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Applied Analysis of Composite Media

Analytical and Computational Results for Materials Scientists and Engineers

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To those who "live not by bread alone"

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Biography

The authors belong to the research scientific group www.materialica.plus

MATERIALICA+
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Piotr Drygaś, is Assistant Professor at the Faculty of Mathematics and Natural Sciences at the University of Rzeszow. He is interested in Boundary Value Problems, describing conductivity of fibrous composites with non ideal contact, and 2D elastic composites of random structure with ideal contact between matrix and inclusions.

Simon Gluzman, PhD, is presently an Independent Researcher (Toronto, Canada) and formerly a Research Associate at PSU, and Researcher at UCLA. He is interested in algebraic renormalization method and theory of random and regular composites. Main achievement is development of novel, analytical Post-Padé techniques for resummation of a divergent series, such as root, factor, additive and corrected Padé approximants. They are proven to achieve high accuracy in calculation of critical properties in a variety of physical and material science problems, see also S. Gluzman, V. Mityushev, W. Nawalaniec, Computational Analysis of Structured Media, Elsevier, 2017.

Vladimir Mityushev is Professor at the Institute of Computer Science of the Pedagogical University of Kraków, Poland. His academic and scientific activity is based on interdisciplinary international research devoted to applied mathematics and computer simulations. His main mathematical result is complete solution to the scalar Riemann–Hilbert problem for an arbitrary multiply connected domain. This result includes, for instance, the Schwarz–Christoffel mapping of multiply connected domains bounded by polygons onto circular domains, Poincaré series for the classical Schottky groups and other objects of the classical complex analysis constructed in other works in particular cases. The main scientific achievements of the group headed by VM concern application of the Riemann–Hilbert problem and of the generalized alternating method of Schwarz to 2D random composites and porous media, analytical formulas for the effective properties of regular and random composites, a constructive theory of RVE, pattern formation, and the collective behavior of bacteria. The developed approach revises the known analytical formulas and precisely answers the question how to determine macroscopic properties of random media.

Wojciech Nawalaniec is Assistant Professor at the Institute of Computer Science of the Pedagogical University of Kraków, Poland. WN is interested in simulation, classification and analysis of random structures. Also interested in application of symbolic-numerical calculations and machine learning to computational materials science. WN also develops algorithms and software modules providing solutions to scientific problems tackled by the Materialica+ Research Group.

Preface

In words of Sergei Prokofiev we define neoclassicism: "I thought that if Haydn were alive today he would compose just as he did before, but at the same time would include something new in his manner of composition. It seemed to me that had Haydn lived to our day he would have retained his own style while accepting something of the new at the same time. That was the kind of symphony I wanted to write, a symphony in classical style."

Classical theory of composites amounts to the celebrated Maxwell formula, also known as Clausius–Mossotti approximation. Actually, all modern self-consistent methods (SCM) perform elaborated variations on the theme, and are justified rigorously only for dilute composites when interactions among inclusions are neglected. In the same time, exact and high-order formulas for special regular composites which go beyond SCM were derived.

Let matrix conductivity be normalized to unity and σ denote the conductivity of inclusions. Introduce the contrast parameter $\varrho = \frac{\sigma-1}{\sigma+1}$. For many years it was thought that Maxwell's and Clausius–Mossotti approximation for the effective conductivity of 2D (3D) composites

$$\sigma_e = \frac{1+\varrho f}{1-\varrho f} + O(f^2) \tag{1}$$

can be systematically and rigorously extended to higher orders in f by taking into account interactions between pairs of spheres, triplets of spheres, and so on. However, it was recently demonstrated (Gluzman et al., 2017, Mityushev et al., 2018b, Mityushev, 2018) that the field around a finite cluster of inclusions can yield a correct formula for the effective conductivity only for non-interacting clusters. Rigorous justification of this fact is given in Appendix A.4 of the present book, based on the paper (Mityushev, 2018). The higher order term(s) can be properly found only after a subtle study of the conditionally convergent series.

The hard experimental evidence accumulated by material scientists and engineers begs for a constructive theory of random composites with explicit account for the geometry. The geometry is, de facto, another important *structural parameter*. As discussed in Nielsen (2005), "In itself the large number of completely different empirical stiffness expressions suggested for porous materials clearly indicates a need for a more rational research on composite properties versus composite geometry. . . Change of geometry will influence any mechanical/physical behavior of composites. Stiffness and viscoelasticity (creep and relaxation) will change. Shrinkage and eigenstress-strain (such as hydro-thermal properties, and heat conductivity are other examples of materials behavior, which will change with geometry. In order to cope rationally with such changes in composite analysis we must increase our freedom to choose other analytical models than the specific, non-variable ones most often used to day." Our new book is dedicated mainly to constructive topics of boundary value problems and their applications to macroscopic properties of composites and of porous media. Symbolic-numerical computations are widely used to deduce new formulas important for engineers and researchers. New formulas for the effective properties are deduced in the form customized for engineering applications.

The outline of typical exposition is given below for the case of 2D elastic composites. Composites with non-overlapping circular inclusions randomly embedded in matrix are investigated. Special attention is paid to critical regimes related to the optimal packing of inclusions and to extreme physical constants (rigid and soft inclusions). Investigation of regular and random structures is based on the general approach of the RVE (representative volume element) and the corresponding structural sums. The proposed method yields an effective algorithm in symbolic-numeric form to compute structural sums as discrete multiple convolutions. In this book, new algorithms are described systematically, codes or pseudo-codes are given, and complexity of computations is studied.

We present also modified averaging computational method applied to the local stresses and deformations. Properly constructed series are reduced to polynomials and rational functions depending on the concentration of inclusions f. But it is not a final solution to the problem. Furthermore, these functions are replaced by asymptotically equivalent expressions. Special methods of resummation suggested in the book and in (Gluzman et al., 2017), bring accurate and compact formulas for all concentrations. Accurate analytical formulas for deterministic and random composites and porous media can be derived employing approximants, when the low-concentration series are supplemented with information on the high-concentration regime. Typical problems we encounter are characterized by asymptotic power laws.

Our first book (Gluzman et al., 2017) may be considered as an neoclassical answer to the question associated to Fig. 0.1, why does James Bond prefer shaken, not stirred martini with ice? Highly accurate computational analysis of structural media allowed us to explain the difference between various types of random composite structures. It is strongly related to the critical exponent s in the asymptotic behavior of the effective conductivity. In the limiting case of a perfectly conducting inclusions, the effective conductivity σ_e is expected to tend to infinity as a power-law, as the concentration of inclusions f tends to $f_c = \frac{\pi}{\sqrt{12}}$, the maximal value in 2D

$$\sigma_e(f) \sim (f_c - f)^{-\mathsf{s}}. \tag{2}$$

The dependence of the index s on the shaken-stirred regime of inclusions is displayed in Fig. 0.1. Similarly, one can consider different effective properties. Universality of the mathematical modeling implies that the same equations hold for the electric and thermal conductivity, magnetic permeability, anti-plane elastic strains and so on.

Scientific classicists are perpetually in search of universal answers to all questions concerning the transport properties of composite materials, which can be simply adjusted to any concrete case. Neoclassical approach includes their classical results as a

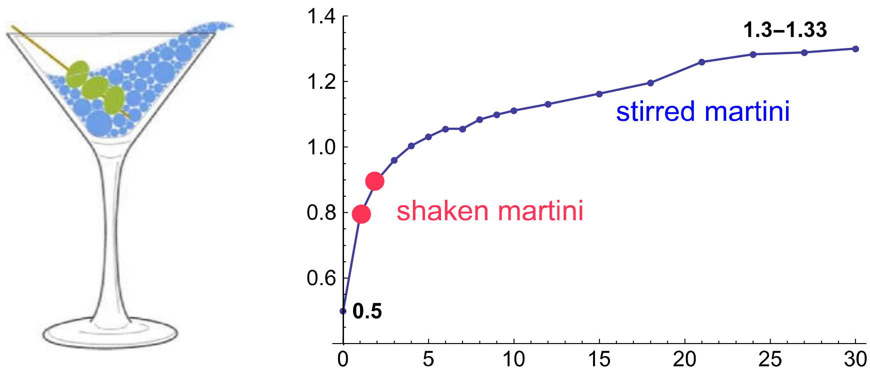

Figure 0.1 Why did James Bond prefer shaken, not stirred martini with ice? Because he sensed in martini the critical exponent s from formula (2). The dependence of s on the degree of disorder measured in steps of random walk is displayed in the graphics.

limit-case, complements it with another limit case of high-concentration percolating inclusions, but does not stop here. The problem now is getting shifted towards methodology (tool-box), concerned with properly matching the limit-cases. On the way one should develop a non-universal, structure-dependent expansions, as well as special approximation methods. From the warm and cosy world where universal answers exist, we are getting to the cold, unfriendly one. In such world each and every problem of the theory of composites should be studied in terms of the particular numerical set of structural sums, the particular large f limit found, and the particular approximation method carefully selected to receive formula for all f.

We are convinced that to derive a new formula, valid in the whole range of relevant variables, is not merely a mathematical exercise, or even a matter of convenience. It provides a fresh insight, since in the majority of cases realistic material sciences problems correspond neither to weak coupling (or low concentration) regime nor to strong coupling (high concentration) limit, but to the intermediate range of parameters. Such regime can be covered by some rather complex formula deduced from asymptotic regimes. It is quite handy for a scientist to possess a general mathematical toolbox to derive asymptotic, typically power laws, as well as explicit crossover formulas for a multitude of processes. Problems discussed in the book can be viewed as asymptotically classical, but in each of them, a neoclassical twist is supposed to make them more agreeable to the modern listener. Besides, they are all interesting and hold a promise in days to come.

Some authors equate an *approximate analytical formula* with a *model*. Such an approach is misleading, since a mathematical modeling involves fundamental governing equations, complemented by interface and boundary conditions. Different approximate formulas/solutions for the mathematical model hold under restrictions usually not discussed by authors. A serious methodological mistake may follow when intermediate manipulations are valid only within the precision $O(f)$, while the final formula is claimed to work with a higher precision, see an explicit example in Appendix A.4. In particular, it follows from our investigations that it is impossible to write a universal higher order formula independent on locations of inclusions. Such a universal formula holds only for a limited class of composites with non-interacting inclusions, e.g., for dilute composites and the Hashin-Shtrikman coated sphere assemblage (Cherkaev, 2009).

Since Einstein, the transport coefficients in random and regular media are expressed as expansions in concentration f. Nevertheless, despite persistent efforts of such outstanding researchers as Batchelor, Bergman, Brady, Jeffrey, Milton, McPhedran, Torquato, Wajnryb the problem still exists of finding correct numerical coefficients in expansions. Besides, the validity of such short series is very limited, and their true value is still remains to be seen.

Let us address the Hashin–Shtrikman bounds and their extensions (Milton, 2002). The dependence of the effective conductivity of a random composite on f corresponds to some monotonous curve, drawn between the bounds. Such a curve can be sketched arbitrarily, and it will correspond to some unspecified distribution of inclusions. Often, we deal with a uniform distribution corresponding to a stir-casting process described by the random sequential addition (RSA) model (Kurtyka and Rylko, 2013, 2017). Thence main theoretical requirement to the geometric model consists not only in writing a formula, but in a precise description of the geometrical conditions imposed on deterministic or random locations of inclusions. The rigorous statement and study of this theoretical problem is necessary for the proper approach to various applied problems, e.g., stir-casting process.

Our formulas for the effective properties of random composites are derived as the mathematical expectation of the effective conductivity over the independent and identically distributed (i.i.d.) non-overlapping inclusions. Even formulas obtained for uniformly distributed non-overlapping balls are not universal, because the effective conductivity depends on the protocol of computer simulations or experimental stirring, meaning that the very notion of randomness is non-universal (Torquato, 2002, Kurtyka and Rylko, 2013, Rylko, 2014, Gluzman et al., 2017).

Some famous formulas turn out to be questionable, in our opinion. The example, why various not rigorous, popular approaches can be questioned, is given in Chapter 6 based on the paper by Mityushev and Nawalaniec (2019). It is demonstrated that the classical Jeffrey formula contains wrong f^2 term. See Chapter 6, where the terms f^2 and f^3 are written explicitly! In particular, we demonstrate that the f^3 term depends on the deterministic and random locations of inclusions. A novel expansion for the random composite with superconducting (perfect conducting) inclusions is obtained, see (6.92) on page 226. It leads to a proper estimate for the critical index for superconductivity. The finding seems to justify the whole body of work on the short series for effective conductivity, and give a physical meaning to the series as a valuable source of estimating critical index s.

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