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Computational Mechanics of Composite Materials

Sensitivity, Randomness and Multiscale Behaviour

Springer

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Preface

Composite materials accompanied the human activity from the beginning of the civilisation. Apart from natural composites, like the wood, applied in various structures people invented many multi−component materials even in ancient times. One of the most famous applications of the old−time composites is the Chinese Wall, whose durability and stability was ensured by contrastively different materials incorporated into a single structure. Next applications worked out and popularised in Central Europe in the Middle Ages was known as the Prussian wall combining the wooden skeleton filled with the bricks. One of the most significant milestones in the history of modern composites was the application of the concrete reinforced with the steel bars in France at the end of the nineteenth century.

Nowadays composites play a very important role in engineering from aerospace technology and nuclear devices to microelectronics or structural engineering applications [37,128,203,286,298,351,367,389]. Considering this fact and the growing role of numerical experiments in the designing of structures and industrial processes, one of the most important purposes of computational mechanics research and direction of progress appeared to be precise numerical modelling of these materials. On the other hand, experimental sciences prove that every structural parameter has a random, in fact stochastic, character. Thus, many probabilistic approaches and methodologies have emerged recently to simulate more accurately the real behaviour of mechanical systems and processes. These methods show that the random character of parameters discussed is very important for the systems simulated [14,121,357]. This conclusion may lead us to the hypothesis, that the random character of the material and physical parameters should play an essential role in multi−component structures [32,34,151,154,275].

Modern computational mechanics of composite materials follows many various ways through different science domains from experimental materials science to advanced computational techniques and applied mathematics. They engage more and more complicated and precise testing methods and devices, stochastic and sensitivity analysis algorithms and multiscale domain theoretical solutions for partial and ordinary differential equations reflecting some practical engineering and physical problems. Commercial computer programs based on the Finite Element Method enable now visualisation of the multifield, multiphase and non-stationary physical and mechanical problems and even introducing uncertainty into computer simulation using random variables (ANSYS, for instance). The growth of computer power obtained from technological progress and advances in parallel numerical techniques practically eliminated the parameter of the cost of computational time in modelling, which resulted in the efficient implementation and use of Monte Carlo simulation.

The basic idea behind this book was to collect relatively up−to−date approaches to the composite materials lying somewhere in between experimental measurements and their opportunities, theoretical advances in applied mathematics and mechanics, numerical algorithms and computers as well as the practical needs of the engineers. The methods are well–documented in the context of computer batch files, scripts and computer programs. It will enable the readers to start from this point and to continue and/or replace the ideas with newer, more accurate and efficient ones. The author believes that this book will appear to be useful for applied mathematicians, specialists in numerical methods and for engineers: civil, mechanical, aerospace and from related branches of industry. Some elements of probabilistic calculus and computation as well as general ideas can also be applied by students, who can incorporate these concepts into new research or into the existing well–documented knowledge dealing with composite materials.

A primary version of the book was completed in Texas, during the author's postdoctoral research at Rice University in Houston in the academic year 1999/2000 under auspices of Prof. P.D. Spanos. The author would like to appreciate the help of many people, whose valuable comments and the time spent enabled finishing of the book. Special thanks are directed to Prof. Michał Kleiber from the Institute of Fundamental Technological Research, Polish Academy of Science in Warsaw, who expressed many precious ideas during a common research in random composites and who promoted this research. Prof. Tran Duong Hien from Technical University of Szczecin influenced the work in the area of stochastic finite elements. The cooperation with Prof. B.A. Schrefler from the University of Padua in Italy concerning numerical analysis of superconducting composites remarkably enhanced the relevant computational illustration included in the book. The help of Mr. Łukasz Figiel, M.Sc. and Mr. Marcin Pawlik, Dr. Eng., two of my younger colleagues, was decisive for finishing of some computations devoted to heat transfer and fracture analysis. The author would like to express his respect to all the colleagues from Chair of Mechanics of Materials at the Technical University of Łódź for their advising voices, too. Last but not least, the role of the unknown reviewers, the editors and the people who commented and criticised this work is also appreciated.

Layout of the Book

Mathematical preliminaries open the book considerations and consist of basic definitions of random events, variables and probabilistic moments as well as description of the Monte Carlo simulation technique with the relevant statistical estimation theory elements. The stochastic perturbation approach (second order second central moment generalised to the *nth* order and higher moments technique) is explained using two examples: a transient heat transfer equation and the solution of the linear elastodynamic problem. The solution to these problems in terms of expected values and standard deviations as well as spatial and temporal cross-covariances is demonstrated and it illustrates the applicability of the method. An important part of this opening chapter is a probabilistic algebraic description of some transforms of random variables, which is necessary for further formulation and development of the stochastic interface defects model. Some of them are valid for the Gaussian variates only, which essentially bounds the application. However, it leads to the specific formulae implemented further in the computer software attached. An important issue raised in this chapter is to show a difference between Gaussian and quasi−Gaussian random variables defined on some unempty and bounded real subsets.

Elastic problems related to deterministic and probabilistic systems are collected in Chapter 2. They are divided into two essentially different parts – the first shows the linear elastic behaviour of some composite materials and structures in boundary value problems connected with their real microstructure. The other part contains description of the homogenisation technique together with the relevant numerical tests documenting the computational determination of so-called homogenisation functions, *a posteriori* error analysis related to homogenisation problems, probabilistic moments of effective material tensors and their variability with respect to some input parameters.

The first part of this chapter starts from the mathematical model of composite, whose material characteristics are given arbitrarily as constant deterministic values or by using the first two probabilistic moments constant through the given component material region (or volume). Further, the stochastic interface defects concept is presented, which originated from some computational contact mechanics models. The interface defects are introduced as semicircles lying on the interface into a weaker material. The radii and total number of these defects are input cut-off Gaussian random variables defined using their expected values and the variances (or standard deviations) with elastic properties equal to 0. The modeling is performed through the following steps: (i) determination of the interphase – a thin film containing all the defects with thickness determined from defect probabilistic parameters, (ii) probabilistic spatial averaging of the defects over the interphase area, (iii) computational analysis of a new composite with the new extra component. Obviously, it is not possible to approximate the real composite with stochastic interface microdefects very accurately. However it can be and it is done intermediately – by comparison with the composites with the weakened interphase or interface, for instance. Computational experiments validating the model are performed using the system ABAQUS [1] (in the deterministic approach) and the specially adapted academic package POLSAP (for the Stochastic Finite Element Method – SFEM needs) [183]. All the results obtained for various composites and various combinations of interface defect parameters demonstrate a high level of structural uncertainty in the case of their presence as well as a significant increase of the structural state functions stresses and displacements around the interface region. The second part of the chapter concerns the homogenisation method both in deterministic and probabilistic context. Computational experiments dealing with a numerical solution of the homogenisation problem are done thanks to the FEM commercial system ANSYS [2], where most of the databases for these experiments are available from the author to be used in further extensions of mathematical and mechanical homogenisation model.

Interface defects model and probabilistic homogenisation using both Monte Carlo simulation techniques are analysed using the authors FEM implementation called MCCEFF. The results of simulation are compared in terms of expected values and variances with analogous results obtained through the stochastic second order perturbation methodology. The appendix to this chapter consists of necessary fundamental mathematical theorems and definitions for the asymptotic homogenisation theorem.

Elastoplasticity of composites discussed in the next chapter is focused on the alternative homogenisation technique, where instead of periodicity conditions imposed on the external boundaries of the RVE, some combination of the symmetry conditions and strain fields are applied to this element. The application of this method to the homogenisation of a periodic superconducting coil cable is also shown – an effective elastoplastic constitutive law is determined numerically and shown as a function of the homogenising uniform strain applied at the RVE boundary. Analogously to the methods typical for elastostatic problems, the closed-form equations for effective yield stresses are formulated in various ways, which can next be extended on probabilistic analysis. This chapter is completed with the transformation matrices algebraic definition, which is the essence of the computational implementation of the method. Probabilistic moments of the effective elastoplastic constitutive law can be obtained as a conjunction of this method with the Monte Carlo simulation technique discussed in the previous chapter. The fundamental issue is however experimental determination of higher order probabilistic moments for the superconductor material characteristics; otherwise the analysis is useful in the context of the sensitivity of the homogenised characteristics with respect to the adopted level of input randomness only.

Sensitivity analysis presented in Chapter 4 is entirely devoted to a relatively new research area – determination of the sensitivity gradients for homogenised material characteristics. For this purpose two essentially different homogenisation methods are used – algebraic approximation and asymptotic methodology. Starting from a traditional description of the effective parameters in both methods, the sensitivity gradients are determined by the symbolic calculus approach and, on the other hand, pure computational strategy based on the Finite Difference Method (FDM). The implementation and results obtained from these two methods demonstrate the basic limitations of the methods, i.e. necessity of closed-form equations for the symbolic approach and numerical instabilities in the FDM simulations. This knowledge is necessary for significant time savings in the extension of this study to the random composite sensitivity analysis where the heterogeneous periodic composites with probabilistically defined material properties are analysed. The probabilistic sensitivity of such structures is defined through the introduction of sensitivity gradients of probabilistic moments of the effective material parameters with respect to the appropriate moments of composite structure parameters – elastic properties of the constituents as well as interface defect data.

Fracture and fatigue – the collection of various fatigue theories with special emphasis placed on the second order perturbation method application are discussed next. The crucial numerical illustration is presented in the case of the Paris Erdogan rule where some of the system input data are treated as random va riables. Therefore, expected values are compared against the deterministic values and standard deviations are added, too. An analogous approach is used to reformulate the well-known fracture criteria applied for composite materials – Tsai−Wu and Tsai−Hill - and to use them in symbolic computations for probabilistic parameters of the composite material fracture parameters. The essential part of this chapter is devoted to the FEM modelling of fracture and fatigue of some composites where analytical solutions are not available. Computational illustrations consist of static fracture of curved composite under shear loading leading to the delamination, fatigue analysis of composite pipe joint as well as thermomechanical fatigue of the curved laminate under thermal and/or static quasistatic load varying in time with constant amplitude. Most of the frequently used theories and equations for fatigue analysis are collected in the appendix to this chapter.

Reliability analysis is included in the Chapter 6 and it consists of a discussion of various order reliability computational approaches together with the Weibull Second Order and Third Moment model (W-SOTM). This methodology is used to compute the reliability index for the composite Hertz contact problem, where elastic spherical inclusion of the reinforcement is loaded by the force to remain in contact with the matrix. Further in this chapter a stochastic process description of the degradation phenomena is also given, which appears to be common for the homogeneous and heterogeneous structures and materials. It can find a broad field of applications together with efficient implementations of stochastic processes (with both spatial and temporal randomness) in the Finite Element Method (or BEM, FDM, meshless as well as hybrid method based) programs.

An application of the wavelet-based multiresolutional approach to composite materials in terms of homogenisation of multiscale media is the extension of previous considerations and concludes the book. The traditional composite materials model consisting of two or three geometrical scales is now rewritten in view of practically infinite number of separate scales (resolutions) that can be linked using interscale wavelet projection (some mathematical transformation). The basic tool necessary for such an analysis development is the basic wavelet basis (a mathematical function varying rapidly in a given geometrical scale), which can be used now to transform between neighboring scales. The homogenised characteristics for the composite can be determined usually in the closed−form equation if and only if the limit of an infinite series of wavelet projections between all geometrical scales exists and is unique. As is illustrated by some wavelet function samples, such an analysis type can be some alternative for the random analysis, because the wavelet functions used in various scale makes, in the coarsest scale, the impression that the relevant material property demonstrates the great level of some kind of uncertainty. It is not underlined clearly that the main limitation of this methodology is that the wavelet projection between the neighbouring scales can be continued through the range of validity of the same physical laws. It is not possible to carry out the passage from the atomistic to the global scale of the composite using the same wavelet projection and, most probably, this is the way that this research area should be extended. The multiresolutional homogenisation is demonstrated for a very general case – a linear ordinary differential equation, which can reflect the linear elastic behaviour of a unidirectional multiscale composite in compression/tension or in bending. On the other hand, this technique can be applied with only small modifications to the unidirectional field problems for heat conduction, seepage flow, electrostatic problems, etc. Further, as is documented by the mathematical derivations, the MRA approach formula reduces to the results obtained in the asymptotic homogenisation technique for the two-scale medium. Since some research is done towards the multiscale analysis and homogenisation for 2D heterogeneous media, the main interest has been directed next to the multiresolutional homogenisation of dynamic and transient problems. Some basic theoretical and computational results are obtained under the assumption that non–stationary and dynamic components of the relevant ODEs can be homogenised independently from the stationary part. In practice it makes possible to calculate effective dynamic structural parameters as the relevant spatial averages for the entire multiscale composite; it is however done for the material properties given *a priori* as some algebraic combination of the elementary wavelets (harmonic, Haar, Gabor, Morlet, Daubechies and Mexican hat functions). Since the homogenisation is the intermediate technique to determine the homogeneous equivalent medium and to replace the real structure with this medium, the results are incorporated next in the classical Finite Element calculus for various boundary value or boundary initial engineering problems. They unambiguously show the limitations of the application of various homogenisation techniques used in engineering computations, i.e. simple spatial averaging, asymptotic approach and multiresolutional method. As can be expected, spatial averaging gives the fastest but least precise approximation for the real structure. The application of the wavelet technique is more recommended to periodic composites having a smaller number of periodicity cells in the Representative Volume Element (RVE), whereas the asymptotic approach gives the best results for increased number of cells in the RVE. Therefore, for most engineering composite structures, where the total number of the periods through their lengths is limited, the proposed multiscale approach seems to be the most efficient. The wavelet functions can be incorporated in the Finite Element Method automatic projection between various scales even for the needs of homogeneous system structural computations – for the fluid flow problems where the profile of the flow is a nonlinear and multiscale complex function (wind pressure profile for high buildings in civil engineering applications). That is why some elementary equations and ideas are collected here and the conjunction of such an analysis with the second order perturbation analysis is presented here to extend the applicability range of traditional wavelet projection on probabilistic analyses, where some input random fields are given using the expected values and the spatial or temporal cross−correlations. The elementary numerical example of cosinusoidal wavelet function implemented in the symbolic package MAPLE demonstrates the computational aspects of this methodology. There is no doubt, however, that the next step will be to make the multiresolutional version of asymptotic homogenisation of the multiscale plane periodic structures where the Daubechies wavelets can find application.

A number of references follow the last chapter. However new valuable conference papers, research and review articles as well as entire books continue to appear on the publishing market. Therefore, it is impossible to appreciate the significant contributions of all the people to this field. The book is completed with the appendix containing the user's manual to the computer code MCCEFF available from the author on the special request. Following the algorithm for data preparation, the reader will be able to solve either deterministic and/or probabilistic homogenisation problems for the fibre–reinforced composite for the rectangular RVE containing a single fibre with the round cross–section. The next part of this appendix is devoted to the batch file for the elastoplastic analysis of the steel–reinforced concrete plate using the commercial FEM system ABAQUS. This file contains the author's comments written in such a manner that the file is ready–to–use by ABAQUS without further processing. Symbolic computation code written in the MAPLE standard concludes the appendix. This script is responsible for a computational mathematic derivation of the homogenised heat conductivity coefficient for the unidirectional multiscale periodic composite structure according to (1) the spatial averaging method, (2) asymptotic homogenisation approach and (3) multiresolutional homogenisation method. It returns for initially specified wavelet functions the values of homogenised parameters, their variability with respect to the contrast parameter and the interface location for two–component RVE. This file can be used without further modifications for sensitivity gradient symbolic computations for the effective parameters returned from these methods with respect to the design parameters mentioned. Probabilistic analysis using Monte Carlo simulation, probabilistic integration technique and perturbation–based analysis is under construction now and will be available also by a special request from the author.

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