Periodic unit cell-based simulation of materials with random microstructure

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Abstract

In this paper a procedure is introduced for the generation of idealized periodic unit cells approximating real complex microstructures. In particular, geometry of such a unit cell is derived from an optimization procedure formulated in terms of statistical descriptors characterizing a microstructure of random multiphase media. Applications to fiber-reinforced composites, woven composites and masonry structures are examined to illustrate the applicability of the presented methodology.

Keywords: Periodic unit cell; Random microstructure; Global stochastic optimization; Fiber-reinforced composites; Woven composites; Masonry structures

1. Introduction

A representative volume element of heterogeneous materials is an important input for qualitative and quantitative multiscale simulation of heterogeneous materials; see, e.g., [7] for a recent overview. Loosely speaking, by a *representative volume* we mean a sample of a microstructure large enough to suitably reflect the stochastic fluctuations of material properties on the scale of observation. The requirement of computational feasibility, on the other hand, calls for as small sizes of the representative volume element (RVE) as possible.

In this paper, an alternative approach to the RVE definition, originated in works of Povirk [1] and Zeman and Šejnoha [2], which essentially relies on microstructural statistics, is introduced. In particular, the original microstructural configuration is first characterized by suitable *geometry-based* statistical descriptors and then a simplified *periodic unit cell* (PUC) is found such that it approximates the target microstructure as close as possible in terms of selected statistical descriptors. Note that the subject of the present work is also closely related to reconstruction of random media with the specified microstructural function(s) (see [3, Chapter 12] for summary and further references).

In general, the proposed procedure consists of following four steps: (i) quantification of microstructure morphology of the original microstructure, (ii) choice of an appropriate idealized microstructure, (iii) determination of parameters of idealized periodic unit cell on the basis of minimization of difference in statistical descriptors related to the original microstructure and the idealized unit cell, (iv) simulation based on geometry of the statistically (sub-)optimal simplified unit cell.[1] Each of these steps will be scrutinized in the following sections.

2. Microstructural descriptors

A variety of statistical descriptors can be introduced to describe the morphology of multi-phase random composites; see, e.g., [3, Part I]. In the present work, the *two-point probability function* S_{rs} and the *lineal path function* L_r are used to characterize geometry of the material as they are reasonably simple to implement and yet capture both short-and long-range order information about microstructure morphology.

To provide general description of geometry of a binary microstructure, we start from the *characteristic function* $\chi_r(\mathbf{x})$, which equals to one when the point $\mathbf{x}$ is contained in the domain occupied by the r-the phase V_r

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and to zero otherwise. Then, the two-point probability function S_{rs} can be defined as:

$$S_{rs}(\mathbf{x},\mathbf{y}) = P(\chi_r(\mathbf{x})\chi_s(\mathbf{y}) = 1) \tag{1}$$

i.e. as the probability that two points **x** and **y**, randomly thrown into a medium, will be found in phases r and s. Similarly, a value of the lineal path function L_r gives the probability that a given segment **xy**, randomly thrown in a medium, is fully contained in the r-th phase,

$$L_r(\mathbf{x},\mathbf{y}) = P(\mathbf{xy} \subset V_r) \tag{2}$$

Under assumption of *ergodicity* and *statistical homogeneity* of the studied material, the statistical descriptors can be efficiently evaluated on the basis of digitized images. In particular, the two-point probability function can be rapidly computed using the fast Fourier transform while the sampling template approach can be used to evaluate the lineal path function; see [3,4] for more details.

3. Optimization problem

Let us assume, for a moment, that an appropriate idealized geometrical model of a periodic unit cell is given; see Section 4 for concrete examples. In the sequel we further assume that a geometrical model is fully characterized by the N-dimensional vector of parameters **x**. Once the geometry of the unit cell is specified, a digital image of the corresponding material can be generated and used to determine the statistical descriptors S_{rs} and L_r. Then, the following measures of similarity between the original microstructure and a periodic unit cell can be introduced:

$$F_s(\mathbf{x}) = \sum_i \sum_j (\bar{S}_{rs}(i,j) - S_{rs}(i,j))^2 \tag{3}$$

$$F_L(\mathbf{x}) = \sum_i \sum_j (\bar{L}_r(i,j) - L_r(i,j))^2 \tag{4}$$

$$F_{s+L}(\mathbf{x}) = F_S(\mathrm{x}) + wF_L(\mathbf{x}) \tag{5}$$

where w is a weighting factor to compensate for the different influence of functions S_{rs} and L_r; $\bar{S}_{rs}$ and $\bar{L}_r$ are functions corresponding to the target medium. The actual parameters **x** are then found by minimizing one of the objective functions, Eqs. (3)–(5).

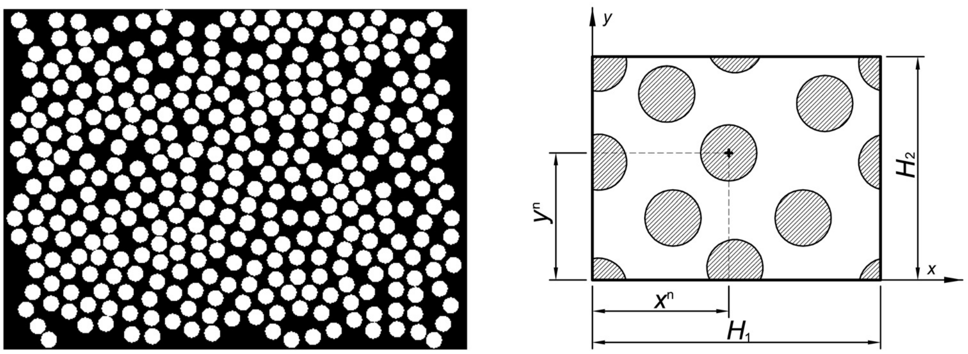
Note that the solution of the introduced optimization problem requires minimization of multi-dimensional and multi-modal objective functions. Therefore, global stochastic optimization methods, such as the RASA algorithm [5], based on a combination of real-coded genetic algorithms and the simulated annealing method, appear to be necessary to solve this problem efficiently.

4. Applications

This section presents particular applications of the previously introduced procedure to distinct material systems. In particular, unidirectional fibrous composites (Section 4.1), woven composites (Section 4.2) and masonry structures (Section 4.3) are discussed in more detail. Finally, the quality of the resulting unit cells is compared from the point of view of effective elastic properties in Section 4.4.

4.1. Unidirectional fiber composites

As in the first example, consider a microstructure characterized by the micrograph taken from the bundle of graphite fibers bonded to the polymer matrix. For numerical analysis the real microstructure is replaced by its idealized binary image, Fig. 1a. Evidently, the microstructure of the material is rather disordered,



(a) (b)

Fig. 1. Fibre-reinforced composite. (a) Target microstructure. (b) Idealized unit cell.

which makes the direct definition of the PUC rather problematic.

As an idealized unit cell, a rectangular region with n particles having identical diameter, see Fig. 1b, is introduced. The geometry of such a unit cell is determined by dimensions H_1 and H_2 and the x and y coordinates of all particle centers. This allows us to determine periodic unit cells with increasing complexity, which in limit correspond to the original medium. See also [2] for further reference. Note that, in the following, the reported results correspond to the five-particle unit cell.

4.2. Plain weave composite

It is a widely accepted fact that the waviness and misalignment of the cross-section of reinforcements play an important role in the overall behavior of textile-reinforced composite materials. Here our attention is limited to a very specific type of imperfections attributed to different heights of individual layers, see Fig. 2a; an interested reader is referred to [4] for more general considerations.

In this case the idealized geometrical model is fully determined by four parameters: a, b, g and h; see Fig. 2b. Note that the model is actually three-dimensional. The scheme in Fig. 2b shows only a two-dimensional section.

4.3. Masonry structures

The last example comes from the field of analysis of historical masonry structures. In particular, the proposed method was used to analyze the sandstone masonry wall of the Charles Bridge in Prague, see Fig. 3a, where a binary image of representative part of the structure is shown.

An idealized unit cell is fully defined once the width of the unit cell, heights of each layer of bricks and thicknesses of individual joints are specified, see Fig. 3b. In summary, the geometry of the chosen unit cell is determined by 12 parameters; see [6] for more detailed discussion.

4.4. Overall behavior

Finally, we present the comparison of effective elastic properties for the target microstructures and corresponding statistically optimized unit cells obtained for various material systems under assumption of linearly elastic behavior of individual phases. For all materials, the results have been obtained by the first-order numerical homogenization procedures (see, e.g. [2,7 and references therein]), which result in a 'homogenized' material stiffness tensor L^{hom}_{ijkl} representing the average response of a heterogenous material. The results are

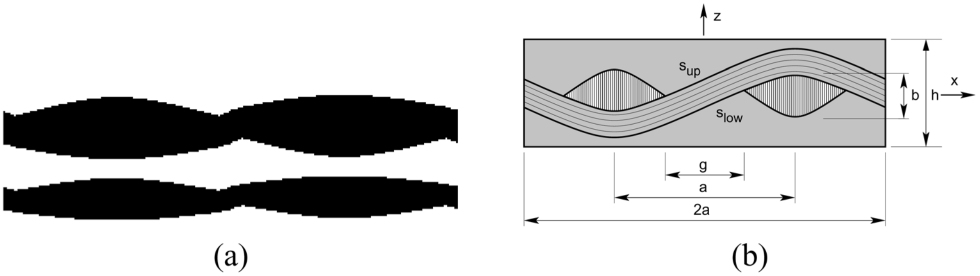


Fig. 2. Plain weave composite. (a) Target microstructure. (b) Idealized unit cell.

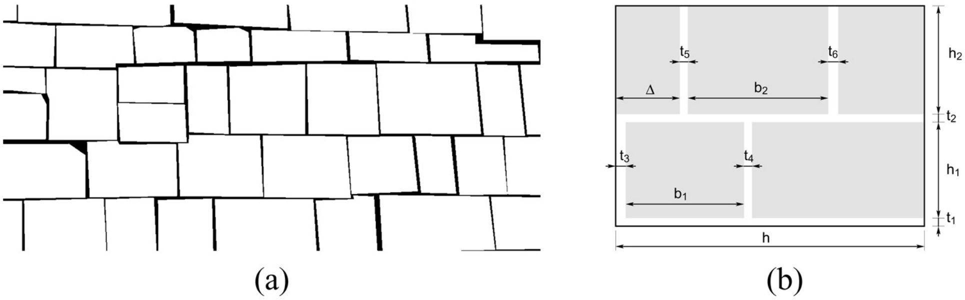


Fig. 3. Masonry wall. (a) Target microstructure. (b) Idealized unit cell.

Table 1
Comparison of homogenized properties

	Woven composite			Fibrous	Masonry
	S_{rs}	L_r	$L_r + S_{rs}$		
N	4	4	4	10	12
L^{hom}_{1111} [GPa]	21.10	22.67	23.33	10.74	9.61
Target	23.32	23.32	23.32	10.74	9.58
L^{hom}_{1212} [GPa]	2.87	2.84	2.93	2.22	3.17
Target	2.96	2.96	2.96	2.22	3.10
Volume fraction	33.86	33.12	35.67	43.57	7.47
Target [%]	36.78	36.78	36.78	43.57	7.43

summarized in Table 1, which stores the selected, most sensitive, components of homogenized stiffness tensors together with comparison of volume fractions and dimensions of vectors of unit cell parameters.

As demonstrated for the case of woven composite analysis, the best results can be expected when a procedure based on a combination of both microstructural descriptors is used. This conclusion also holds for the remaining material systems. As evident, the obtained match between target and optimized values is rather satisfactory and justifies the introduced procedure.

5. Conclusions

In this paper, a conceptually simple and well-defined procedure for the approximation of real-world disordered materials by periodic unit cells was introduced. The applicability of this methodology was demonstrated for a variety of material systems and lengthscales spanning the range of micrometers (fibrous composites), millimeters (woven composites) and meters (masonry structures). The numerical results suggest that the procedure works rather well, at least in the case of linearly elastic materials. Its extension to more complex inelastic materials, however, deserves a detailed numerical investigation. This will be the subject of future work.

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Notes

[1] In other words, we claim that if two microstructures are similar in the sense of statistical descriptors their overall response will be similar as well. This hypothesis can be supported by a large body of literature relating microstructure and collective properties of heterogeneous materials, where these descriptors play a central role; see, e.g., [3, Part II] for an exhaustive overview.

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