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VIRTUAL MODEL GENERATION OF REPRESENTATIVE VOLUME ELEMENT FOR UNIDIRECTIONAL COMPOSITE

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Abstract. *Composite materials are widely used in different industries because of their unique characteristics that can be adapted depending on the application. Prediction of mechanical properties before the production process enables time saving and optimization of geometry and materials. The purpose of this paper is to show the steps in virtual modeling of the elementary unit of the unidirectional composite. The first step is the computer generation of the virtual domain that needs to geometrically match the experimental sample. After that, the mesh of finite elements must be defined and apply algorithms for periodic border conditions. The next step is setting the boundary conditions and forces. After obtaining contour plots (homogenization method) mechanical characteristics and effective elastic constants of the composite can be predicted.*

Thanks to the implementation of the finite element method in the ABAQUS program, it is possible to predict the mechanical characteristics of the composite depending on the variation of different parameters of the composite.

Key words: *Unidirectional composite, finite element method, simulation, algorithm.*

1. INTRODUCTION

Simulations of complex physical phenomena in the field of composite materials have led to a better understanding of the mechanical characteristics of the composite on the microscale. Composites are modeled from microscale to macroscale while taking into account the replication of a representative volume element (RVE). Thanks to finite element simulations, it is possible to predict the values of mechanical characteristics and elastic constants as well as macroscale fracture [1, 4 - 6]. In aerospace, where project values are measured in millions of dollars, it is very important to initially test the high load zone under the given operating conditions. After that, there are several corrections to the model with the aim of reducing the critical zones.

Figure 1a shows a micrograph of a unidirectional composite that can be represented as a reference structure when creating a model. In practice, it is more convenient to use the algorithm for the random generation of fibers, which must fulfill several conditions that will be discussed later. It is necessary to create a model that realistically represents the micrograph (Figure 1a) as well as the internal stress fields (Figure 1b, Figure 3).

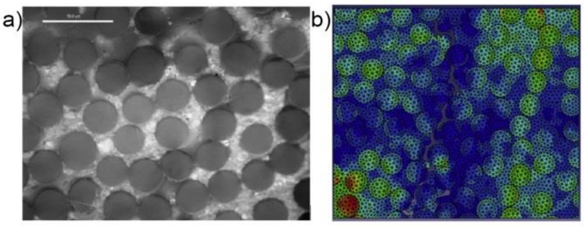

Figure 1. *a) An micrograph of unidirectional hybrid kenaf/glass fiber composites [3], b) internal stress fields and fracture of RVE[6]*

The nature of the manufacturing process shows that the fibers in the composite are randomly distributed. The computer model must not have perfectly distributed fibers at equal distances - composite fibers must have a random layout that cuts edges of the RVE domain to avoid the wall effect. In the work of Gitman et al it has been shown that there are deviations of 95% (for small dimensions of RVE

25x25) for the case of shear loading composite if there is a wall effect.

In order to avoid this unwanted effect and achieve a representative picture of reality, it is better to avoid the wall effect by applying periodicity rather than increasing RVE size with the aim of reducing the unwanted wall effects. This paper will be based on the algorithm that generates random fiber positions of the unidirectional composite for a given volume fraction and takes into account cross-sections of fibers with domain boundaries and fiber transformation along the x and y axis to always equal the number of the fibers in each RVE.

2. VOLUME FRACTION

The volume fraction of the carbon fiber in this case directly affects the mechanical characteristics of the composite. For this reason, it is necessary to compare the same volume fraction for different RVE sizes (figure 2). The goal is to determine the minimum value of the ratio between domain and fiber, where deviations from experimental results are minimal. Also, in future papers, the "strength" function can be determined, which will represent a change in mechanical characteristics depending on the volume fraction.

In the case of 2D RVE, the fiber volume is calculated by the formula $(R^2\pi*N)/(W*H)$, where R is the radius of fiber, N number of fibers, W width and H height of the RVE domain. The algorithm is able to generate fiber positions up to a 68% volume fraction, which is one of the high-density composites. Figure 2 represents domains with a volume fraction of 50.2% while RVE sizes are 25x25, 75x75, 125x125 and 175x175 micrometers. In accordance with the previously mentioned formula and the values of the volume fraction of fiber in the composite, going from the smallest to the highest RVE size, the numbers of fibers are 1, 9, 25, and 49, which can be seen in figure 2. All fibers are randomly generated to ensure a real correlation to the microscopic view (figure 1a).

3. MESH CONVERGENCE

When a domain is defined, defining the parameters of the finite element mesh is also necessary before running the simulation. The common step in applying the finite element method is the determination of numbers where the results are converging. A coarse mesh causes shorter simulation times, but this must not lead to results that deviate from the experimental sample. In order to obtain a mesh that has optimal size (number of elements), it is necessary to analyze several different models for the given 75x75 micrometer domain.

When the results achieve convergence, a mesh that has a minimum number of elements will be chosen so that the simulation time is minimal. At the same time, there is a sufficient number of finite elements that the results from the experiment deviate within any given range. Today's computers are powerful but it is up to the engineer to always optimize the system in order to make the process cost and time effective.

4. RANDOM GENERATOR

The randomly generated fiber position algorithm consists of two steps. The first step is the generation of a random center of the circle and checking conditions for not intersecting fibers. The second step is applying a periodic boundary conditions algorithm that replicates the fibers to the corresponding edges of the domain in case the fiber cuts the domain edge.

The randomly generated non intersecting algorithm is based on Pythagorean theorem: $Distance_{min}^2 = (x_2-x_1)^2+(y_2-y_1)^2$, where (x_1,y_1) and (x_2,y_2) are coordinates of circles. $Distance_{min} = R_1+R_2+\Delta$, where R_1 and R_2 are radius of circles and the Δ is the value of the minimum distance between the circles. The algorithm starts from the random coordinates x_1 and y_1 of the first circle where $x_1 \in [0,W_{comp}]$ and $y_1 \in [0,H_{comp}]$. After you enter the first set of numbers in the list, the next coordinates are generated for x_2 and y_2.

If the distance between centers is greater than the sum of their radius and the previously defined Δ, it means that circles are not intersecting and that coordinates should be added to the list. If the distance is less than $R_1+R_2+\Delta$, the coordinates are discarded and the algorithm generates the new coordinates for x_2 and y_2 until successfully generated nonintersecting. For practical reasons (generation of a mesh of finite elements) it is desirable to define the minimum distance between the circles that the finite element in that position is not significantly smaller than the surrounding elements.

4.1. Periodic boundary conditions

The periodic boundary condition is essentially a characteristic of RVE that nodes and fibers on opposite sides of the domain behave in exactly the same way in working conditions. Each fiber that cuts RVE edges must be mirrored on the other side of the domain so that there is exactly one fiber in the total. In case this step is ignored, when connecting two or more nearby representative volume elements there will be a visible wall effect after applying force - the real material does not have the characteristic that it is limited within the box (domain). Figure 2 shows that each fiber that cuts the domain edge has its matching pair from the other edge of the domain. If we replicate RVE from figure 2a and place eight identical copies around it, there would be no intersection between the domain fibers, which is important because they are common nodes (figure 3).

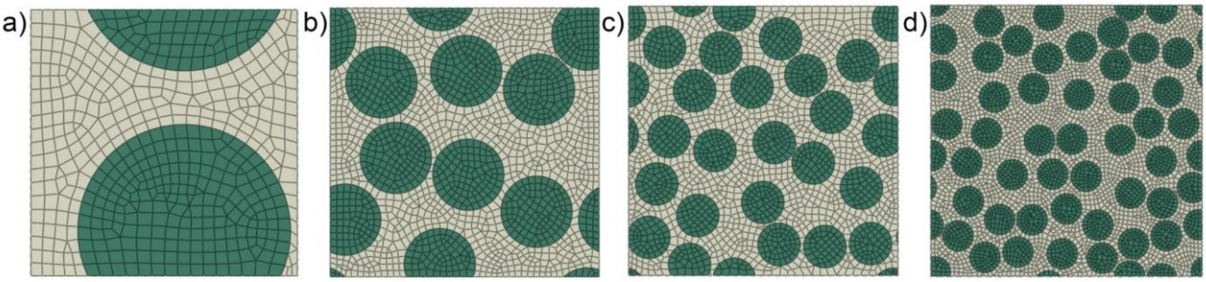

***Figure 2.** Different RVE sizes with constant volume fraction of 50,2% a) 25x25μm b) 75x75μm c)125x125μm d) 175x175μm. All the images show a mirroring of the fibers that cut the domain edge*

The circle intersection and replication of elements (fibers) will be shown for the given value. Suppose the center of the first generated fiber is in position $(R, H_{comp}/2)$. If the next generated center has coordinates $(W_{comp}, H_{comp}/2)$ it means that the circle cuts the right border in two parts, it needs to be mirrored to the left edge. As the first circle is already close to the left edge, mirroring of the second generated circle is impossible so it must be discarded. The algorithm randomly generates the next coordinate until there is enough room for each newly generated mirrored circle so there couldn't be any intersection. If a randomly generated center is located at the intersection of two domain edges, at the coordinate (W_{comp}, H_{comp}) by applying periodicity, it must also be replicated to coordinates $(0, H_{comp})$, $(0,0)$ and $(W_{comp}, 0)$.

The generalized form of the periodic boundary conditions algorithm (Python script for the Abaqus) which was previously generated, can be presented in the following form - there are 9 cases of replication the randomly generated fiber center, where $x \in [0, W_{comp}]$ and $y \in [0, H_{comp}]$:

1) if $x<R$ and $y \in [R, H_{comp}-R]$, replicated circle center is $(x+W_{comp}, y)$leva ivica
2) if $x<R$ and $y<R$, mirrored (replicated) circles have this coordinates $(x+W_{comp}, y)$ $(x+W_{comp}, y+H_{comp})$ $(x, y+H_{comp})$
3) if $x<R$ and $y>H_{comp}-R$, mirrored circles have this coordinates $(x+W_{comp}, y)$ $(x+W_{comp}, y-H_{comp})$ $(x, y-H_{comp})$
4) if $y>H_{comp}-R$ and $x \in [R, W_{comp}-R]$, mirrored circle has this coordinate $(x, y-H_{comp})$
5) if $y>H_{comp}-R$ and $x>W_{comp}-R$, mirrored circles are $(x, y-H_{comp})$ $(x-W_{comp}, y-H_{comp})$ $(x-W_{comp}, y)$
6) if $x>W_{comp}-R$ and $y \in [R, H_{comp}-R]$, mirrored circle has this coordinate $(x-W_{comp}, y)$
7) if $x>W_{comp}-R$ and $y<R$, mirrored circles have this coordinates $(x-W_{comp}, y)$ $(x-W_{comp}, y+H_{comp})$ $(x, y+H_{comp})$
8) if $y<R$ and $x \in [R, W_{comp}-R]$, mirrored circle has this coordinate $(x, y+H_{comp})$
9) if $x \in [R, W_{comp}-R]$ and $y \in [R, H_{comp}-R]$, the circle does not intersect domain edge

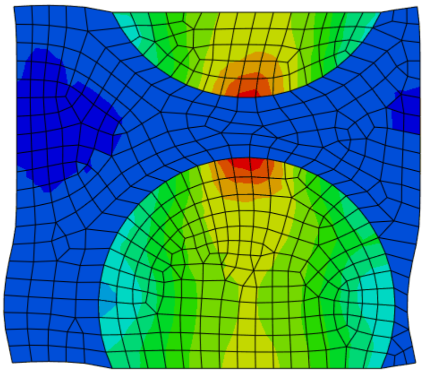

***Figure 3.** Internal stress fields of unidirectional composite (volume fraction 50,2%, domain size 25x25 μm)*

When modeling the interaction between nearby RVEs, because they have common nodes, the displacement of the node on one edge must correspond to the displacement of the corresponding node on the other edge, as shown in figure 3.

4.2. Reliability of results

The algorithm that has been created should be tested several times at the same input parameters (such as domain size, volume fraction, applied forces and boundary conditions, size, and a number of finite elements) to check whether identical results of mechanical characteristics are obtained. In the case that the results are repeated from simulation to simulation with each new random generated fiber arrangement, it can be considered that the algorithm is suitable for the virtual analysis of composite materials.

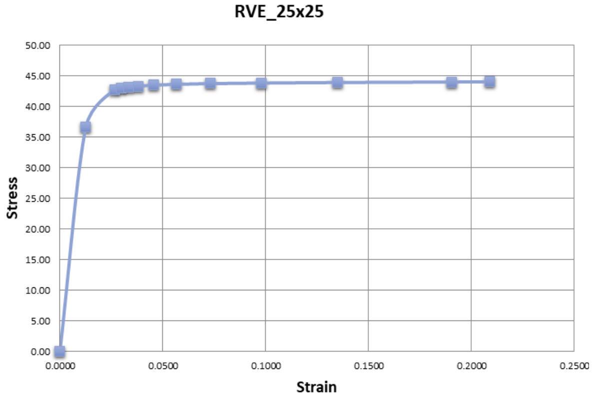

Figure 4. Stress-strain curve after RVE homogenization

5.CONCLUSION

The micromechanical analysis enables not only analysis of the elastic characteristics of the composite, but also the mechanical characteristics of the composite in any working conditions. Codes for algorithms are generated that enable an analysis of the mechanical characteristics of unidirectional composite materials. The algorithm can generate a high-density composite model of up to 68% volume fraction. The paper presents all the major steps in coding the Python script. It also explains and graphically presents fiber interactions via nodes on the opposite side of the representative volume element.

The concept of the paper should be extended to analyze the differences between experimental data and simulations. The idea is to get the optimal domain size for the given input parameters, which is small enough for faster simulation and at the same time large enough to obtain results that are repeatable and to an acceptable extent deviate from experimental results. In the future, attention may be focused on finding the same coefficient for short-fiber composites (2D), 3D RVE unidirectional composites, hybrid composites as well as other forms of composite structures. Attention can be also focused on analyzing the initiation and growth of the cracks in the matrix depending on loading conditions and determining the impact of the matrix material on damage initiation and propagation.

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