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Research Paper

Automatic three-dimensional geometry and mesh generation of periodic representative volume elements for matrix-inclusion composites

Konrad Schneider[a,*], Benjamin Klusemann[b,c], Swantje Bargmann[a,c]

[a] Institute of Continuum Mechanics and Material Mechanics, Hamburg University of Technology, Hamburg, Germany
[b] Institute of Product and Process Innovation, Leuphana University of Lüneburg, Lüneburg, Germany
[c] Institute of Materials Research, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany

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ABSTRACT

This paper introduces an efficient method to automatically generate and mesh a periodic three-dimensional microstructure for matrix-inclusion composites. Such models are of major importance in the field of computational micromechanics for homogenization purposes utilizing unit cell models. The main focus of this contribution is on the creation of cubic representative volume elements (RVEs) featuring a periodic geometry and a periodic mesh topology suitable for the application of periodic boundary conditions in the framework of finite element simulations. Our method systematically combines various meshing tools in an extremely efficient and robust algorithm. The RVE generation itself follows a straightforward random sequential absorption approach resulting in a randomized periodic microstructure. Special emphasis is placed on the discretization procedure to maintain a high quality mesh with as few elements as possible, thus, manageable for computer simulations applicable to high volume concentrations, high number of inclusions and complex inclusion geometries. Examples elucidate the ability of the proposed approach to efficiently generate large RVEs with a high number of anisotropic inclusions incorporating extreme aspect ratios but still maintaining a high quality mesh and a low number of elements.

1. Introduction

A crucial aspect in the development and optimization of high performance materials is the utilization of heterogeneous materials such as particle or fiber reinforced composites. For simulating and predicting the mechanical deformation behavior most accurately, it is essential to incorporate information of the underlying microstructure. The research field of computational micromechanics deals with this topic and the issues of how this should be conducted. A major interest in this field lies in the prediction of effective material properties or in the deduction of constitutive laws via multiscale methods [14,18,35]. One sophisticated approach is addressed to the investigation of unit cells that act as RVEs[1] of the material of interest [17,18]. The guiding idea is the computation of material responses on sample RVEs by solving a boundary value problem using numerical methods. The numerical method of choice throughout this work is the finite element method representing a state-of-the-art technology in computational engineering. For employing finite element simulations in this context, a discretization of the unit cells is inevitable. This rises the important question on what the RVE should look like and what the requirements of a proper finite element mesh are.

The geometric information of real microstructures gained from experimental observations, such as image reconstruction, are only partially suitable for numerical simulations due to their abundance and complexity [7,13]. For simulation purposes it is often necessary to artificially generate geometrically simpler RVEs which feature relevant properties of the real material. In this regard, the microstructures may be interpreted as the result of a stochastic process [35]. Generating a RVE can therefore be sourced by an artificial stochastic process which in turn leads to artificial microstructures. To verify and to ensure the quality and compliance of the generated geometry a stochastic equivalence between the real and artificial microstructures is desirable [28]. Considering the general

* Corresponding author.
E-mail address: Konrad.Schneider@tuhh.de (K. Schneider).

[1] Following [2] we associate the terminus unit cell with any volume that is capable of forming a periodic microstructure via congruence mappings (translation, mirroring, rotation). As a limiting case a unit cell might be a RVE.

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computational feasibility, only a few meaningful geometric parameters and their corresponding distributions might be included in such a process. A common approach to generate randomized artificial RVEs is the utilization of random sequential absorption processes [15,26,33] that successively built up the microstructure.

One major class of microstructured heterogeneous materials are matrix-inclusion composites featuring non-overlapping inclusions to which this paper addresses. Many authors dedicated their work to these materials considering various types of inclusions such as spherical particles [3,4,11,22,23], ellipsoids [3,5,12,24] or cylinders [1,8]. A cumbersome task in the generation process is placing the inclusions randomly while preserving the non-overlapping requirement. For this task intersection tests or distance queries between two inclusions need to be conducted. Especially the generation of unit cells with high volume fractions is difficult to manage [see e.g. 3, 24, 8]. More sophisticated approaches like molecular dynamic methods [12], geometric adaption of the particles [1], dynamic simulation of densification [34] or simulated annealing [26] are necessary to circumvent this problem.

Besides the geometry generation itself the geometric discretization is an important step for subsequent simulations. Especially for finite element simulations this becomes a non-trivial task. In context of the underlying boundary value problem, with respect to homogenization purposes, the application of periodic boundary conditions is favorable [18,21]. A drawback of this method is the inevitable requirement of a periodic mesh topology. Although there exist some software packages that feature a periodic mesh generation, e.g., NETGEN [27] or commercial meshing packages which allow mesh copying and constrained meshing, there is no straightforward way of generating such meshes. Problems may arise from the restriction to very simple inclusion geometries, such as spheres. Unstable boolean operations, which are likely to fail in the process of constructing the geometry, might be an inevitable obstacle. On the other hand, the mesh size can easily increase, resulting in finite element models too large for efficient simulations. In [3–5] the authors investigated random RVEs with different types of inclusions using NETGEN. It was revealed that for small number of inclusions very large number of elements result from the discretization process (e.g., 15 inclusions yield 100.000 elements). To circumvent this problem, [24] divided the meshing process into several steps. However, they were only able to consider spheroids with aspect ratios smaller than three. The recent work of [8] shows an approach featuring a large number of inclusions with infinite length. A combination of multiple software packages is applied to circumvent the drawback of using boolean operations. However, neither the generated microstructure nor the mesh feature a periodic topology. In this regard, the publication of [32] reveals a promising approach. By successively treating each inclusion individually a periodic mesh is obtained. However, their method requires the utilization of polyhedral finite elements, which requires non-standard software.

Another noticeable class of microstructured heterogeneous materials are polycrystals with a pronounced grain topology. [10,17,25] investigated their generation, discretization and effective mechanical properties by approximating the granular structure via Voronoi-diagrams. Again, only non-standard methods [10] result in a periodic mesh topology suitable for periodic boundary conditions.

These examples highlight the demand for a proper method for generating randomized matrix-inclusion RVEs featuring a periodic mesh topology. The central contribution of this paper is an algorithm that automatically generates a periodic tetrahedralization of cubic matrix-inclusion RVEs for the use in finite element simulations. The outline of this paper is as follows: First, we describe the microstructure geometry generation process. Thereafter, the individual inclusions are incorporated into a constructive solid geometry model, thus, taking care of potential intersections with the unit cell. The difficulties of discretization are solved by meshing the inclusions successively, hence, breaking down the meshing process into smaller subtasks. Therefore, the generated surface meshes of the constructive solid geometry representations of all inclusions are periodically distributed in the RVE, master edges and surfaces are created, resulting in a waterproof surface mesh. Afterwards, a volume mesh of high quality tetrahedrons is generated to obtain a discretization of the whole structure. Finally, we elucidate the quality of the generated mesh, and compare it to meshes from available software packages, e.g., NETGEN.

2. Microstructure generation

Exemplarily, the considered microstructures possess ellipsodial inclusions of revolution, namely spheroids. The examined RVEs exhibit a cuboid like shape featuring translational periodicity with these spheroids inside. Before the actual microstructure generation process is explained, we introduce an accurate description of the geometric setting, the significant geometric primitives and their randomized placement.

2.1. Mathematical description of geometric setting

One corner of the cuboid shaped RVE is located at the origin of the global coordinate system with edges aligned parallel to the coordinate axes as shown in Fig. 1. The side lengths of the cuboid are denoted by a_x, a_y and a_z. The faces of the RVE are interpreted as subsets of planes P_i. We describe these planes by the Hessian normal form

$$P_i = \{\boldsymbol{x} \in \mathbb{R}^3 \,|\, \boldsymbol{x}^{\mathrm{T}} \cdot \boldsymbol{n}_p + d = 0\}, \tag{1}$$

with $\boldsymbol{n}_p$ being the outward pointed normal vector and $|d|$ being the distance of the plane from the origin. With this description the six faces of the cuboid are addressed by

$$\begin{aligned}
P_{x_0} &= \{\boldsymbol{n}_{x_0} = [-1, \ \ 0, \ \ 0]^{\mathrm{T}}; d = 0\},\\
P_{x_1} &= \{\boldsymbol{n}_{x_1} = [\ \ 1, \ \ 0, \ \ 0]^{\mathrm{T}}; d = -a_x\},\\
P_{y_0} &= \{\boldsymbol{n}_{y_0} = [\ \ 0, -1, \ \ 0]^{\mathrm{T}}; d = 0\},\\
P_{y_1} &= \{\boldsymbol{n}_{y_1} = [\ \ 0, \ \ 1, \ \ 0]^{\mathrm{T}}; d = -a_y\},\\
P_{z_0} &= \{\boldsymbol{n}_{z_0} = [\ \ 0, \ \ 0, -1]^{\mathrm{T}}; d = 0\},\\
P_{z_1} &= \{\boldsymbol{n}_{z_1} = [\ \ 0, \ \ 0, \ \ 1]^{\mathrm{T}}; d = -a_z\}.
\end{aligned} \tag{2}$$

The edges of the cuboid are defined by subsets of lines L_i

$$L_i = \{\boldsymbol{a} + r\,\boldsymbol{n}_L \,|\, r \in \mathbb{R}\}, \tag{3}$$

where $\boldsymbol{a}$ is a point on the line and $\boldsymbol{n}_L$ the direction vector. Additionally, all 12 edges of the cube are interpreted as subsets of the intersection of two planes and expressed as

$$\begin{aligned}
&\left.\begin{aligned} L_{y_0z_0} &= \{P_{y_0} \wedge P_{z_0}\}, L_{y_0z_1} = \{P_{y_0} \wedge P_{z_1}\},\\ L_{y_1z_1} &= \{P_{y_1} \wedge P_{z_1}\}, L_{y_1z_0} = \{P_{y_1} \wedge P_{z_0}\}\end{aligned}\right\} \text{ with } \boldsymbol{n}_L = \begin{bmatrix}0\\1\\0\end{bmatrix},\\
&\left.\begin{aligned} L_{x_0z_0} &= \{P_{x_0} \wedge P_{z_0}\}, L_{x_0z_1} = \{P_{x_0} \wedge P_{z_1}\},\\ L_{x_1z_1} &= \{P_{x_1} \wedge P_{z_1}\}, L_{x_1z_0} = \{P_{x_1} \wedge P_{z_0}\}\end{aligned}\right\} \text{ with } \boldsymbol{n}_L = \begin{bmatrix}0\\1\\0\end{bmatrix},\\
&\left.\begin{aligned} L_{x_0y_0} &= \{P_{x_0} \wedge P_{y_0}\}, L_{x_0y_1} = \{P_{x_0} \wedge P_{y_1}\},\\ L_{x_1y_1} &= \{P_{x_1} \wedge P_{y_1}\}, L_{x_1y_0} = \{P_{x_1} \wedge P_{y_0}\}\end{aligned}\right\} \text{ with } \boldsymbol{n}_L = \begin{bmatrix}0\\0\\1\end{bmatrix}.
\end{aligned} \tag{4}$$

The eight corners C_i of the cuboid are described as the intersection of three planes by

$$\begin{aligned}
C_{x_0y_0z_0} &= \{P_{x_0} \wedge P_{y_0} \wedge P_{z_0}\}, \ C_{x_0y_1z_0} = \{P_{x_0} \wedge P_{y_1} \wedge P_{z_0}\},\\
C_{x_1y_1z_0} &= \{P_{x_1} \wedge P_{y_1} \wedge P_{z_0}\}, \ C_{x_1y_0z_0} = \{P_{x_1} \wedge P_{y_0} \wedge P_{z_0}\},\\
C_{x_0y_0z_1} &= \{P_{x_0} \wedge P_{y_0} \wedge P_{z_1}\}, \ C_{x_0y_1z_1} = \{P_{x_0} \wedge P_{y_1} \wedge P_{z_1}\},\\
C_{x_1y_1z_1} &= \{P_{x_1} \wedge P_{y_1} \wedge P_{z_1}\}, \ C_{x_1y_0z_1} = \{P_{x_1} \wedge P_{y_0} \wedge P_{z_1}\}.
\end{aligned} \tag{5}$$