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Computation of effective electrical conductivity of composite materials: A novel approach based on analysis of graphs

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ABSTRACT

In this work we continue the investigation of different approaches to conception and modelling of composite materials. The global method we focus on, is called ‘stochastic homogenization’. In this approach, the classical deterministic *homogenization* techniques and procedures are used to compute the macroscopic parameters of a composite starting from its microscopic properties. The *stochastic* part is due to averaging over some series of samples, and the fact that these samples fit into the concept of RVE (Representative Volume Element) in order to reduce the variance effect.

In this article, we present a novel method for computation of effective electric properties of composites – it is based on the analysis of the connectivity graph (and the respective adjacency matrix) for each sample of a composite material. We describe how this matrix is constructed in order to take into account complex microscopic geometry. We also explain what we mean by homogenization procedure for electrical conductivity, and how the constructed matrix is related to the problem. The developed method is applied to a test study of the influence of micromorphology of composites materials on their conductivity.

1. Introduction/ motivation

Composite materials and more generally heterogeneous media appear in various real-life situations. The latter represent the matter from microscopic scale to perfectly observable macro objects, while the former play an important industrial role in the last decades. The incredibly fast development of composite materials in most of the branches of modern technology is due to their exceptional properties in comparison with pure materials. The process of conception and production of composites is however far from being simple: while a lot of tests are needed to be able to validate the technology before going to industrial applications, the experimental work is still expensive and not easy to carry out. All this results in a strong demand for efficient mathematical modelling techniques that can be applied to predict and optimize effective properties of composite materials. Moreover in the recent years computational facilities have become much more accessible, that resulted in a great number of works dealing with development of methods and implementation of algorithms for such studies.[1] Out of all possible approaches to the problem we focus on the method which is usually called *stochastic homogenization*.

The key idea of *homogenization* as a modelling technique[2] is to be able to estimate measurable macroscopic parameters of a composite material (or heterogeneous medium) starting from its microscopic geometry. In a sense, one computes the parameters of an equivalent homogeneous material that can “replace” the studied heterogeneous medium in the experiment. Various techniques based on different mathematical and algorithmic approaches have been proposed. In what follows, we will see that it is very important to carefully choose suitable methods, and this choice is greatly influenced by the problem one is solving or by a property one is studying, and also by availability and type of the input data. In our previous papers we have observed for example, that the methods based on Fast Fourier Transform proposed initially in [1,2] for 2D problems, are perfectly suitable for studying elastic properties in 3D ([3]), but they have to be modified to be applied to thermal phenomena ([4,5]). It became clear from the previous studies ([6]) that they are practically not efficient to estimate electrical conductivity, which is the main motivation for the method we describe in this paper.

We would like to dedicate this article to Vojislav Golo…

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[1] Similar logic goes far beyond the subject of composite materials: one can for example recall the Nobel Prize 2013 in chemistry, that was given more or less for advances in computer simulations.

[2] Not to be confused with an industrial process.

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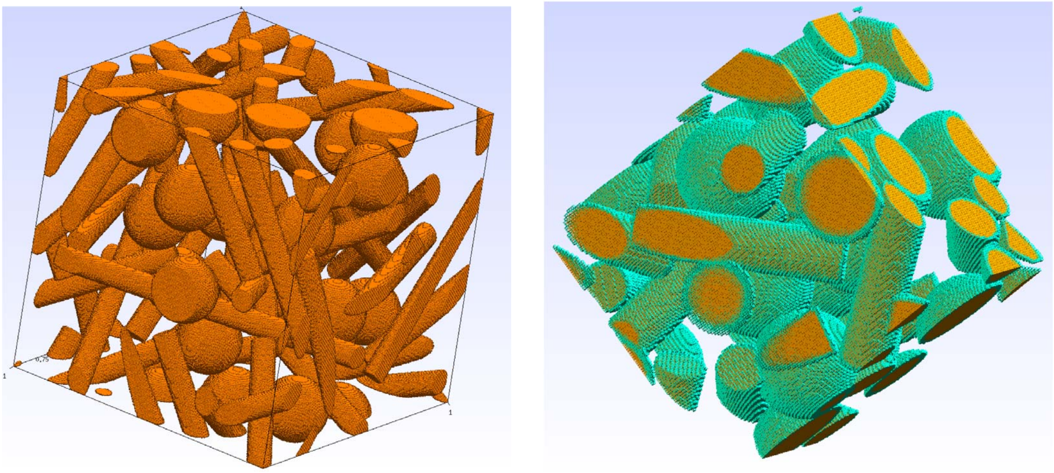

(a) Non-overlapping inclusions (b) Highlighted zone corresponds to overlaps

Fig. 1. 3D view of an RVE: spherical and cylindrical inclusions, periodic boundary conditions.

The *stochastic* part in the name of the method is due to the fact that each given sample of a medium does not capture exactly the behavior of the composite material. One is thus forced to average the results on a reasonable sampling with some common properties. The idea is coming from a very classical approach of Monte Carlo simulations. For our purposes, it means that an efficient algorithm of generation of such samples should be implemented. We profit from the flexibility of the methods we have developped in [7,8] to use them in the analysis of electrical conductivity.

Our interest in the subject is also motivated by some very concrete applications related to aeronautic equipment, a project carried out in close collaboration with industrial partners. Some part of this contribution will thus be devoted to explaining in what way the techniques can indeed be applied and to potential difficulties that arise in "true-to-life" situations, and to possible ways out.

The main goal of this paper is to provide a tool that can be applied "out of the box" in order to study effective properties of heterogeneous media or composite materials. Therefore we present the "building blocks" for such a tool, that are sufficiently flexible and can be then "assembled" depending on the available input data and the problem under consideration. For each method that is discussed here, we give ideas of some mathematical background, that is necessary for understanding and application, we do not however go into much details not to overload the presentation.

To sum it up, the text is organized as follows: In the next Section (2) we briefly recall the tools we have developped for generating samples of composite materials/heterogeneous media with rather complex microscopic geometry; we explain how they can be easily adapted to cover the situations arising typically in the studies of electrical conductivity. In the Section 3 the novel (deterministic) homogenization procedure is presented – it is based on the analysis of the connectivity graph of a material and is perfectly suitable for the type of samples we produce. The last Section (4) is devoted to application of the developped method to some test examples, it also contains some discussion about its adaptation to industrial problems.

2. Stochastic part – sample generation

A composite material, or what is the same in our analysis, a heterogeneous medium, is a material composed of several constituents often called phases. Typically one thinks about some "matrix", say made of a polymer, into which inclusions of a different nature are inserted. For electrical conductivity the matrix would be made of an insulator (or a material with rather low conductivity) and inclusions would be microparticles chosen to conduct electricity (typically containing a metal/alloy or some other material with high conductivity). It is intuitively clear (and also confirmed by a lot of studies) that effective properties of composite materials strongly depend on the volume fraction of inclusions, but sometimes even in a more pronounced way on the *morphology* of the material, i.e. microgeometry and repartition of inclusions. For modelling, it is thus important to be able to generate samples that are close enough to the actual microstructure of the material. But since we talk about stochastic homogenization, i.e. averaging the results over a big series of tests, this process should not take too much time. Not going much into details, let us just say that the usual way out is to replace the inclusions by simple geometric objects and handle their repartition inside the sample. And certainly a lot of work has been done in this direction (see [7,8] and references therein).

The concrete tool we have at hand permits to place spherical and cylindrical inclusions into the matrix, that already gives a very rich "true-to-life" microscopic geometry. The key feature that we need throughout all the studies is the ability to control contacts and overlaps of inclusions. In the previous studies (elastic and thermal) we were rather focusing on non-overlapping or slightly overlapping inclusions – the machinery had been developped mostly for that. Let us be slightly more specific about the algorithm. There are essentially two methods how to generate samples with non-intersecting inclusions: RSA- and MD-based ones. RSA ([9]) stands for "random sequential addition" – the inclusions are generated one after another, and only those that do not intersect with previously generated ones are kept. MD ([10]) stands for "molecular dynamics" – all the inclusions are generated simultaneously, and then repulsive forces are introduced to position them correctly. Both algorithms have been adapted to the case of spherical and cylindrical inclusions and implemented in [7]. The input of the algorithms consists of the desired volume fraction, the respective number of spheres and cylinders and their geometric parameters. The output is a list of non-intersecting inclusions with coordinates of their centers and angles responsible for orientation, this can be used directly in computations or converted to a 3D image like Fig. 1. (a).

Let us note that the numbers should be chosen in order to fit the concept of a Representative Volume Element (RVE, [11]): the sample should be large enough to effectively capture the properties of the material, like isotropy for example, but sufficiently small to make the computation doable. We have performed a detailed study of the effective elastic properties of composite materials in [3] and it included also some tests to choose the size of the RVE. Let us just mention here that if