Generating of Random Structures for Mathematical Modelling of Composite Materials

Tomáš Pospíšil
Brno University of Technology, Faculty of Mechanical Engineering, Department of Mathematics, Technická 2, 616 69 Brno, Czech Republic.
e-mail: tomposp@seznam.cz

Abstract

Real fibre composite materials often used in technology do not have periodic structure as is supposed in many mathematical methods. The contribution deals with generating random structures similar to real ones, four new algorithms are introduced.

1 Introduction

Composite materials are formed by at least two different phases, particularly two-phase fibre composite material consists of the so called stiffening phase in the shape of fibres included into the second one, called matrix. By various distribution of inclusions we can develop materials with special properties and that is the reason, why they are intensively used in engineering. We are interested in prediction damage initiation, propagation of a discontinuity and consequently in final failure of such material. Experimental measurements are very expensive and that is the reason, why it is very useful to compute effective parameters from the knowledge of properties of phases and their distribution.

Solving of boundary-value problems modelling the behavior of composite materials is very demanding since we have to solve PDEs with highly oscillating coefficients. Their numerical computation thus needs very fine triangulation and successively large systems of equations. The reason of this problem is a fine structure of such material. Let us remark that using simple averages of the coefficients leads to incorrect results.

Let us remind a mathematical method called homogenization for solving the problem. Adopting the assumption of periodic structure of the material, this method enables to compute its effective parameters from the knowledge of properties of the phases and their geometric distribution. It means that strongly heterogeneous material is replaced by a fictional homogeneous material “equivalent” in sense of having globally the same properties. From the mathematical point of view the equation with highly oscillating periodic coefficient is replaced by a constant coefficient equation.

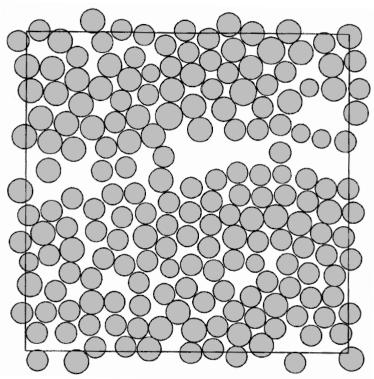

Figure 1: Real sample of a composite material taken from [1].

Real composite materials do not have periodic structure — distribution of the fibres in the matrix is not periodic, see [1]. The paper [5] studies question what error we do (in computations of boundary-value problem), if we replace random structure by an equivalent periodic one.

The base for modelling of non-periodic composite materials is generating of random structures, see the following picture. The aim of this contribution is to present four new algorithms (**AI**)–(**AIV**) for generating of random structure with the same volume fraction.

2 Simulation of Random Structure

We shall deal with random structure of two phase fibre composite materials. Most of present papers dealing with generating these structures assume that the fibres has the constant diameter. Algorithms generating such samples are based on the so called spatial point processes, see [2], [6]. These algorithms do not allow to deal with non-constant diameter of the fibres. For modelling samples with non-constant fibres new algorithms were developed. Of course, in all samples the volume fraction is conserved.

An input argument for generating samples was the side of the square domain in μm, volume fraction and probability distribution of diameters of the fibres. According to [1], the following parameters were chosen: normal distribution N$(6,78\mu\text{m};0,38\mu\text{m}^2)$, length of the sample's side 100μm and the volume fraction 0,55.

3 Description of Algorithms

- Algorithm (**AI**) – the algorithm uses the so called Karhunen-Loève expansion, see [3], of the stochastic process having a character of a white noise process. A detailed procedure can be described in several steps: First of all, "curved lines" using a special stochastic process are generated. These lines are fictional positions of the fibre's centers. In the case of overlying, new position is generated by shifting the fibre(these fibres are marked by arrows in the next figure). The number of generated lines depends on the requested volume fraction.

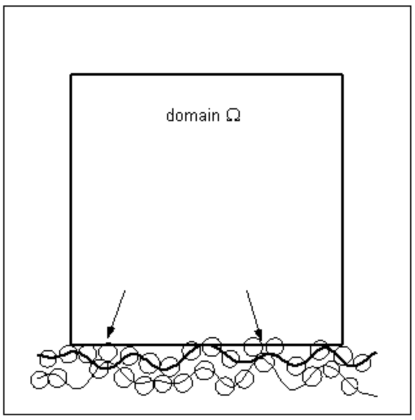

Figure 2: To the description of the Algorithm (**AI**).

- Algorithm (**AII**) – the algorithm consists of several steps. We start with placing of one fibre (with random diameter) into the interior of the sample domain. Then random direction and distance of new fibre is generated. In case of overlaying of fibres, new position is generated. These steps are repeated until the resulting volume fraction is not reached.

- Algorithm (**AIII**) – the algorithm is quite different from the previous ones. It is based on the Brownian motion of the suspended particles. We start with periodic structure with constant diameters of fibers. Then we change the diameters to be random with normal distribution. Then each fiber is shifted by the Brownian motion and simultaneously excluded their overlaying. The fibers are randomly deflected only in tenths of fiber's diameter. In contrast to the real Brownian motion we do not consider collisions of fibers.

- Algorithm (**AIV**) – the algorithm is similar to the algorithm (**AIII**). The difference is in processing overlaying of fibers: if the shift will cause overlaying with neighboring fiber, the shift is canceled – the fiber stays in its old position. It causes, that the final structure is not so random as in the case of algorithm (**AIII**), but computing time is several times shorter.

We have to note that in each of the previous algorithms the diameters of the fibres are driven by a known probability distribution. In our cases it was normal distribution described above. In the following pictures we can see the results of the introduced algorithms (**AI**)–(**AIV**):

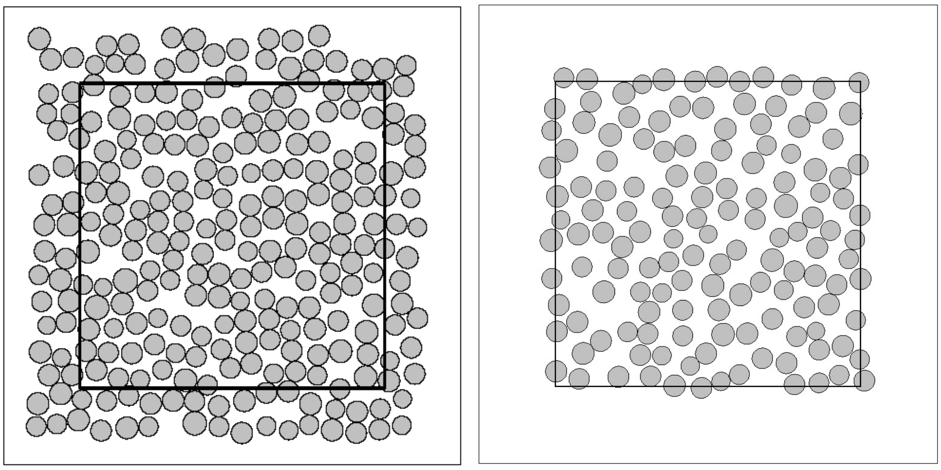

Figure 3: A STRUCTURE GENERATED BY ALGORITHM (**AI**) AND (**AII**).

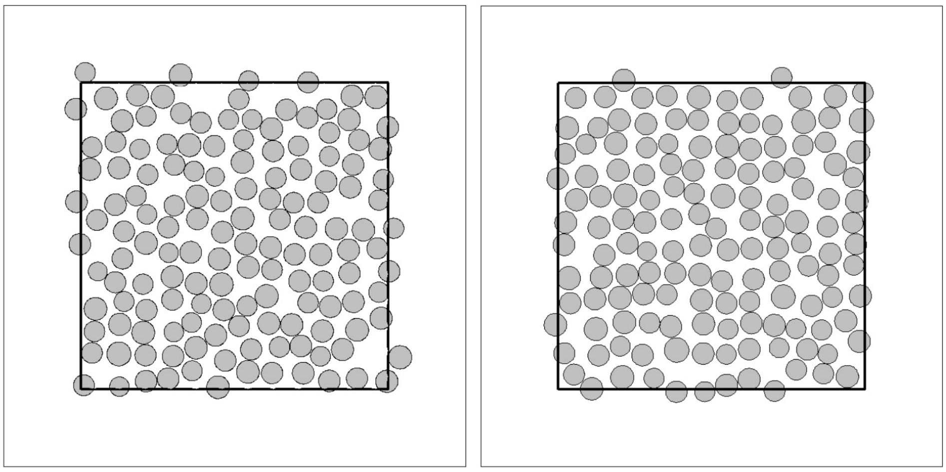

Figure 4: A STRUCTURE GENERATED BY ALGORITHM (**AIII**) AND (**AIV**).

4 Analysis of algorithms

The random structures generated by the introduced algorithms can be compared by different methods, see [4]. Let us introduce one of them. As we said above, the requested volume fraction was 0.55. After simulating 1500 different samples by the algorithm (**AI**), we obtained average volume fraction 0.5514. Then the detailed analysis was proceeded. On the left figure there is one generated sample with a grid.

In each element of this grid it was computed so called local volume fraction. On the right figure there is contour plot of computed local volume fraction from the left figure.

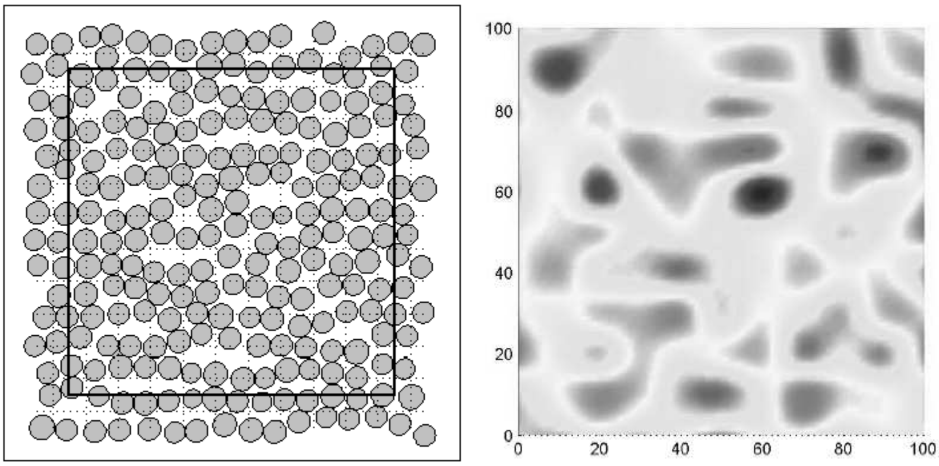

Figure 5: The structure generated by Algorithm (**AI**)and its shadow contour lines.

5 Conclusion

Mathematical modelling of materials with periodic structure brings important savings by creating new composite materials: although the experiments cannot be excluded, their number can be substantially diminished. It enables optimize their properties and experimentally verify the final optimal variants. Nevertheless, modelling of real composite materials brings several problems.

To generate a random structure of a fibre-composite material similar to the real one is quite difficult, because we have to know the real structure from many viewpoints, e.g. volume fraction of each phases or stickiness parameter, see [7]. It means that an accurate analysis of a real material must be proceeded before simulations, see [1]. Although the volume fraction is constant for statistically homogeneous media, on a spatially level it fluctuates.

The aim of this contribution was to show several algorithms for generating random structure of two-phased fiber composite material. Comparing these four algorithms, one can say, that the (**AIV**) is fastest, but the structure is not "so random". The following open problems are more sensitive comparison these algorithms based on statistical means, their likelihood to the real samples and efficiency of the simulation. These problems will be the subject of next paper.

References

[1] Babuška, I., Andersson, B., Smith, P.J.: *Damage Analysis of Fiber Composites, Part I: Statistical Analysis on Fiber Scale*, Comput. Methods Appl. Mech. Engrg. 172 (1999) 27-77.

[2] Diggle, P. J.: *Statistical Analysis of Spatial Point Patterns*, Oxford University Press Inc., 2003.

[3] Kloeden P. E., Platen E., Schurz H.: *Numerical Solution of SDE Through Computer Experiments*, Springer-Verlag Berlin Heidelberg 1997.

[4] Sofia Mucharreira de Azeredo Lopes: *Statistical Analysis of Particle distributions in Composite Materials*, PhD thesis, Dept. of Probability and Ststistics, University of Sheffield, 2000

[5] Pospíšil, T.: *On Mathematical modelling of Composite Material with Random Structure*, submited to Mathematics and Computers in Simulation.

[6] Ripley, B. D.: *Spatial Statistics*, John Wiley & Sons, Inc., 2004.

[7] Torquato S.: *Random Heterogeneous Materials, Microstructure and Microscopic Properties*, Springer-Verlag, 2002.