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AN ALGORITHM TO GENERATE MICRO MECHANICAL MODELS COMPOSED BY CIRCULAR INCLUSIONS

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Abstract. An algorithm to generate random representative volume elements (RVE) of the microstructure of materials with a large number of circular inclusions of constant diameter is described. The type of problem that the algorithm addresses belongs to the class of sphere packing problems, with important industrial and academic applications. In fact, statistical mechanics of hard-sphere systems has generated considerable interest by the scientific community from Boltzman (1898) [20] to the Bernal (1959)[2] works on the model of the structure of liquids using random close packing (RCP), and many researchers have contributed to this subject.
In this work, the general propose algorithm developed is able to generate models that define the internal structure of unidirectional fiber reinforced composites and other materials, but can also be used for other types of applications. The proposed algorithm has a linear complexity and it is based on a new and innovative geometric concept to distribute the inclusions. The computational efficiency of this algorithm was compared with the efficiency of other existing algorithm ([18]) revealing the advantages of the method. The generated models have been combined with finite element analysis of materials subjected to periodic boundary conditions and showed transversal isotropy of the material and good agreement with experimental results.

1 INTRODUCTION

To describe the behavior of the materials attending to their internal structure, homogenization techniques have been applied in the last decades. See for instance [3, 4, 5, 6, 7, 8, 9, 10, 11].
The endeavor on homogenization research is motivated by the increment of the computational power available, the advances of the simulation models, the interest of industry to

improve the reliability of predictions, and the aim to design tailored materials for specific proposes. Important classes of tailored materials are: (1) dispersed particle microstructures, (2) continuous fiber microstructures, (3) discontinuous fiber, whisker or elongated single crystal microstructures, (4) fabric woven braid microstructures. [12]
Many studies such as [13] and [14] conclude that the generation of representative volume elements (RVE) is an important issue in the simulations, because can be a time costly procedure and because over simplifications can induce a pour representation of important phenomena leading to bad results.

In this work a new algorithm with linear complexity that is able to generate distributions of 2D disks, randomly packed is proposed. The algorithm can easily be extended for 3D or other dimensional problems.
Preformance analysis of the algorithm is presented. The generated models have been used for finite element analysis of materials subjected to periodic boundary conditions and showed transversal isotropy of the material and a good agreement with experimental results.

2 DESCRIPTION OF THE ALGORITHM

The algorithm described in Figure 1 follows the random sequential addition (RSA) scheme, with some important modifications. The basic idea of the algorithm is to introduce each inclusion (fiber) after another in a sequential manner. However, the ability to introduce new inclusions and the regions of the RVE where those new inclusions can be placed is wisely evaluated after each new inclusion is introduced. In this way, the position where each new inclusion is placed is directly chosen without collision tests. The absence of collision tests results in a huge reduction of the algorithmic complexity.

3 PERFORMANCE ANALYSIS analysis

In order to verify the performance of the algorithm and compare it with others, tests have been performed with different RVEs. For a constant inclusion volume fraction $\phi_c = 0.58$, models with different ratios of edge length a and inclusion radius R have been generated and the time has been measured. The results obtained for different relations (a/R) with the present algorithm and the one proposed in [18] are described in Table 1.

It can be concluded that the proposed algorithm, in comparison with the referenced algorithm, allows to produce RVE models in significant less time.

4 STATISTICAL CHARACTERIZATION OF THE MODELS

The randomness of the inclusion distribution can be quantified numerically, using statically procedures. A review of such statistical procedures can be found in [18].
In order to compare the statistical characterization of the proposed algorithm with the one in [18], the same statistical procedures and variables were adopted.

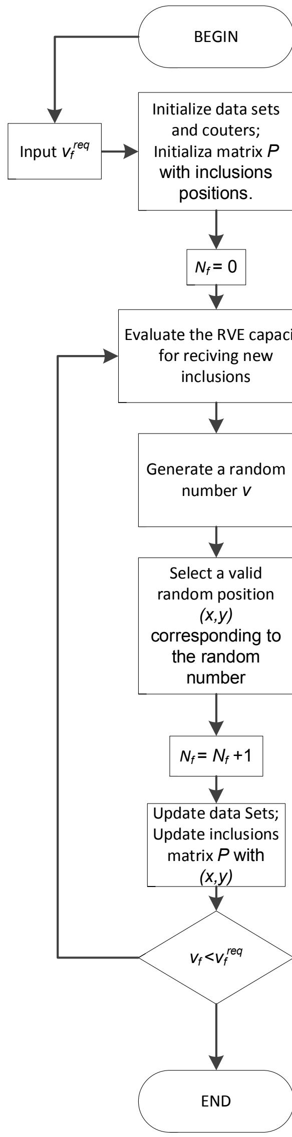

Figure 1: Flowchart of the overall algorithm

Five models were generated with the described algorithm considering an RVE size of 50 inclusion radius ($50R$) and a fraction of inclusions $\phi_c = 0.56$. For each of the models a distribution of Voronoi areas and a distribution of neighboring inclusion distances was been obtained. For each distribution, the coefficient of variation of the the areas (ρ_A) and distances (ρ_D) was computed, according the expression (1).

$$\rho(\chi) = \frac{\sigma(\chi)}{\mu(\chi)}, \tag{1}$$

Table 1: Time required to generate the models (inclusion volume fraction $\phi_c = 0.58$) for different edge length per radius relations (a/R)

RVE size	Computation Time (min)	
a/R	Proposed method	Melro[18]
30	0.07	0.36
50	0.17	0.62
70	0.35	1.09
100	0.64	1.71
120	0.98	2.95
150	1.76	6.10

where χ is the random variable, $\sigma(\chi)$ is the standard deviation and $\mu(\chi)$ is the mean. Table 2 presents the average values obtained for the described algorithm, together with the ones provided by [18].

Table 2: Coefficient of variation for Voronoi polygon areas and distances to neighbor inclusions

Method	ρ_A	ρ_D
Proposed method	0.144	0.193
Melro[18]	0.137	0.196
Wongsto[16]	0.129	0.190
Matsuda's Y-distribuition[30]	0.106	0.190
Matsuda's point distribuition[30]	0.135	0.256

For the Voroni areas, the proposed method appears to originate higher values of variation than the other methods. For the distance to the neighbor inclusion, the proposed method obtains values near to the ones obtained with the other methods except in the case of Matsudas point distribution, where the variation is much larger than in the other methods.

5 MICROMECHANICAL CHARACTERIZATION OF THE MODELS

5.1 Material definition

Panels of a unidirectional E glass fiber/913 epoxy resin composite described in [29] were considered. The material has a fibre radios of $R = 15\mu m$ a fibre volume fraction $\phi_c = 0.54$ and the elastic properties of the matrix and fibres are defined in the table 3.

5.2 Model definition

A set of 400 models has been generated using the algorithm described in the previous sections. The generated models have a square shape with the edge of 50 radius of inclusions (50R). It was assumed that the real material is a repetition in a periodic pattern of the

Table 3: Material properties

Propreties	Young's moduli E(Gpa)	Poison's ratio ν
Epoxy resin	5.32	0.365
E-glass fiber	72.5	0.20

generated models. Therefore, the left and bottom edges must match geometrical with the right and top respectively. A model generated with the proposed algorithm is depicted in Figure 2.

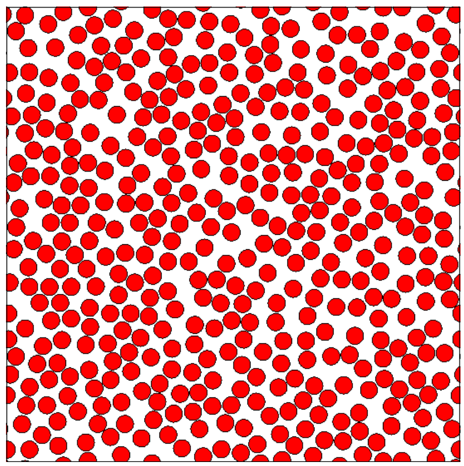

Figure 2: Model allowing a geometrical periodic pattern assumption for the real material ($a = 50R$ and $\phi_c = 0.54$).

A plane strain state was considered and isoparametric planar triangular elements with 3 nodes and 1 gauss point have been used. An average of 73000 nodes and 145000 elements per model have been used. A detail of the refinement of the generated meshes is presented in Figure 3. The meshes have been generated using Delaunay tessellation according to the process suggested in [18].

5.3 Homogenization strategy

The simulations have been performed with a user developed academic software of micro-scale simulation based on FEM. In the calculations, the strain field is prescribed to the RVEs using boundary conditions and the equivalent homogenized stress is computed. Periodic boundary conditions have been employed in the current study, which have been enforced such that the displacement on a pair of opposite nodes of the boundary surface (with their normal along the Y_i axis) is given by expression (x) according to [1].

$$u_i^{j+} - u_i^{j-} = \bar{\varepsilon}_{ik}(y_k^{j+} - y_k^{j-}) = \bar{\varepsilon}_{ik}\Delta y_k^j. \tag{2}$$

In equation (2), the index $j+$ means along the positive Y_j direction, while the index $j-$ means along the negative Y_j direction and Δy_k^j is constant representing the edge length

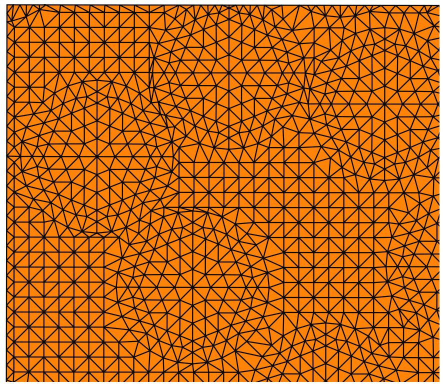

Figure 3: Detail of the refinement of the used mesh

of the RVE in the direction j.

For each model three different small deformations corresponding to three small strains ε have been applied and the respective stress σ has been computed.

The obtained stress and strain allows the determination of the compliance matrix C of the material that respects the relation (3).

$$\sigma = C\,\varepsilon \tag{3}$$

The homogenized properties have been obtained directly from the compliance matrix C components according the expression (4).

$$\begin{aligned} E_1 &= 1/C_{11} \\ E_2 &= 1/C_{22} \\ \nu_{12} &= -C_{21}\,E_1 \\ \nu_{21} &= -C_{12}\,E_2 \\ G_{12} &= 1/(2\,C_{66}) \end{aligned} \tag{4}$$

Where E is the the Yong's moduli, ν is the Poisson's ratio and G is the shear modulus, the numeric indexes 1 and 2 denote the directions orthogonal to the fibres.

5.4 Results

The table 4 shows the experimental measured properties and a summary of the numerical analysis.

The transversal isotropy is verified by the relations $E_1 = E_2$, $\nu_{12} = \nu_{21}$ and $G_{12} = G_{12}^{calc} = \frac{E_1}{2(1+\nu_{12})}$ that are expressed in term of ratios in the table 5.

The results show a good agreement between the experimental results and the numerical predictions. The relations between homogenized properties confirm that the use of the proposed algorithm conducts to isotropic models.

Table 4: Comparison of experimental and numerical determined properties

	Experimental‡	Mean	Std. Dev.	Error(%)	Gusev‡
E_1(GPa)	17.1	16.816	0.1295	1.7	16.0
E_2(GPa)	17.1	16.792	0.1675	1.8	16.0
ν_{12}	0.391	0.444	0.00421	13.6	0.410
ν_{21}	0.391	0.442	0.00627	13.1	0.410
G_{12}(GPa)	6.07	5.829	0.0517	4.0	5.61

‡ values mentioned in [29] and assumption of traversal isotropy

Table 5: Verification of transversal isotropy

	$\frac{E_1\nu_{21}}{E_2\nu_{12}}$	$\frac{E_1}{E_2}$	$\frac{\nu_{12}}{\nu_{21}}$	$\frac{G_{12}^{calc}}{G_{12}}$
Mean values	1.006	1.001	1.005	1.001

6 CONCLUSIONS

A new algorithm which is able to generate a geometrical definition for the internal structure of unidirectional fiber reinforced composites was presented. This algorithm can be applied in many other types of engineering problems. Because of the linear complexity ($O(n)$) of the algorithm it is highly efficient in the generation of large models. Which was confirmed by performance testes. Simulations to predict the mechanical behavior of a composite fiber glass material, using the FEM method and homogenized techniques have been performed. The results show a good agreement with the experimental data. The transversal isotropy of the generated models was also confirmed.

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