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ASPECTS OF RVE TOPOLOGY, MESH DISCRETIZATION AND BOUNDARY CONDITIONS IN PRACTICAL MULTISCALING FOR MATRIX INCLUSION COMPOSITES

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Summary. A fully periodic representative volume element featuring a periodic topology, a periodic mesh and periodic boundary conditions is known to perform the best for determining effective material properties. However, the set-up of such finite element model can become a cumbersome task and might significantly reduce the overall efficiency.

In this contribution we examine multiple methodologies of setting up finite element models for homogenization purposes that extenuate these difficulties. A systematic study indicates that a fully periodic topology and mesh discretization with periodic boundary conditions is not necessary in order to identify effective macroscopic material parameters.

1 Introduction

Modern and complex materials are developed to serve the needs of modern machinery and their components. These materials often possess a distinctive microstructure at a certain length scale which significantly influences the macroscopic material behavior. The prediction of the mechanical deformation behavior to enhance the material design and production process is challenging, if it is necessary to consider microstructural information.

State of the art methodology is to only consider a small, but representative part of the structure, namely a representative volume element (RVE), featuring all relevant characteristics of the microstructure[1,4,6]. Within finite element simulations fully periodic RVEs featuring a periodic topology, a periodic mesh and exact periodic boundary conditions are known to perform best[4]. However, setting up such models and integrating these in the engineering practice might become cumbersome.

The aim of this contribution is a systematic evaluation of the influences on the macroscopic responses when relaxing the strong requirements of full periodicity[3].

2 Model setup

We follow the efficient RVE generation process described in Schneider et. al[2] to create and mesh three-dimensional, random, non-overlapping matrix-inclusion RVEs with arbitrarily placed spheroidal particles. The used algorithm is very efficient, robust and automized to produce high quality meshes while keeping the total number of elements at a manageble minimum.

Linear elastic and elastic-plastic behavior for the matrix material is considered. We investigate the behavior of two phase contrasts $\alpha = {}^{E_{\text{Matrix}}}/_{E_{\text{Inclusion}}} = {}^{G_{\text{Matrix}}}/_{G_{\text{Inclusion}}}$ with $\alpha = 100$ (soft inclusions mimicing rubber toughened polymerblends) and $\alpha = 0.01$ (stiff inclusions mimicing short fiber reinforced materials).

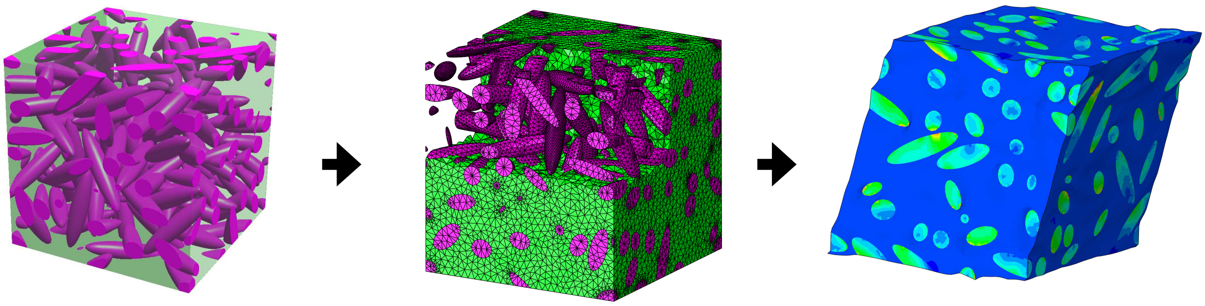

Figure 1: RVE with 100 inclusions under shear loading, exemplarily shown: periodic tetrahedral mesh under periodic boundary conditions.

Three different RVE sizes are considered via 10, 50 and 100 inclusions, respectively the characteristic ratio of RVE size to inclusion size $l/d = 0.49, 0.28$ and 0.23. The microstructural generation process yields periodic and non-periodic RVEs. Furthermore we investigate three variants of discretization, namely periodic tetrahedral meshes (PMESH), non-periodic tetrahedral meshes (NPMESH) and voxel meshes (VOXEL). For the determination of macroscopic material responses kinematic uniform boundary conditions (KUBC), periodic boundary conditions (PBC) and static uniform boundary conditions are applied to all finite element models. Due to the fact of the requirement of a periodic mesh, when applying periodic boundary conditions, a form of approximate periodic boundary conditions (PBCTIE) are introduced to the models with non-periodic meshes.

Following the suggestions of Yuan[5], a constraint formulation typically available in commercial finite element software is utilized[1]. A statistical study is given to support the results and extenuate artificial findings due to the randomness of the RVE generation process in considering 20 random RVEs per realization. Tensile and shear loadings are applied.

3 Conclusion

Figure 2 exemplarily shows the normalized shear modulus of all realizations for different shear contrasts. All simulations are normalized to the fully periodic reference solution with

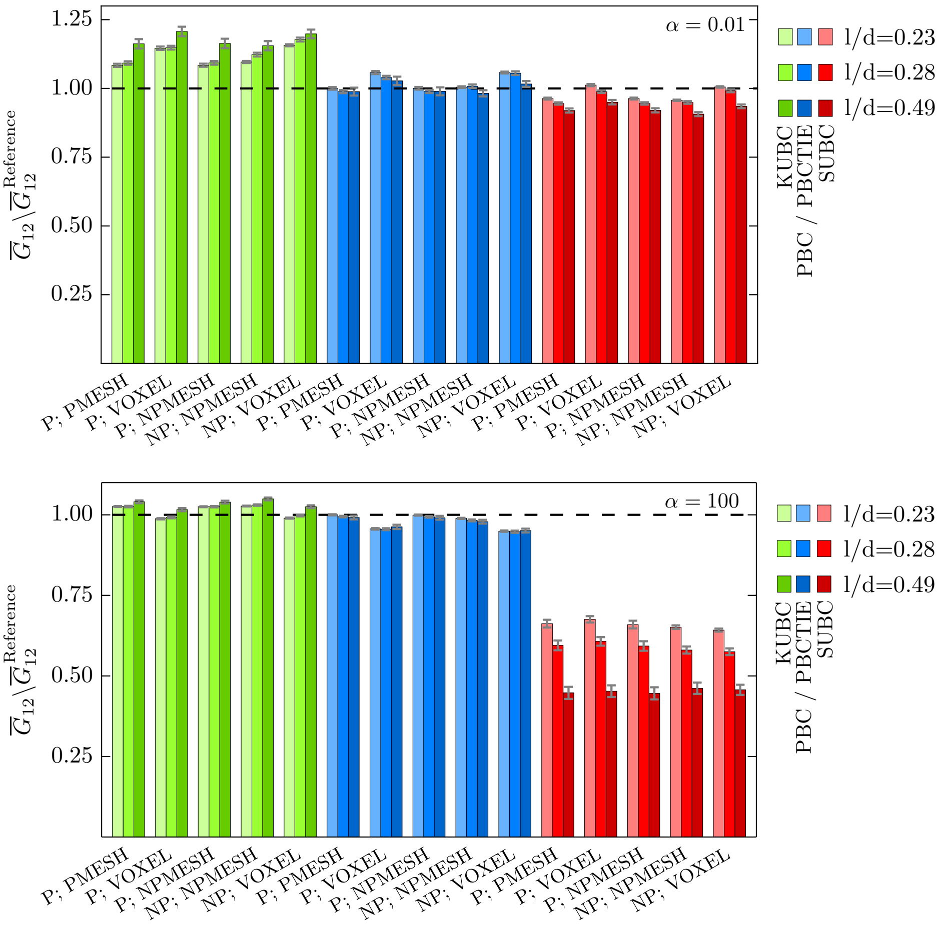

Figure 2: Normalized macroscopic shear modulus for all realizations for different phase contrasts α.

100 inclusions.

Amazingly the macroscopic responses are seemingly independent of the chosen combi-

[1]In the used software ABAQUS the TIE-constraint formulation is applied.

nations of periodic and non-periodic topologies or meshes. Very similar material behavior is predicted in each case with variations of only a few percent independent of the phase contrast.

With regard to the boundary conditions the phase contrast plays an important role. For a small phase contrast α static uniform boundary conditions perform better than kinematic uniform boundary conditions and vice versa. However, the approximate periodic boundary conditions are a good choice in either case.

In summary, good alternatives exist to circumvent the cumbersome task of setting up a fully periodic RVE, questioning the indispensable necessity of fully periodic RVEs.

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