVE for heterogeneous microstructures by studying the averages and standard deviations of specific factors like particle size, dissipated energy and strain concentration. This methodology was also used by Ren and Zheng (2004) to define the minimum RVE size for random composites. The real application of the statistical method is studied by Thomas *et al*. (2008) for carbon–epoxy composite with high–fiber volume fraction and Pelissou *et al*. (2009) for random quasi–brittle composites. The RVE was generated using the microstructure of optical images. The size of different RVE ranges from 691.1µm x 748.9µm to 1129.2µm x 785.5µm. The statistical parameters defined for each RVE are; the covariance, the pair correlation function and the voronoï diagram. These treatments make a strong case for the use of statistical descriptors in the development of the statistical RVE. According to Moussaddy *et al*. (2013), the RVE edge length was found to be around half the fiber length for aspect ratios larger than 10, allowing firsthand quick estimations of RVE sizes.

The effect of volume fraction of particles on the RVE size was studied by EL Moumen et al (2015a) using the statistical approaches. For each configuration 200 realizations were generated in order to ensure the representativity of the results. The volume fraction of particles ranges from 5% to 23% of spherical and ellipsoidal inclusions. It is concluded that the RVE size depends on the volume fraction, type of inclusion and the composite properties. It is concluded that the minimum RVE is obtained with 50 particles. Mirkhalaf et al. (2016) presented a methodology to construct the RVE of composites. This methodology based on the statistical and numerical approaches. It was concluded that for both cases of inclusion volume fraction equal to 10% and 15% the RVE size could be considered 15µm. Sukiman et al. (2017) studied the effect of microstructures on the RVE size of composite made up of randomly oriented short fibers using a computational homogenization technique. It appears that some microstructures with fibers do not respect the convergence of the apparent properties calculated under different boundary conditions because their RVE size is very large. Hua et al. (2018) proposed a statistical approach to determine RVE size to simulate a given property with the desired precision dependent on the volume fraction of particles and the number of realization. Using this technique, the mean of many realizations of a small RVE instead of a single large RVE can retain the desired precision of a result with much lower computational cost. Mohan et al. (2020) studied the RVE generation and its size determination. The minimum size is determined and integrated in the algorithm based

on the random sequential adsorption technique. This algorithm has been exploited to generate
the 3D RVEs.

In literature, much attention has been paid to construction of various parameters that affects the RVE size. The important examined parameters are particles volume fraction, morphology of particles (sizes and shapes) and distribution, effective properties and contrast in properties. However, all definitions reveal that the RVE should contain enough information's about the microstructure and should be sufficiently smaller than the macroscopic structural dimensions. Obviously these definitions need to be completed introducing the statistical parameters of random microstructures.

Motivated by the work Moussaddy et al. (2013) and Hu et al. (2018) the contribution of this paper is the numerical and statistical demonstration of the existence of RVE for random microstructures. This is because coupling numerical and statistical methods can give rise to marked differences in the macroscale response. The idea is to make a connection between the RVE size and all microstructure parameters. Having a general expression of the RVE of heterogeneous materials, a procedure to find its variation versus particle volume fractions and contrasts can be determined.

After this general introduction, Section 2 outlines the different microstructural parameters which influence the RVE size. Section 3 presents the microstructures used in this investigation, benefits of identifying and using statistical parameters and the methodology used for RVE determination. The paper then discusses the results and Section 5 lastly presents the conclusions.

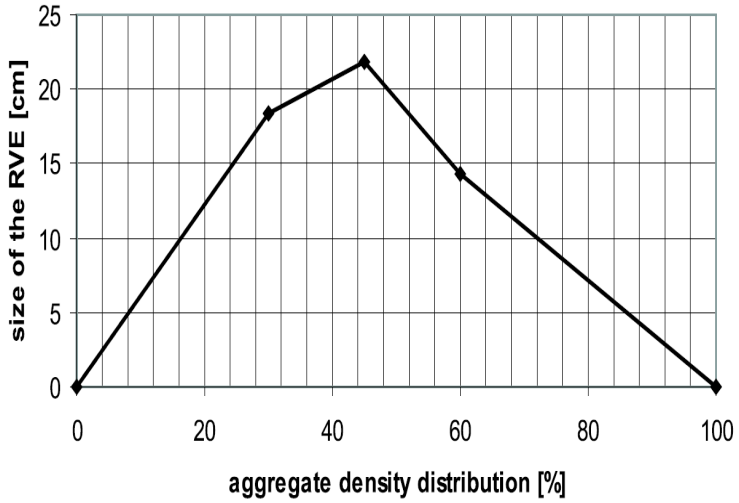
2. RVE size versus microstructural parameters

The objective of this section is to present the results of some works concerning the effect of microstructural parameters on the size of the RVE. The evolution of the RVE as a function of the volume fraction, contrasts and morphology of particles is presented.

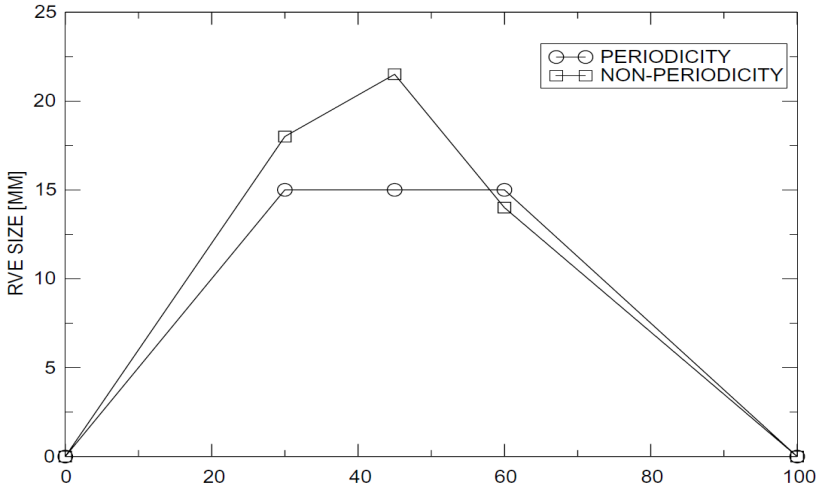
2.1. RVE size versus particle volume fractions

In many investigations, the evolution of the RVE size as a function of particles volume fraction was studied. This is because changing the particle volume fractions changes the RVE

size. Figure 1 presents the results obtained by Gitman et al. (2004) and Gitman et al. (2007) for the variation in the RVE size as a function of the volume fraction of inclusions. It appears that the RVE of periodic microstructures with volume fractions ranging from 30% to 60% is the same. For non periodic microstructures, it appears that the RVE size increases by increasing the particle volume fractions until 50% of inclusions and then decreases. The maximum length of RVE is 22 cm. It should be mentioned that the proposed methodology by Gitman *et al*. (2004) and Gitman et al. (2007) do not give a precise size of the RVE because the evolution is discontinuous. El Moumen *et al*. (2013), El Moumen *et al*. (2014) and El Moumen *et al*. (2015a, 2015b) have investigated on the variation of the RVE size as a function of the particle volume fractions, for elastic and thermal properties of random microstructures. Figure 2 presents the example of the evolution of RVE size for different values of contrasts. In this study, the authors consider the case of higher contrast, for that the RVE size becomes important. It appears that by increasing the volume fraction of inclusions, the size is increased. This RVE reaches a maximum value at 67% of inclusions and then decreases again.

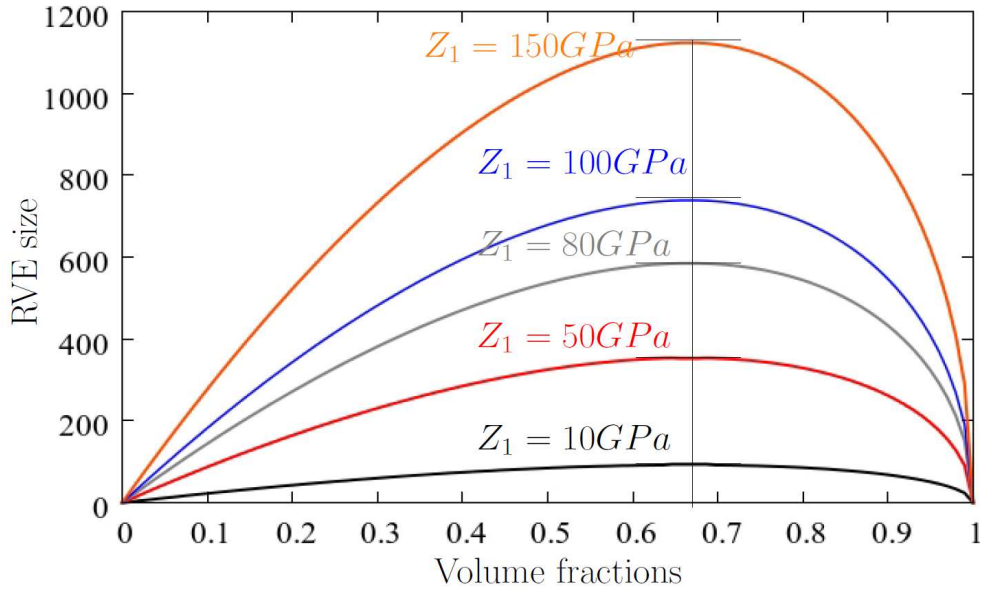


(a) Gitman et al. (2004)



(b) Gitman et al. (2007)

Figure 1: Variation of the RVE size versus volume fraction of inclusions as proposed by: (a) Gitman et al. (2004) and (b) Gitman et al. (2007).



El Moumen et al. (2015a, 2015b)

Figure 2: RVE size vs particle volume fractions for different values of contrasts.

2.2. RVE size versus effective and apparent properties

In this sub–section, we present the variation of the RVE size depending on the computed mechanical properties. Generally, there is two types of estimated properties, apparent properties

obtained on the volume size less than RVE and effective properties obtained on the volume larger than RVE. The question is what is the RVE size regarding the estimated properties ? Kanit et al. (2003) and Phu–Nguyen et al. (2010) give the variation of the RVE as a function of the estimated properties for different boundary conditions. Figure 3 shows that the RVE size is achieved if the estimated properties do not depend on the used boundary conditions. It should be stated these are boundary conditions, the results being based on variational principles and certain statistical properties of random microstructures, see Huet (1990).

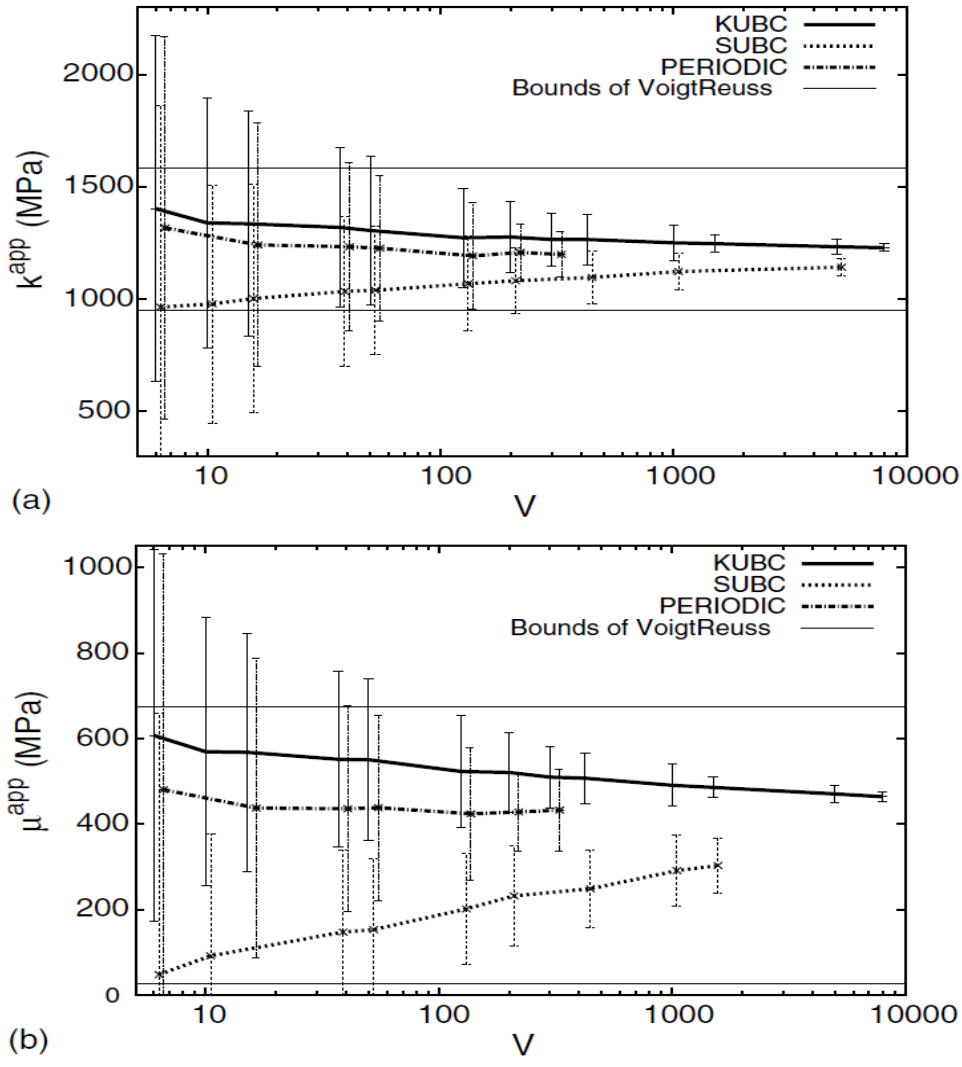


Figure 3: RVE size vs estimated properties for different boundary conditions as proposed by Kanit et al. (2003): Kinematic Uniform Boundary Conditions (KUBC), Static Uniform Boundary Conditions (SUBC).

The notion of realizations and statistical methods are introduced by El Moumen et al. (2014) to estimate the properties of heterogeneous materials and to determine the RVE size. In the case of the RVE, it appears that one realization is sufficiently for representativeness of the results, conversely to the case of volumes less than RVE for which the number of realizations, about 100 realizations, is important to achieve the effective properties. It should be mentioned that the RVE size of the thermal conductivity is small than the RVE size of mechanics properties, because the contrast and the number of degree of freedom. The statistical methods were also used in other works to investigate the RVE size for two–dimensional 2D and three–dimensional 3D viscoplastic composite materials as Madi et al. (2006). They found as conclusion that the size of the RVE in 2D is larger than the size of the RVE in 3D and the size of the RVE seems to be smaller in the nonlinear case than in the linear case.

2.3. RVE size versus morphology of particles

It is mentioned that the particles morphology (or shape of inclusions) has an important effect on the RVE size. Several articles have studied the effect of reinforcement shape on the physical properties and RVE size of heterogeneous materials, El Moumen et al. (2014) for example. The authors show that the RVE size of composites reinforced with random distribution of particles is increased if the geometrical shape becomes more complex, keeping the same contrast. The minimum RVE size is one of composites containing spherical particles. This is can be explained by the non–existence of preferred orientation in the case of spheres. Furthermore, Dirrenberger et al. (2014) have shown that there are some microstructures, with gigantic fibers or infinitely long fibers, can lead to gigantic RVE sizes, or even no RVE at all i.e. yield non–homogenizability in the sense of Auriault (1991). Figure 4 gives the scale variation of the RVE size for different particle shapes generated using Poisson process.

The large RVE is given by gigantic fibers and the small one by spherical particles, while maintaining the same contrasts between physical properties. It should be mentioned that the repulsion distance between neighboring particles has also an effect on the RVE size. For example, El Moumen et al. (2013) have shown that the RVE of microstructures based hard spheres models, with non–overlapping particles, is 13 times the RVE size of microstructures based Boolean models, with overlapping spheres. Figure 5 illustrates the morphological description of the effect of repulsion distance on the RVE size as proposed by El Moumen et al.

(2013).

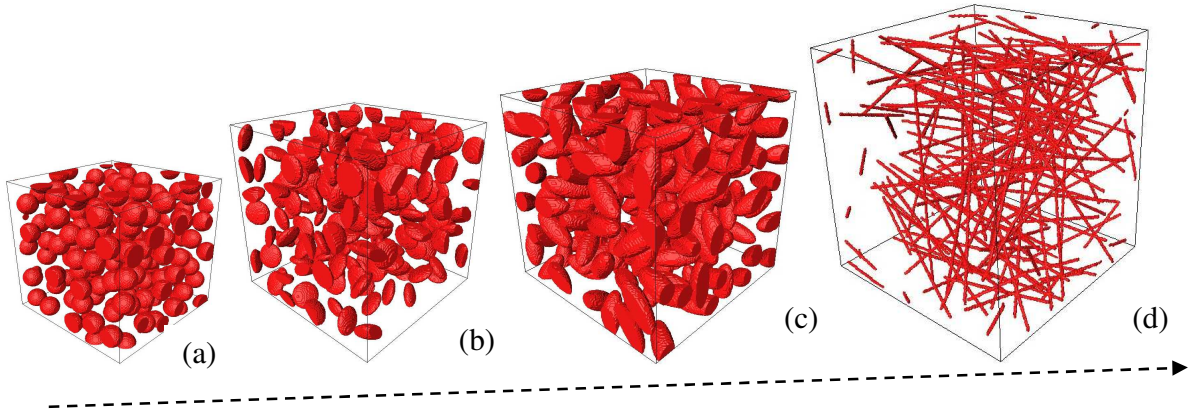


Figure 4: Sense of the RVE size increasing for different reinforcement shapes: (a) spherical particles, (b) oblate spheroïds, (c) prolate spheroïds and (d) gigantic fibers (infinitely long fibers).

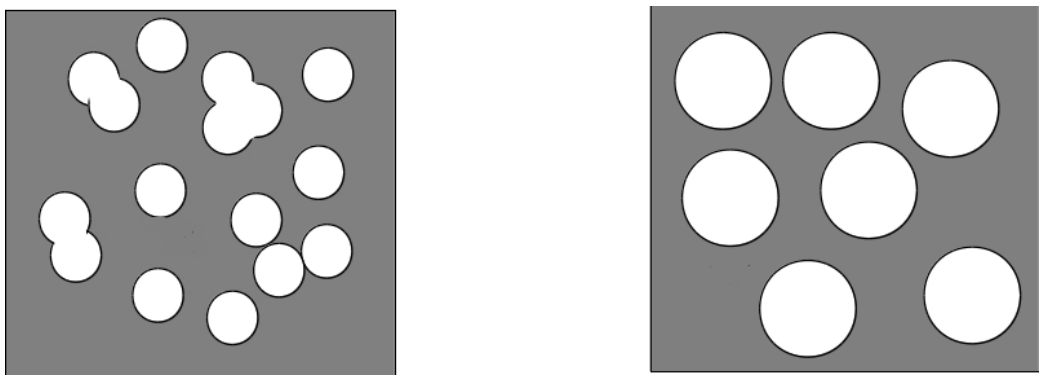


Figure 5: Morphological equivalence between RVE of overlapping and non–overlapping spheres as proposed by El Moumen et al. (2013).

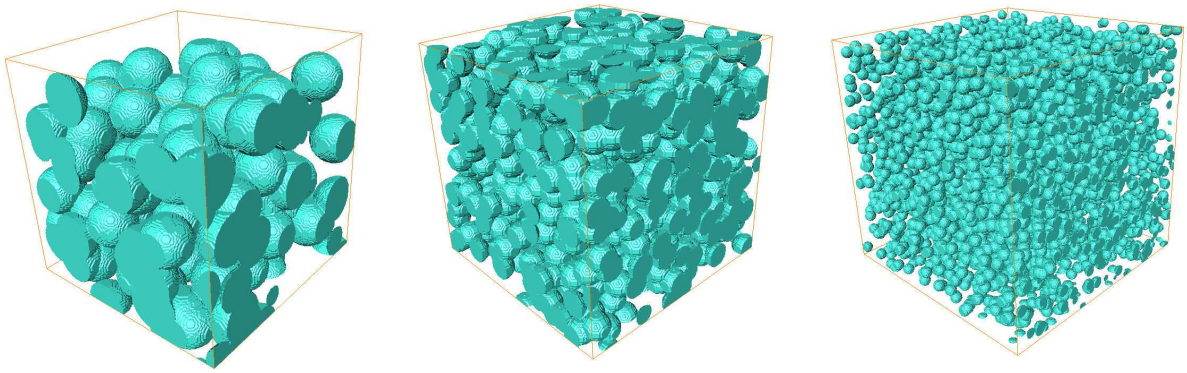
3. Description of the investigated microstructures

In this investigation, various microstructures are used for numerical and statistical characterization. The microstructures are made of so–called Boolean models of spheres and hard spheres model. The Boolean models are obtained by a random implantation of primary inclusions, pores; grains; rigid particles; fibers; .., with possible overlaps. The hard spheres model is obtained by a sequential implantation of inclusions, keeping only the particle without any contact. The hard model does not give the microstructure with high volume fraction because the jamming limit. The maximum fraction obtained with this model is 27%. For the microstructures

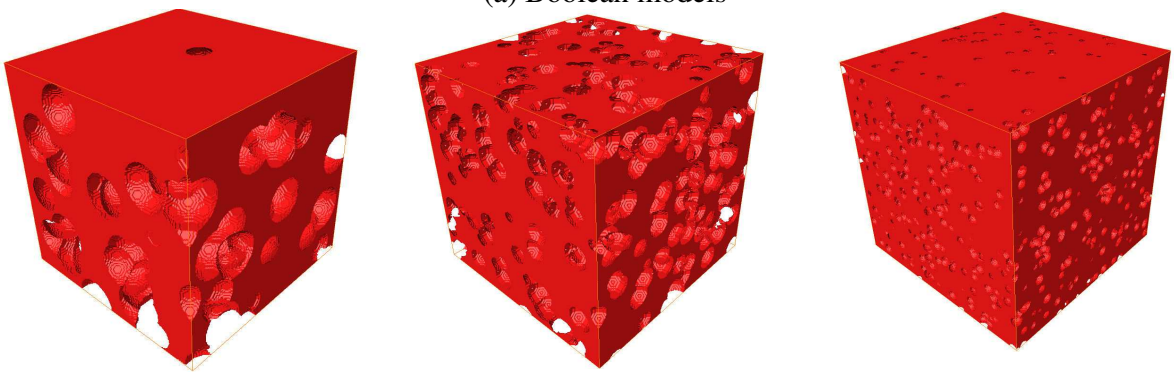
with the volume fractions of particles more than 27%, the inclusions are allowed to overlap and in the case of volume fraction less than 27%, the overlapping is possible but not imposed in the algorithm.

The composite microstructures are modeled by a random set. To generate the simulated microstructures, first pick points M_1, M_2, ..., M_i, ..., M_n in space at random, according to a Poisson process. Next, construct inclusion i of each center M_i, while respecting a given repulsion distance between neighboring inclusions in the microstructure based hard spheres model and without respecting any repulsion distance for a microstructure based Boolean model. Figures 6 and 7 present an example of the investigated microstructures, generated by a Poisson process using the Boolean model and the hard spheres model.

In our computation, an RVE with 200 particles randomly distributed in the matrix are generated with the possibility of overlapping for the case of high volume fraction. This RVE clearly reveals the multiscale microstructure of the composite with three scales: spherical particles, the aggregates phase, and the matrix



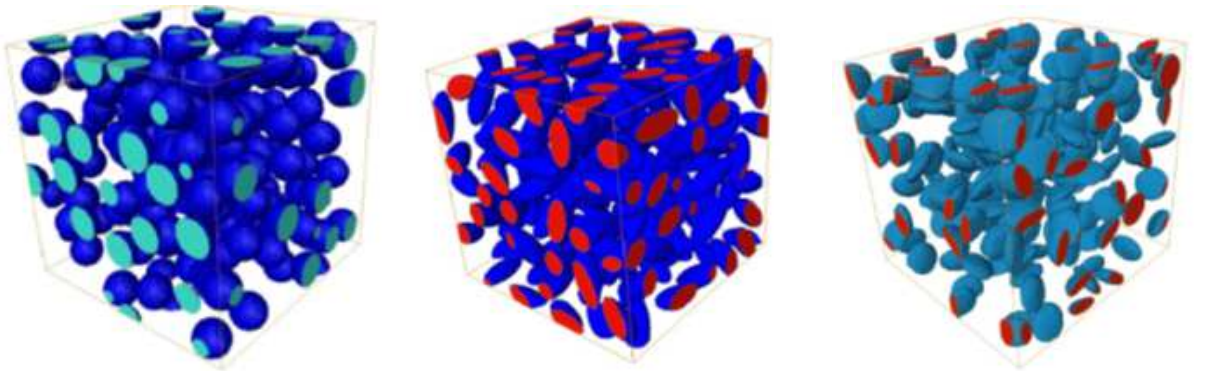
(a) Boolean models



(b) Complementary of Boolean models

Figure 6: 3D simulated microstructures of Boolean models, with 30% of volume fraction,

obtained using Poisson Process.



(a) Hard models

(b) Complementary of hard models

Figure 7: 3D simulated microstructures of hard model, with 10% of volume fraction, obtained using Poisson Process.

The combination of basic models and their complementary leads us to generate composite structures with different particle volume fractions. Figure 8 gives an example of the simulated microstructure based Boolean model and its finite element FE meshes. The number of FE mesh used for the simulation was 100000 EFs.

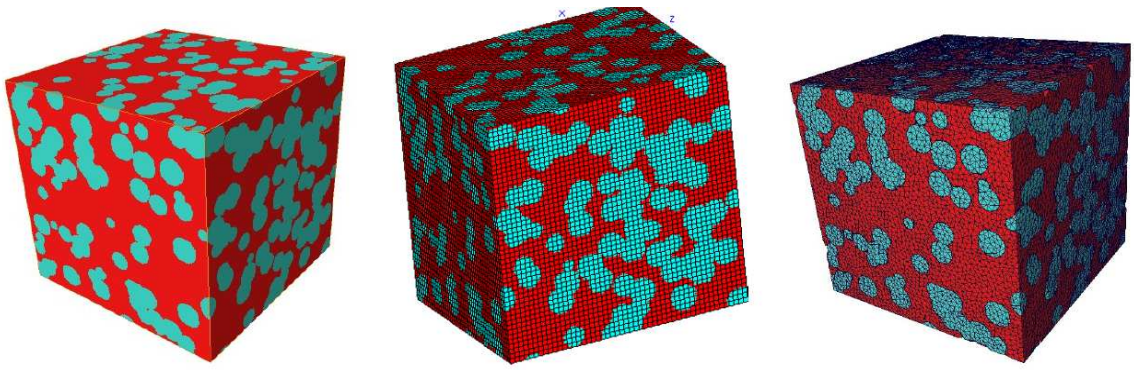


Figure 8: Example of 3D microstructures based Boolean models and their FE meshes with different resolutions.

4. Numerical and statistical evaluation of RVE size

4.1. Expression of the RVE size

Combined numerical and statistical methods offer a good balance between general applicability on the one hand and the possibility of automated testing of different samples on the other, Gitman et al. (2007). For this reason, a combined numerical–statistical approach was chosen in this study to determine the fluctuation of the RVE size as a function of the microstructure properties. It should be mention here that the FE computations presented in El Moumen et al. (2014) and El Moumen et al. (2015a, 2015b) are used in this section to study the fluctuation of the RVE size. These computations are reinforced introducing some laws of mathematical morphology. A computational procedure is proposed by which the fluctuation of the RVE can be determined for random microstructures. To achieve this objective, we apply the results of Kanit et al. (2003), Jeulin (2012) and El Moumen et al. (2013) in the case of composite materials and make use of the key notion of the integral range A. This geostatistical parameter is used to relate the size of the RVE with other microstructure parameters. This parameter was defined by various workers as follows.

- Matheron (1971): It is possible to define a range which gives information on the domain size of the structure for which the parameters measured in this volume have a good statistical representativity. This range is called the integral range.
- Kanit *et al*. (2003): In the microstructure of Voronoï mosaics, the integral range depends on the size of grains in RVE.
- Jeulin (2012): The integral range A does not depend on volume V, it is large enough to insure the stationarity of the field by minimizing the effect of boundary conditions.
- El Moumen *et al*. (2013): It means that, the integral range A is a morphological parameter, depends for the random microstructure, on the volume of inclusion in RVE.

- El Moumen *et al*. (2014): The integral range A depends on the volume of one inclusion in the RVE. This volume of inclusion was integrated in the particle volume fraction p. The authors have studied several configurations with changing the contrast, the particles distribution and the particles volume fractions. It appears that for random microstructures with volume fraction p, the integral range can be written as:

$$A = \frac{p}{V_{RVE}} \quad [1]$$

In order to obtain a good prediction of the effective properties, it is necessary to relate the size of RVE with all morphological and mechanical, or thermal, parameters of microstructures. The main parameters are the mechanical properties of phases Z_1 and Z_2, or thermal conductivity λ_1 and λ_2, the particle volume fractions p and some statistical parameters.

In geostatic, based on the work of Jeulin (2012) it is well known that for an ergodic stationary random function Z, we can compute the variance $D_Z^2(V)$ over the volume V as a function of the integral range A and the point variance S_Z^2 by:

$$D_Z^2(V) = S_Z^2 \frac{A}{V} \quad [2]$$

We now consider a random microstructure made of two phases F_1 with volume fraction p and F_2 with volume fraction $(1-p)$ having real properties Z_1 for phase F_1 and Z_2 for phase F_2. In the case of a two–phase material, the point variance S_Z^2 of the random variable Z is given by Cailletaud *et al*. (1994) as:

$$S_Z^2 = p(1-p)(Z_1 - Z_2)^2 \quad [3]$$

Considering now that the mechanical properties is the random function Z, we finally reach at the following equation:

$$D_Z^2(V) = p(1-p)(Z_1 - Z_2)^2 \frac{A}{V} \quad [4]$$

Where $D_Z^2(V)$ is the variance of the volume V and A is the integral range.

Several methods were used to determine the RVE parameters. The first group lists the number of realizations n determination criteria, while the second group lists the number of

inclusions N determination criteria, Moussaddy *et al*. (2013). In this study, we use the first criterion for which the variance $D_Z^2(V)$ is expressed introducing the absolute error ε_{abs} and realizations n as proposed by Lantuéjoul (1991):

$$\begin{cases} 2D_Z(V) = \varepsilon_{abs}\sqrt{n} \\ 4D_Z^2(V) = \varepsilon_{abs}^2 n \end{cases} \quad [5]$$

It is to be noted that the size of the RVE can be defined as the volume for which the number of realizations is equal to 1, see Willot and Jeulin (2009). We have:

$$n(V = RVE) = 1 \quad [6]$$

Therefore the combination of Equations 1, 4, 5 and 6 gives:

$$RVE = \frac{4p(1-p)(Z_2 - Z_1)^2 A}{\varepsilon_{abs}^2} \quad [7]$$

$$RVE = \frac{4p(1-p)(Z_2 - Z_1)^2 p}{\varepsilon_{abs}^2 RVE}$$

Using Equation 7, we can deduce the variation of the RVE as a function of particle volume fractions p and the contrast c in mechanical properties. The contrast c is defined as $c=Z_1/Z_2$. This volume size gives the representativity of the estimated properties in random microstructures, for desired error ε_{abs} as:

$$V_{RVE} = RVE = \sqrt{\frac{4p^2(1-p)(Z_2 - Z_1)^2}{\varepsilon_{abs}^2}} \quad [8]$$

The unit of the RVE is the Voxel. Therefore, the variation of the RVE size versus the volume fraction p and the contrast c in random microstructures is equivalent to the fluctuation of the bivariate function $f(p,c)$ as follows:

$$f(c,p) = \frac{2Z_2|1-c|p\sqrt{1-p}}{\varepsilon_{abs}} \quad [9]$$

Where $c=Z_2/Z_1$ and Z_2 is the matrix property. Developing Equation 8, we finally come at:

$$RVE(c,p) = \frac{2Z_2|1-c|p\sqrt{1-p}}{\varepsilon_{abs}} \quad [10]$$

The relative error is given as $\varepsilon_r = \frac{\varepsilon_{abs}}{Z_2}$, and the final expression of the RVE is:

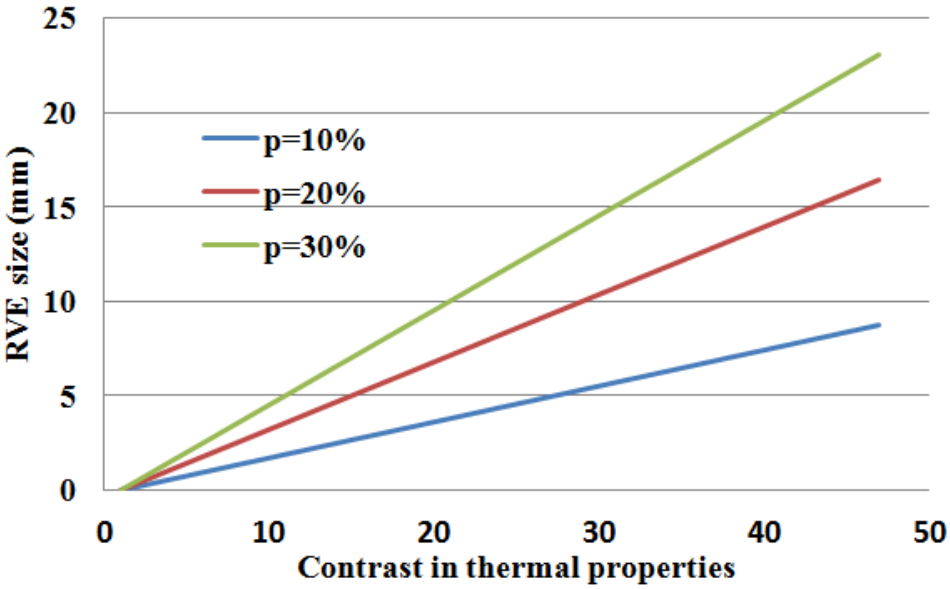
$$RVE = \frac{2|1-c|\, p\sqrt{1-p}}{\varepsilon_r} \qquad [11]$$

Using this equation, the unit of the RVE is the voxel. This equation is used to describe the variation of the RVE of random microstructures as a function of the volume fraction and as a function of the contrast for desired and fixed absolute error.

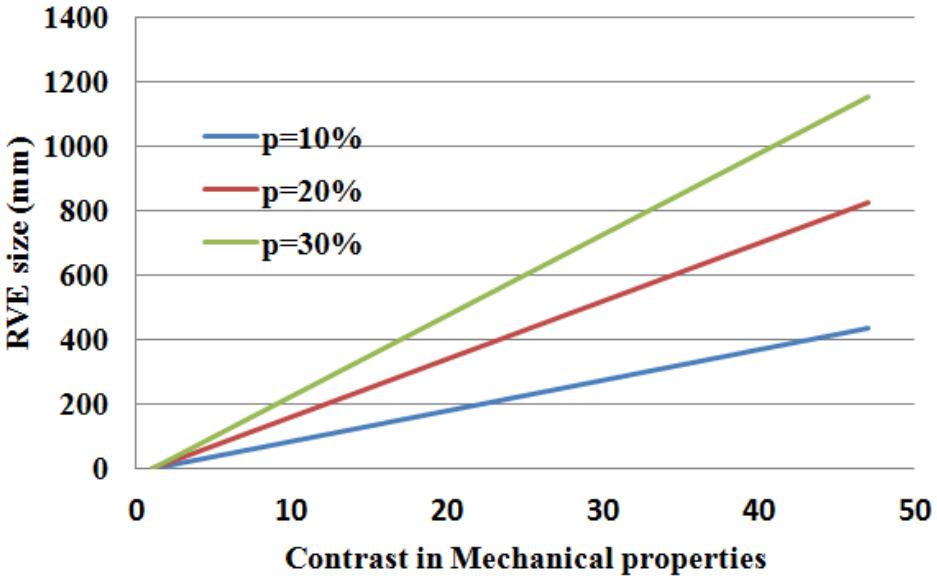
4.2. Fluctuation of the RVE as a function of contrasts and volume fractions

Considering the variation of Equation 11 as a function of the contrast c. We can determine the linear variation of the RVE size versus contrast for different fixed values of particle volume fractions p and the variation of the RVE as a function of the volume fraction for different values of c. These fluctuations are presented for contrasts defined on the range [0 50] in Figure 9 and for the variation as a function of p in Figure 10. Figure 9 gives these variations for different values of volume fractions 10%, 20%, 30% and 0.4. It appears that, by increasing the contrast c, the size of the volume for which the obtained numerical results are statistically representative and isotropic is increased. This RVE reaches a maximum value at $c \mapsto \infty$. It also appears that if the volume fraction increases the RVE becomes important.

The variation of the RVE size as a function of the volume fraction is presented in Figure 10. The size increases with increasing the volume fraction and reach the maximum value for 67% of particles and then decreases. This distribution provides a large RVE. Corresponding values of the RVE for all different volume fractions are 22 x 22 mm^2, except the theoretical values p=0 and p=1, purely homogeneous materials. We can also deduce that, for any value of the contrast, the RVE size increases and reaches its maximum for 67% of inclusions and then decreases. Finally, it should be mentioned that the RVE size changes depending on the accuracy of the results (relative error). If the error is small the RVE becomes large.



(a) Thermal conductivity $Z_2 = \lambda = 0.1W/mk$



(b)Mechanical property $Z_2 = E = 5Gpa$

Figure 9: Variation of the RVE size versus contrast for an error of 2%. The results are converted to mm.

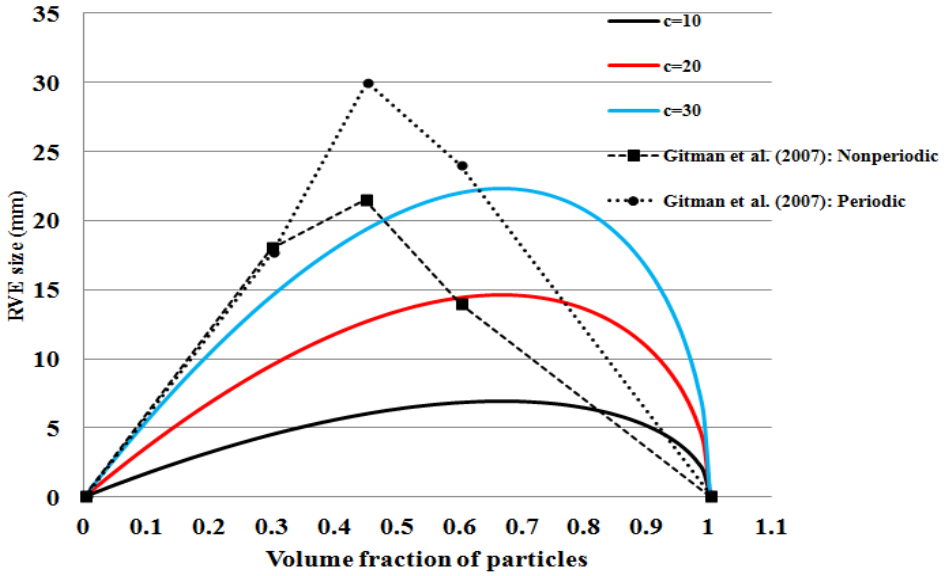


Figure 10: Variation of the RVE size as a function of the particle volume fractions: comparison between existing data and the results of this paper.

5. Conclusion

Several RVE determination methods have been presented for the computation of accurate effective properties. As noted at the outset, the methodology is used for virtual microstructures based Boolean and hard spheres models generated using Poisson process. This paper focuses on variation in the representative volume element size taking into account the all microstructure parameters.

Based on a statistical and numerical analysis conclusions are drawn about the RVE existence and fluctuations. The key notion of the integral range is introduced. It appears that the RVE variation increases with increasing particle volume fractions, until 67% of particles, and then decreases. It is also found that the maximum RVE size is obtained by a random distribution of 67% of particles. Attention was subsequently given to the RVE size variation as a function of contrast. It may be concluded from a comparison of different results that the microstructure with a larger RVE is the one with the greatest contrast. The most important finding of this work is that a larger RVE is obtained with a random distribution of 67% of the particles and a high contrast.

In this study, it was demonstrated that new definition can determine accurate the size of the RVE for random microstructures, particularly, the composite and porous materials. The size is given for each particle volume fractions taken into account the absolute error and the contrast in

properties. The set results are compared with the obtained results by other studies as presented in Figure 10. It appears that the new definition is in agreement with earlier results from RVE variations.

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