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Random Microstructure Generation

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Abstract. This paper presents a method for automatically generating three-dimensional (3D) microstructures of composites with a view to predicting their effective properties by finite element (FE) methods. The loads are modeled by dispersed and randomly oriented ellipsoids using the random sequential adsorption (RSA) algorithm developed under Matlab. The advantage of this method is its good applicability to a large number of heterogeneities of different sizes and shapes (grains, wafers, voids, needles, fibers, etc.). The geometric of the microstructure is converted into STL (Standard Tessellation Language) format commonly in rapid prototyping (i.e., 3D printing, additive manufacturing) and can be exported to a finite element calculation software package

Keywords: Microstructure, Random composites, Random Sequential Adsorption, Standard Tessellation Language.

1. Introduction

Recently, composite materials have attracted a lot of attention due to their various potential applications, especially in fields that require customizable properties. Depending on the application under consideration, the nature, size, and/or aspect ratio of the loads can be adjusted to see performance aspects. For example, stronger and lighter materials can be produced by dispersing carbon nanotubes uniformly in a polymer matrix [1], just as the electroactive properties of a piezoelectric polymer which can be significantly improved by incorporating nanoparticles [2], also the thermal conductivity of a building material can be reduced by adding different types of insulating aggregates to the cement matrix [3,4], etc. to achieve mutual enrichment between experimental results and theoretical studies of these materials and for rational conception, we would like to model their real microstructure and understand the influence of the geometric factor on their effective properties. In this respect, numerical homogenization techniques [5] make it possible to predict the effective properties of these materials based on knowledge of the properties of the various components and by simulating boundary conditions on Representative Volume Element (RVE)[5-7] of the material. Homogenization based on the finite element method (FE) [1,8] is suitable for complex microstructures [9] and hyper elastic materials [10], but asymptotic homogenization based on perturbation expansion or fast Fourier transformation (FFT) [11] could also be used. All these methods share a common point, which consists in exploring the average response and isotropy of the 3D representative volume elements (RVE), associated with a given precision of the estimate of the desired global property. Table 1 provides examples of some technologically relevant physical properties governed by the Laplace's equation.

Table 1. Some Effective Physical Properties Governed by Laplace's Equation (For multiphase materials with anisotropic constituents, the phase properties are given by second-rank symmetric 3 x 3 tensors), [8].

| Phase property | Local variable | Laplace's equation |
|---|-------------------------------|--|
| Dielectric constants, $\boldsymbol{\varepsilon}(\vec{r})$ | Electric potential, φ | $\text{div}(\boldsymbol{\varepsilon}(\vec{r})\overline{\text{grad}}(\varphi)) = 0$ |
| Thermal conductivity, $\boldsymbol{\lambda}(\vec{r})$ | Temperature, T | $\text{div}(\boldsymbol{\lambda}(\vec{r})\overline{\text{grad}}(T)) = 0$ |
| Electric conductivity, $\boldsymbol{\sigma}(\vec{r})$ | Electric potential, φ | $\text{div}(\boldsymbol{\sigma}(\vec{r})\overline{\text{grad}}(\varphi)) = 0$ |
| Solute diffusion Coeff, $\boldsymbol{D}(\vec{r})$ | Concentration, C | $\text{div}(\boldsymbol{D}(\vec{r})\overline{\text{grad}}(C)) = 0$ |

It is essential to incorporate as real as possible the information of the microstructural characteristics of the real material. There are mainly three methods for constructing 3D microstructure using random generation algorithms [12] such as: random sequential adsorption algorithm (RSA)[13][14], Monte Carlo simulations [15], and molecular dynamics [16].

Many theoretical methods have been successfully applied to the prediction of the effective properties on composites. In particular, the improved Mori-Tanaka (MT) homogenization method, which is an incremental theory formulation based on the generalized Eshelby's tensor, have the advantage of high computational efficiency [17]. Furthermore, among the modelling approaches, commonly used to predict the actual behavior of composites, those known as Halpin-Tsai equations based on the "self-consistent micromechanics method" [18] these equations demonstrate, in agreement with the experimental data, the importance of the effect of load geometry on the thermal and mechanical properties of the composite materials [19,20].

The present work focuses on a method for generating a large quantities of 3D microstructure with random inclusions (both position and orientation), applicable to a large number of heterogeneities with different sizes and shapes (grains, wafers, voids, needles, fibers, etc). The constructed RVEs are used to create STL models that can be imported into any conversion software such as CATIA, and then export the created model as any solid format such as CATpart, STEP, or IGES, to calculate the effective properties using finite element techniques

2. Generation of microstructures

2.1. Geometric representation of loads at different aspect ratios

Ellipsoidal objects are appropriate for modeling the loads typical of many composites; Figure 1 shows examples of sketches of geometric objects that can be obtained from an ellipsoid by a simple change in aspect ratio.

The proposed geometries highlight their potential utility in generating 3D microstructure for a wide range of heterogeneous materials, Figure 2 shows three examples of composites with particulate inclusions of various aspect ratios.

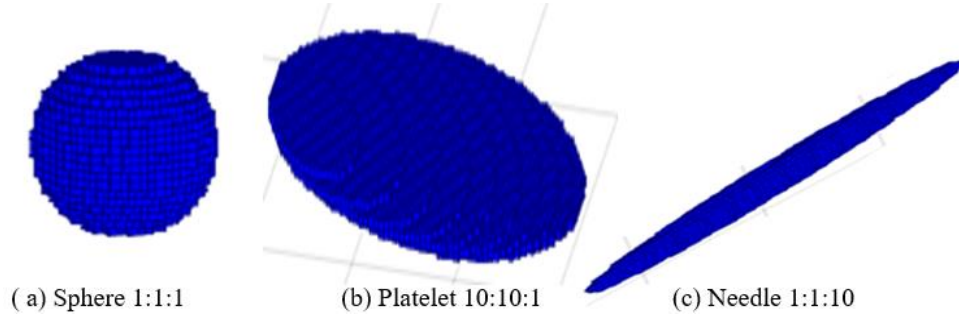


Figure 1. Geometric representation of the loads used in this work to generate a synthetic 3D composite microstructure with ellipsoidal inclusions of different aspect ratios.

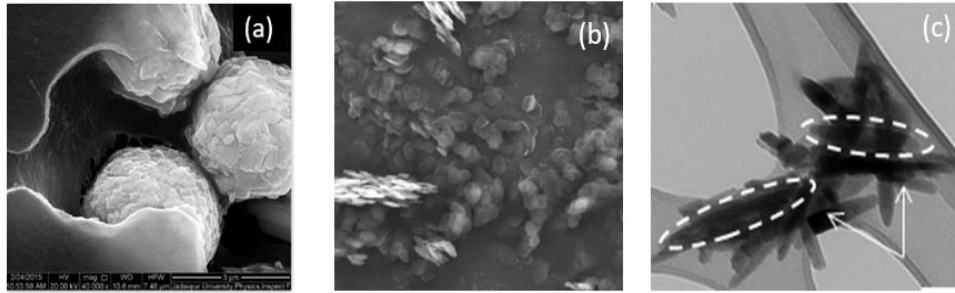


Figure 2. Examples of composites with particulate inclusions of various aspect ratios:(a) FESEM images of WO_2, H_2O nanoparticle loaded poly(vinylidene fluoride)[17](b) SEM images of Zirconium phosphate nanoplatelets [18](c) TEM micrographs of Biomimetic Nanoscale Hydroxyapatites [19]

The rotation matrix, based on the Euler angles ψ_1 , ψ_2 and ϕ , used to create the ellipsoids is:

$$\begin{pmatrix} \cos(\Psi_1) * \cos(\Psi_2) - \sin(\Psi_1) * \sin(\Psi_2) * \cos(\phi) & \sin(\Psi_1) * \cos(\Psi_2) + \cos(\Psi_1) * \sin(\Psi_2) * \cos(\phi) & \sin(\Psi_2) * \sin(\phi) \\ -\cos(\Psi_1) * \sin(\Psi_2) - \sin(\Psi_1) * \cos(\Psi_2) * \cos(\phi) & -\sin(\Psi_1) * \sin(\Psi_2) + \cos(\Psi_1) * \cos(\Psi_2) * \cos(\phi) & \cos(\Psi_2) * \sin(\phi) \\ \sin(\Psi_1) * \sin(\phi) & -\cos(\Psi_1) * \sin(\phi) & \cos(\phi) \end{pmatrix}$$

2.2. Algorithm description

The random sequential adsorption algorithm (RSA) is the methodology commonly used to generate random 3D microstructure because of its simplicity. The random placement of loads is performed by interpreting the placement procedure as a six-parameter stochastic process: three coordinates of the ellipsoid center (x_0, y_0, z_0) and the three angles describing orientation (ψ_1, ψ_2, ϕ) , and the method can be performed by the following steps:

Step 1: Initialization of the variables used in the generation of the 3D microstructure: the orthogonal distances of the ellipsoid (a, b, c), the desired volume fraction V_f_{max} and the size of the unit cell V.

Step 2: the first load is placed and oriented in a random position of the matrix. Once placed, the position of this particle is fixed and it cannot be modified.

Step 3: the following loads are randomly placed one after another in a sequential manner, and if the test particle overlaps with the previously placed particle(s), then this attempt is rejected. Otherwise, the placement is accepted.

Step 4: The following loads are added using the same method until the predetermined volume fraction is attained or jamming limit is attained. Jamming limit or volume saturation occurs when it is no longer possible to place a particle in the cavities between the other deposited particles. The generated microstructure should be able to create a periodic and continuous medium, which requires any ellipsoid that intersects with the boundary of the cube to be extended on the opposite side. The adopted RSA algorithm is presented in Figure 3.

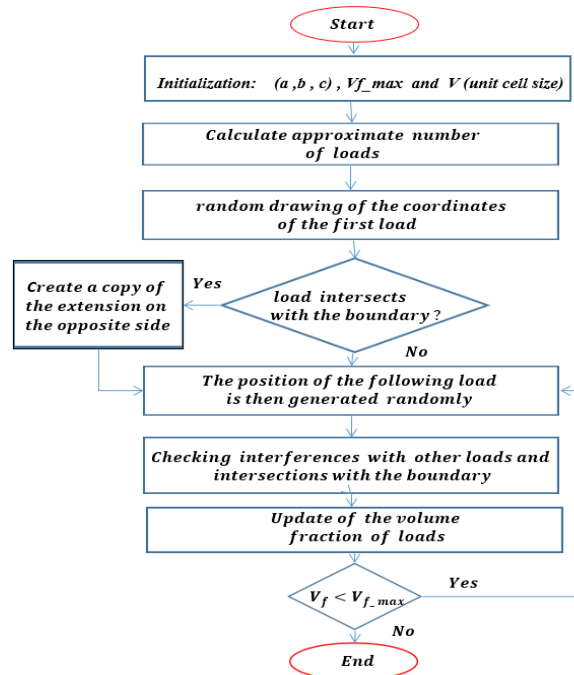


Figure3: Flowchart of the RSA algorithm used to generate 3D microstructure of various volume fractions and particles shapes

2.3 Program Code

```
% Generate Synthetic 3D Structure with Ellipses
clear all; clc;
% Initialize variables used in generation of 3D
microstructure used RSA algorithm that varies
% ellipse volume fraction, size, aspect ratio, and
%orientation
tic
Vf = 0;
% Vf_max = 0.05;
prompt={'entrer Vf_max'};
name='Vf_max';
numlines=1;
answer=inputdlg(prompt,name,numlines);
Vf_max=str2double(answer{1,1})
prompt={'entrer a'};
name='a';
numlines=1;
answer=inputdlg(prompt,name,numlines);
a=str2double(answer{1,1});
prompt={'entrer b'};
name='b';
numlines=1;
answer=inputdlg(prompt,name,numlines);
b=str2double(answer{1,1});
prompt={'entrer c'};
name='c';
numlines=1;
answer=inputdlg(prompt,name,numlines);
c=str2double(answer{1,1});
% a = 12; b = 6; c = 6;
nparticles = 0;
I = false(256,256,256);
image_size = size(I);
% Calculate approximate Vf of particle and approximate
number of particles to generate the specified volume
fraction.
% Assign random orientation
psi1 = 2*pi*rand; psi2 = 2*pi*rand; phi = acos(rand);
I_ellipse = image_ellipse_3D_fast(a,b,c,psi1,psi2,phi);
Vf_particle = sum(I_ellipse(:)) / numel(I);
```

```

approx_nparticles = Vf_max/Vf_particle;
disp(['Approximate      #      of      particles:      '
num2str(approx_nparticles)]);
% Main loop for generating microstructure
h = waitbar(0, 'Ellipsoid placement');
while Vf < Vf_max
psi1 = 2*pi*rand;
psi2 = 2*pi*rand;
phi = acos(rand);
I_ellipse = image_ellipse_3D_fast(a,b,c,psi1,psi2,phi);
x0 = ceil(rand*image_size(1));
y0 = ceil(rand*image_size(2));
z0 = ceil(rand*image_size(3));
diam = size(I_ellipse,1);
%Merge circle matrix with synthetic microstructure image
nlo = x0 - floor(diam/2); nhi = x0 + ceil(diam/2)-1;
ix = mod(nlo:nhi,image_size(1));ix(ix==0)=image_size(1);
nlo = y0 - floor(diam/2); nhi = y0 + ceil(diam/2)-1;
iy = mod(nlo:nhi,image_size(2));iy(iy==0)=image_size(2);
nlo = z0 - floor(diam/2); nhi = z0 + ceil(diam/2)-1;
iz = mod(nlo:nhi,image_size(3));iz(iz==0)=image_size(3);
Itest = logical(I(ix,iy,iz));
if sum(Itest(I_ellipse)) == 0
Itest(I_ellipse) = 1;
I(ix,iy,iz) = Itest;
accept = 1;
else
accept = 0;
iter = 0;
while accept == 0 && iter <= 10
iter = iter + 1;
x0 = ceil(rand*image_size(1));
y0 = ceil(rand*image_size(2));
z0 = ceil(rand*image_size(3));
diam = size(I_ellipse,1);
% Merge circle matrix with synthetic microstructure
nlo = x0 - floor(diam/2); nhi = x0 + ceil(diam/2)-1;
ix = mod(nlo:nhi,image_size(1));
ix(ix==0)=image_size(1);
nlo = y0 - floor(diam/2); nhi = y0 + ceil(diam/2)-1;
iy = mod(nlo:nhi,image_size(2));
iy(iy==0)=image_size(2);

```

```

nlo = z0 - floor(diam/2); nhi = z0 + ceil(diam/2)-1;
iz = mod(nlo:nhi,image_size(3));
iz(iz==0)=image_size(3);
Itest = logical(I(ix,iy,iz));
if sum(Itest(I_ellipse)) == 0
Itest(I_ellipse) = 1;
I(ix,iy,iz) = Itest;
accept = 1;
end
end
end
if accept;
nparticles = nparticles + 1;
Vf_particle = sum(I_ellipse(:)) / numel(I);
Vf = Vf + Vf_particle;
ellipse(nparticles,1:10) = ...
[x0 y0 z0 a b c psi1 psi2 phi Vf_particle];
end
waitbar(Vf/Vf_max)
end
close(h)
disp(['3D Digital Slices (sec): ' num2str(toc)]);
disp(['Number of particles: ' num2str(nparticles)]);
% Write ellipse parameters to Excel
% Store all ellipse parameters in Excel so that the 3D
structure
% can be generated without worrying about overlap.
image_save_flag = 1;
if image_save_flag
string_path = pwd;
Excel_fileName
=
sprintf('%s\3D_ellipses.xlsx',string_path);
sheet = sprintf('ellipse_%dvf_%da_%db_%dc_%05d',...
round(100*Vf),a,b,c,nparticles);
warning off MATLAB:xlswrite:AddSheet;
ColHeaders
=
{'x0','y0','z0','a','b','c','psi1','psi1','phi'};
xlswrite(Excel_fileName, ColHeaders, sheet, 'A1');
xlswrite(Excel_fileName, ellipse, sheet, 'A2');
deleteEmptyExcelSheets(Excel_fileName);
end
% View slices of a 3D section

```

```

j=1;
close all;
Ix=1:256;
Iy=Ix;Iz=Ix;
% [Ix,Iy,Iz]=meshgrid(Ix,Iy,Iz);
figure()
box on
grid on
PATCH_3Darray(I,Ix,Iy,Iz);
view([155 11])
figure()
subplot 121
box on
grid on
PATCH_3Darray(I,Ix,Iy,Iz);
view([155 11])
subplot 122
while j
for i = 1:image_size(3)
J = 1-I(:, :, i);
image_view(J);
title(['Slice ' num2str(i)])
pause(0.05)
end
end
% Hit control-C to exit
% Save individual slices as jpegs for animated gifs
tic
close all; figure;
sheetname = sprintf('ellipse_%dvf_%da_%db_%dc_%05d',...
round(100*Vf), a,b,c,nparticles);
if ~isdir(sheetname), mkdir(sheetname); end
copyfile('image_view.m',sheetname)
cd(sheetname)
fid = fopen([sheetname '.txt'],'w');
figure
for i = 1:image_size(3)
K = reshape(1-I(:, :, i),image_size(1),image_size(2));
J = K;
image_view(J);
pause(0.05)
image_filename = [sheetname, sprintf('_%03d.jpg',i)];

```

```

fprintf(fid,'%s \n',image_filename);
if image_save_flag; imwrite(J,image_filename,'jpg'); end
end
fclose(fid);
delete('image_view.m')
cd ..
% Save to *.mat file as well
save([sheetname '.mat'],'I')
disp(['Image viewing and saving (sec): ' num2str(toc)]);
% *.mat file is useful for subsequent operations in
MATLAB or writing
% files, *.jpg is useful for visualization, *.tif
binaries are a useful
% if lossless compression is desired, *.txt contains a
list of images,
% *.xls contains spreadsheet with all ellipse parameters,
if desired

CONVERT_voxels_to_stl('toto.stl',I,Ix,Iy,Iz)
% READ_stl('toto.stl')

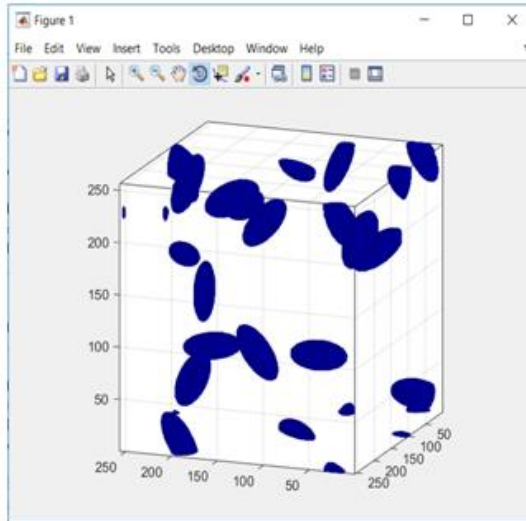
```

2.4 Geometric generation

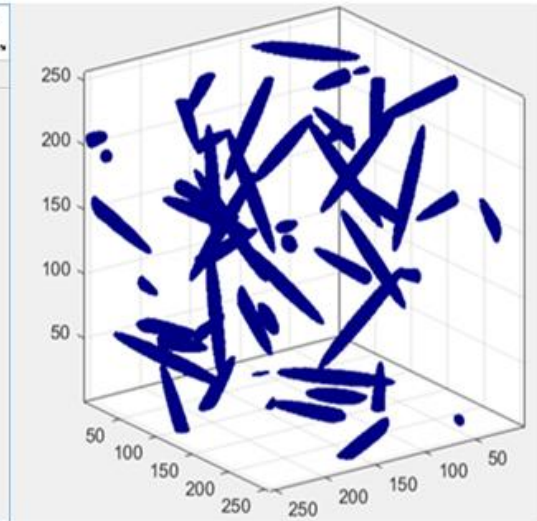
2.4.1 3D microstructure

A tool for generating ellipsoids randomly dispersed in a periodic cube has been developed under Matlab. Figure 4 shows examples of 3D microstructures containing ellipsoids dispersed and randomly oriented in a cube generated using this tool.

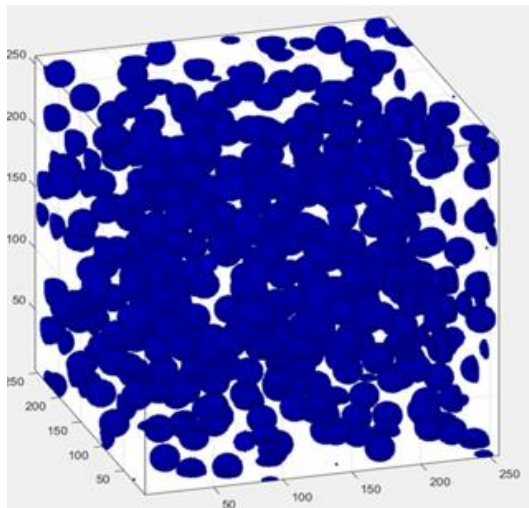
The ellipsoid parameters are saved in Excel (figure 5) so that the 3D structure can be generated without worrying about overlap.



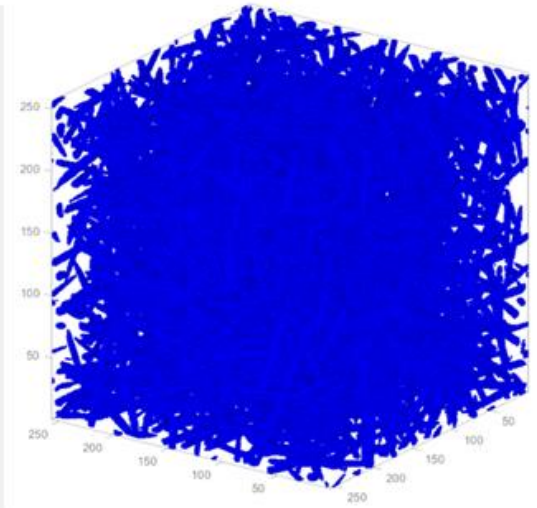
$V_{fmax} = 2\%$
 Approximate # of particles: 17.8168
 3D Digital Slices (sec): 45.5301
 Number of particles: 18
 Aspect ratio 1:2:4



$V_{fmax} = 1\%$
 Approximate # of particles: 32.9627
 3D Digital Slices (sec): 23.863
 Number of particles: 33
 Aspect ratio 1:2:10



$V_{fmax2} = 10\%$
 Approximate # of particles: 403.3954
 3D Digital Slices (sec): 16.9137
 Number of particles: 403
 Aspect ratio 1:1:1



$V_{fmax2} = 10\%$
 Approximate # of particles: 1167.5168
 3D Digital Slices (sec): 2123.0664
 Number of particles: 1168
 Aspect ratio 70:3:2

Figure 4 Generated microstructures using the modified RSA method

| 3D_ellipses.xlsx | | | | | | | | | | | | |
|------------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|------------|--------|--------|
| DellipsesS2 | | | | | | | | | | | | |
| | x0 | y0 | z0 | a | b | c | psi1 | psi2 | phi | VarName10 | | |
| Number | Number | Number | Number | Number | Number | Number | Number | Number | Number | Number | Number | Number |
| 2 | 207 | 18 | 244 | 10 | 10 | 6 | 5.1459 | 3.9265 | 0.7399 | 1.4955e-04 | | |
| 3 | 213 | 41 | 118 | 10 | 10 | 6 | 3.1264 | 4.7447 | 0.7341 | 1.4895e-04 | | |
| 4 | 230 | 150 | 150 | 10 | 10 | 6 | 3.8836 | 5.8571 | 0.5825 | 1.4967e-04 | | |
| 5 | 105 | 10 | 192 | 10 | 10 | 6 | 5.3717 | 0.2191 | 0.4834 | 1.4919e-04 | | |
| 6 | 66 | 83 | 103 | 10 | 10 | 6 | 0.9728 | 0.9042 | 0.9198 | 1.4955e-04 | | |
| 7 | 43 | 49 | 25 | 10 | 10 | 6 | 2.5533 | 2.4265 | 0.9150 | 1.4943e-04 | | |
| 8 | 190 | 178 | 211 | 10 | 10 | 6 | 2.0306 | 4.8355 | 1.3345 | 1.4931e-04 | | |
| 9 | 134 | 84 | 213 | 10 | 10 | 6 | 5.2023 | 1.8433 | 1.2563 | 1.4979e-04 | | |
| 10 | 175 | 60 | 117 | 10 | 10 | 6 | 5.0912 | 3.4997 | 1.3047 | 1.4907e-04 | | |
| 11 | 194 | 251 | 61 | 10 | 10 | 6 | 2.4163 | 3.3841 | 0.1289 | 1.4836e-04 | | |
| 12 | 155 | 220 | 253 | 10 | 10 | 6 | 3.3210 | 0.3232 | 0.7123 | 1.4848e-04 | | |
| 13 | 139 | 54 | 57 | 10 | 10 | 6 | 5.8401 | 2.5731 | 1.5705 | 1.4955e-04 | | |
| 14 | 192 | 140 | 87 | 10 | 10 | 6 | 2.0471 | 0.6029 | 0.7265 | 1.4800e-04 | | |
| 15 | 229 | 92 | 140 | 10 | 10 | 6 | 5.2297 | 3.4719 | 0.2924 | 1.4895e-04 | | |
| 16 | 191 | 33 | 211 | 10 | 10 | 6 | 2.1783 | 3.9132 | 0.6491 | 1.4967e-04 | | |
| 17 | 201 | 95 | 191 | 10 | 10 | 6 | 0.1580 | 2.6039 | 0.7504 | 1.4931e-04 | | |
| 18 | 58 | 90 | 74 | 10 | 10 | 6 | 5.6063 | 1.5243 | 1.4408 | 1.4883e-04 | | |
| 19 | 42 | 215 | 43 | 10 | 10 | 6 | 5.8276 | 0.3224 | 0.9364 | 1.4979e-04 | | |
| 20 | 13 | 55 | 102 | 10 | 10 | 6 | 3.1554 | 6.2790 | 1.2074 | 1.4943e-04 | | |
| 21 | 175 | 247 | 113 | 10 | 10 | 6 | 2.0965 | 1.4426 | 0.3594 | 1.5038e-04 | | |
| 22 | 206 | 60 | 239 | 10 | 10 | 6 | 5.9083 | 0.0367 | 0.9143 | 1.4955e-04 | | |
| 23 | 203 | 85 | 58 | 10 | 10 | 6 | 4.7957 | 5.1927 | 0.9601 | 1.4883e-04 | | |
| 24 | 75 | 104 | 221 | 10 | 10 | 6 | 1.9628 | 3.6727 | 0.5918 | 1.5014e-04 | | |
| 25 | 212 | 174 | 64 | 10 | 10 | 6 | 3.8625 | 6.2278 | 1.3657 | 1.4943e-04 | | |
| 26 | 216 | 91 | 111 | 10 | 10 | 6 | 2.9894 | 2.5075 | 0.9280 | 1.4943e-04 | | |
| 27 | 195 | 100 | 110 | 10 | 10 | 6 | 3.5955 | 4.4034 | 0.7340 | 1.4931e-04 | | |
| 28 | 71 | 160 | 151 | 10 | 10 | 6 | 6.0089 | 3.6001 | 0.5553 | 1.4955e-04 | | |

Figure 5: ellipsoid parameters.xlsx

2.4.2 2-D slices from a 3-D microstructure

A set of 2D slices from a 3D microstructure can be visualized as orthogonal 2D planes in the 3D microstructure as a function of depth. Figure 6 illustrates a two-dimensional slice of a 3D microstructure containing 401 particles with an aspect ratio (1:1:4) and a 5% volume fraction.

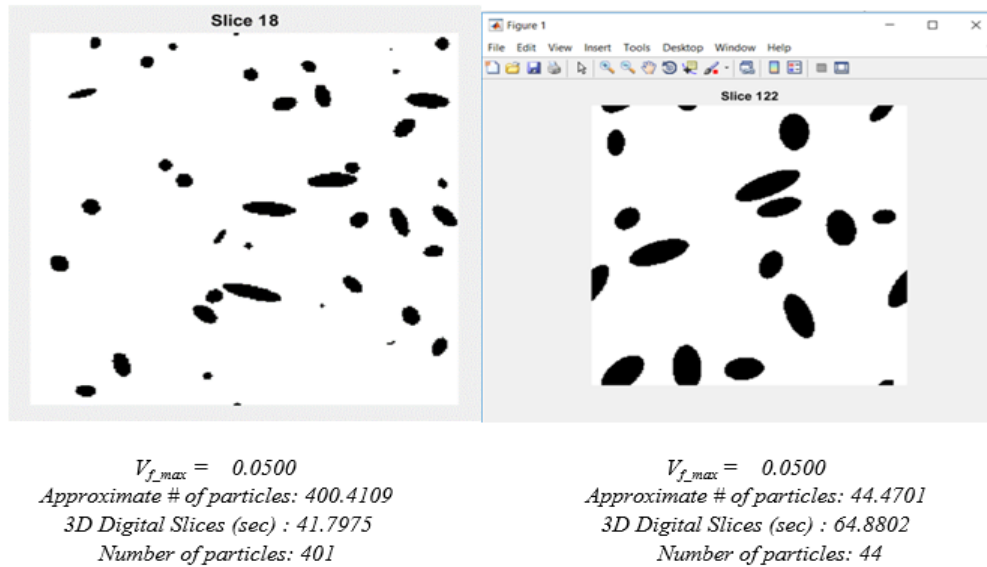


Figure 6 slice of 3D microstructure

On a slice the microstructure seems to have particles with a distribution of aspect ratios, but in reality, the particles are identical which shows the difficulty to deduce the 3D structure from the 2D the periodic limits are visible on the example in Figure 7 for some particles that cross the square limits.

2.5 Conversion of the 3D microstructure into STL format

To achieve a consistent transfer of geometric information, the microstructure is converted to STL format (Figure 8), which is widely used in the context of additive manufacturing, and can be exported into a software package to determine the effective properties of the materials considered by finite element techniques.

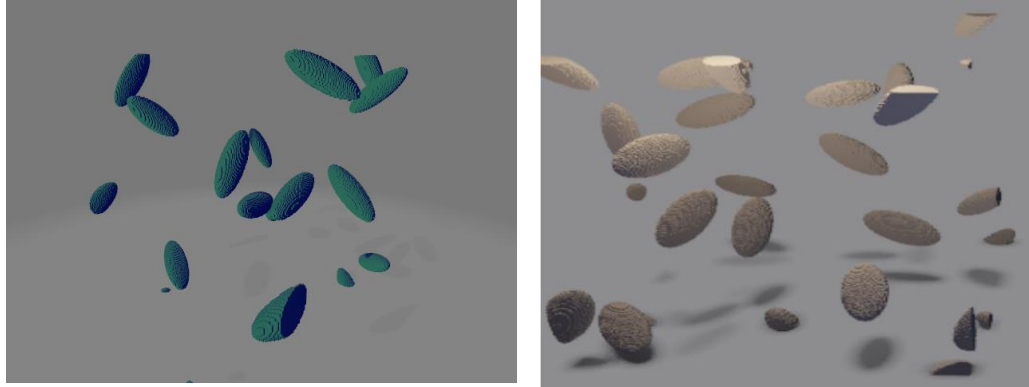


Figure 7: STL format of the microstructure

The STL file can be imported directly into ABAQUS or it is imported into CATIA, then the created model is exported into ABAQUS in CATpart, or STEP format (Figure 8).

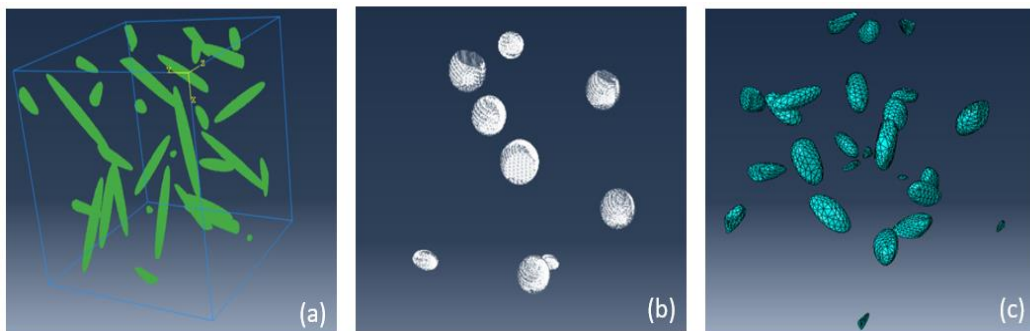


Figure 8. Illustration of geometric models:(a) STL, (b) CATpart, (c) STEP

2.6 Meshing

Periodic boundary conditions (PBCs)[5][24][25] have been shown to provide a better estimate of effective properties for random microstructure composite materials. However, their application requires meshes with maps of almost identical opposite sides, i.e. coupling a large number of nodes randomly distributed on two opposite surfaces, since they will ensure that the external surfaces deformed by the RVE remain periodic. Therefore, a periodic microstructure, such that any ellipsoids that intersect the boundary of the volume have been extended to the opposite surface (see Figure 9), is necessary for the implementation of PBCs in the context of the FE method. Figure 10 shows two periodic mesh volumes with a 10% volume fraction.

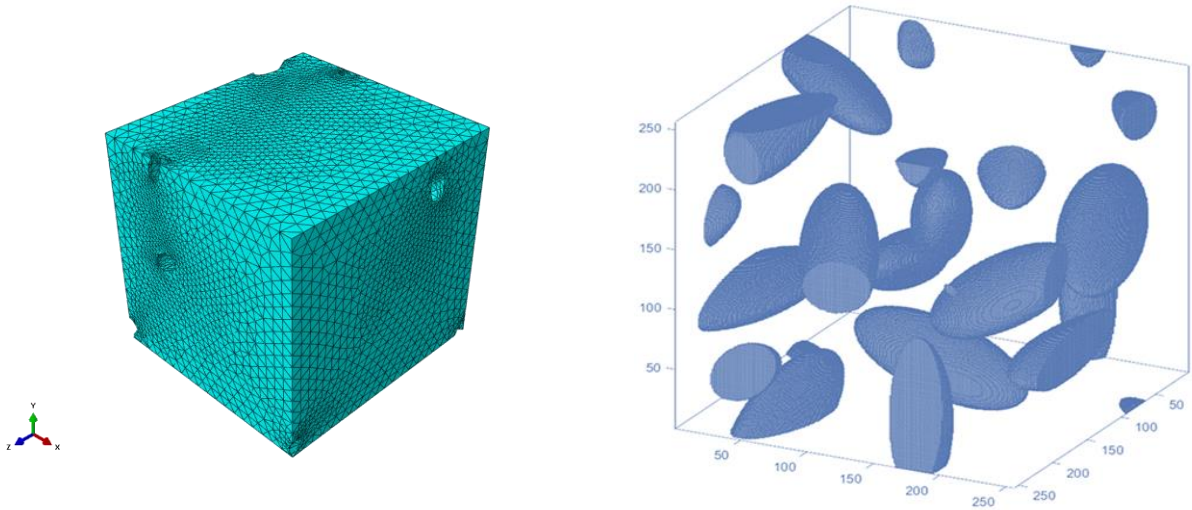


Figure9. Periodic microstructure

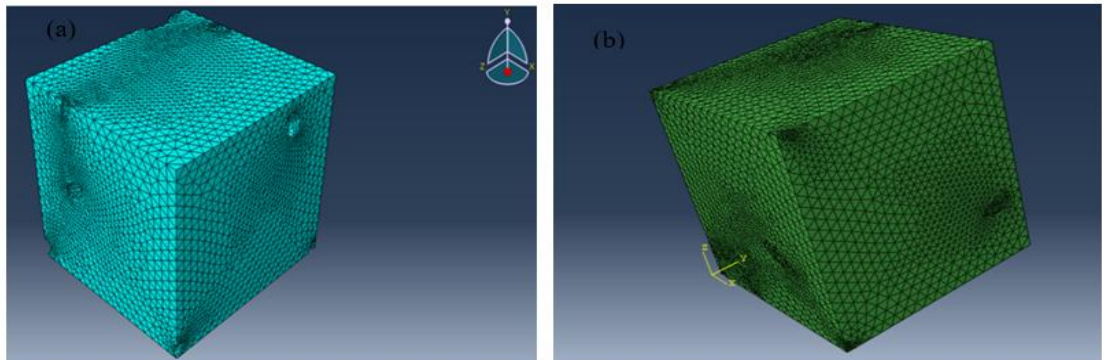


Figure. 10 Meshing of the microstructure:

(a) of a porous material and (b) a composite obtained by a matrix/inclusion assembly

Conclusion and perspectives

Geometric information of real microstructures is necessary for the study of the effective behavior of random heterogeneous materials. In this paper we have provided a method for generating 3D microstructure preserving the non-overlapping requirement, and creating STL models that can be imported into any conversion software such as CATIA, and then export the created model as any solid format such as STEP or CATpart or IGES, to calculate the effective properties using finite

element techniques. As perspectives for this work, the generated models will be used, on the one hand, to predict the mechanical and electrical properties of Poly(vinylidene fluoride)-based scaffolds, and on the other hand to study the thermal response of a clay-based composite construction materials.

References

- [1] H. R. Lusti and A. A. Gusev, Finite element predictions for the thermoelastic properties of nanotube reinforced polymers, *Modelling and Simulation in Materials Science and Engineering*. vol.12 (3) (2004) 107–119.
- [2] B. Dutta, N. Bose, E. Kar, S. Das, and S. Mukherjee. Smart , lightweight , flexible NiO / poly (vinylidene flouride) nanocomposites film with significantly enhanced dielectric , piezoelectric and EMI shielding properties. *J Polym Res* vol. 24 (220) (2017) 1-15
- [3] M. Faye, B. Lartigue, and S. Kane, Influence of structural and thermophysical parameters of insulating aggregates on the effective thermal conductivity of lightweight concrete. *J. Build. Eng.* Vol. 21 (2018). 74–81.
- [4] S. Mounir, A. Khabbazi, A. Khaldoun, Y. Maaloufa, and Y. El Hamdouni, Thermal inertia and thermal properties of the composite material clay-wool, *Sustain. Cities Soc.* vol. 19 (2015) 191–199,.
- [5] T. Kanit and S. Forest, Determination of the size of the representative volume element for random composites: statistical and numerical approach. *International Journal of Solids and Structures*. vol. 40 (2003) 3647–3679
- [6] H. Moussaddy. D. Therriault and M. Lévesque. A new definition of the representative volument element in numerical homogenization problems and its application to the performance evaluation of analytical homogenization models. *International Journal of Solids and Structures*. vol. 50(24) (2013) 3817-3828.
- [7] S. L. Omairey, P. D. Dunning, and S. Sriramula, Development of an ABAQUS plugin tool for periodic RVE homogenisation, *Eng. Comput.* vol. 35 (2) (2019) 567–577.
- [8] A. A. Gusev, Numerical Identification of the Potential of Whisker- and Platelet-Filled Polymers. *Macromolecules*. vol. 34 (2001) 3081–3093.
- [9] L. Chen, B. Gu, J. Tao, and J. Zhou, The average response and isotropy of 3D Representative Volume Elements for random distributed short fibers reinforced elastomer. *Composite Structures*. vol.216 (2019) 279-289.
- [10] M. T. Abadi, Characterization of heterogeneous materials under shear loading at finite strain. *Compos. Struct.* vol. 92 (2) (2010) 578–584.
- [11] S. Lucarini and J. Segurado. DBFFT: A displacement based FFT approach for homogenization of the mechanical behavior. *International Journal of Engineering Science*. vol. 144 (2019) 1–26.
- [12] S. Bargmann *et al.* Generation of 3D representative volume elements for heterogeneous materials: A review. *Prog. Mater. Sci.* vol. 96 (2018) 322–384.
- [13] M. A. Tschopp. 3-D Synthetic Microstructure Generation with Ellipsoid Particles 3-D Synthetic Microstructure Generation with Ellipsoid Particles. *US Army Research Laboratory*.vol. 0789 (2016) 1-26 .
- [14] E. Ghossein and M. Lévesque. Homogenization models for predicting local field statistics in ellipsoidal particles reinforced composites: Comparisons and validations fibers. *International Journal of Solids and Structures*. VOL. 58 (2015) 91-105.
- [15] H. R. Lusti, A. A. Gusev, and O. Guseva, “The influence of platelet disorientation on the barrier properties of composites: A numerical study,” *Model. Simul. Mater. Sci. Eng.*, vol. 12 (6) (2004) 1201–1207.
- [16] A. A. Mousavi, B. Arash, X. Zhuang, and T. Rabczuk. A coarse-grained model for the

- elastic properties of cross linked short carbon nanotube/polymer composites. *Composites Part B: Engineering*. vol. 95 (2016) 404-411.
- [17] P. Thakur, A. Kool, B. Bagchi, N. A. Hoque, S. Das, and P. Nandy. RSC Advances Improvement of electroactive b phase nucleation loaded poly (vinylidene fluoride) thin films. *RSC Adv*. vol. 5 (2015) 62819-62827.
- [18] H. Zhang, L. Chen, X. Han, F. Jiang, H. Sun, and D. Sun. RSC Advances Enhanced mechanical properties of Nylon6 nanocomposites containing pristine α -zirconium phosphate nanoplatelets of various sizes by melt. *RSC Adv*. vol.7 (2017) 32682-32691.
- [19] P. Gentile, C. J. Wilcock, C. A. Miller, R. Moorehead, and P. V Hatton. Process Optimisation to Control the Physico-Chemical Characteristics of Biomimetic Nanoscale Hydroxyapatites Prepared Using Wet Chemical Precipitation. *Materials*. vol. 8 (2015) 2297-2310.
- [20] W. Wu and J. Owino. Applying Periodic Boundary Conditions in Finite Element Analysis. *Simulia Community Conf*. (2014) 707-719.