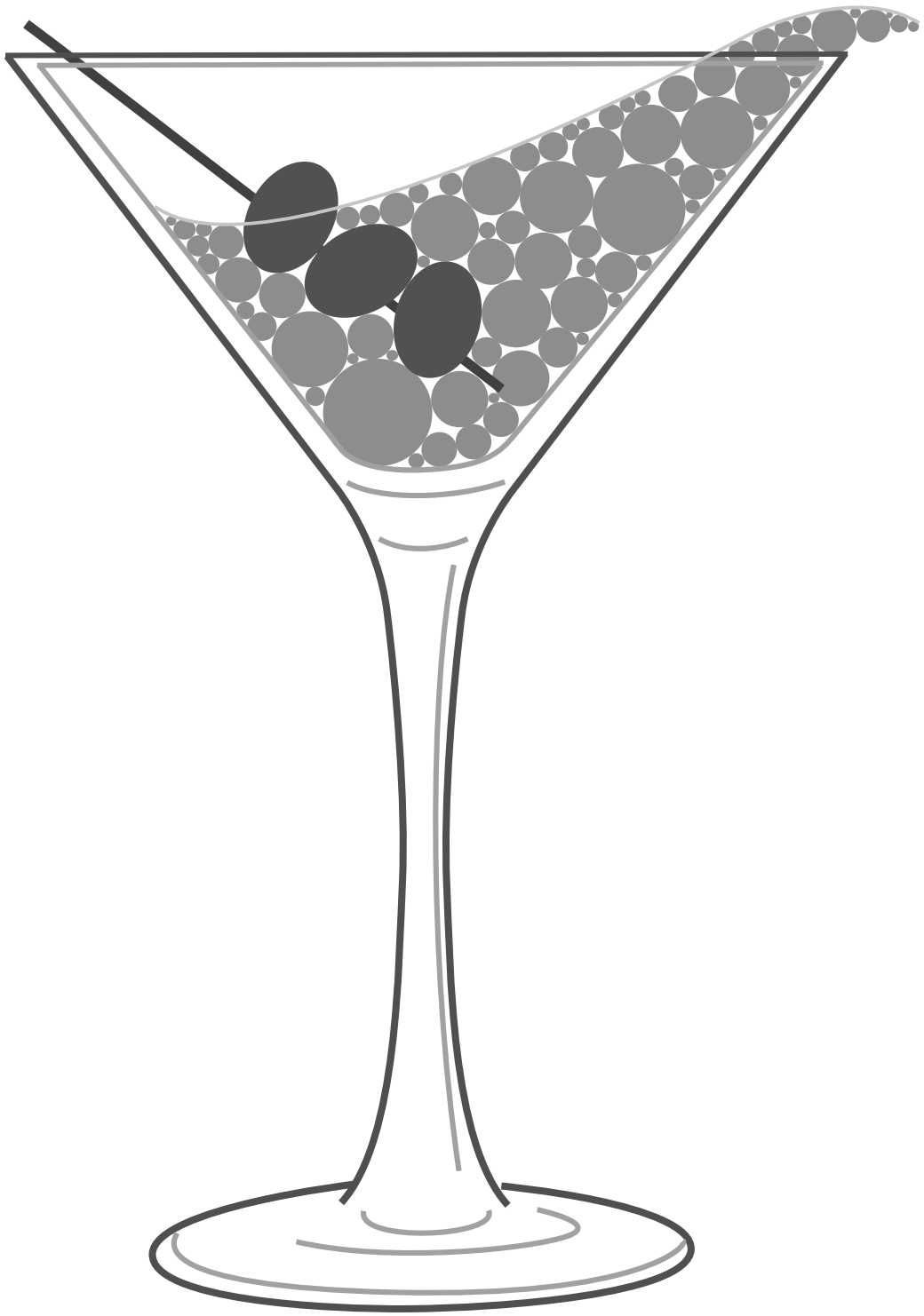

For Our Families

CONTENTS

This page intentionally left blank

ACKNOWLEDGMENT

We thank our friends and colleagues, Pierre Adler, Igor Andrianov, Leonid Berlyand, Piotr Drygaś, Barbara Gambin, Leonid Filshtinsky, Alexander G. Kolpakov, Pawel Kurtyka, Natalia Rylko, Ryszard Wojnar, Vyacheslav Yukalov, for all their support and useful discussions. We are also indebted to the whole Elsevier team for their help and guidance throughout the publishing process. We are grateful to the editor for carefully reviewing the book during this process. The authors (V.M. and W.N.) were partially supported by Grant of the National Centre for Research and Development 2016/21/B/ST8/01181.

Simon Gluzman, Vladimir Mityushev, and Wojciech Nawalaniec
April 2017

This page intentionally left blank

PREFACE

Four legs good, two legs bad

— George Orwell, Animal farm

The present book may be considered as an answer to the question associated to the picture on the last front matter page. Why does James Bond prefer shaken, not stirred martini with ice?[1] Highly accurate computational analysis of structural media allows us to explain the difference between various types of random composite structures.

We are primarily concerned here with the effective properties of deterministic and random composites. The analysis is based on accurate analytical solutions to the problems considered by respected specialists as impossible to find their exact solutions. Consensual opinions can be summarized as follows: " It is important to realize that solution to partial differential equations, of even linear material models, at infinitesimal strains, describing the response of small bodies containing a few heterogeneities are still open problem. *In short, complete solutions are virtually impossible*" (see [5, p. 1]).

Of course, it is impossible to resolve all the problems of micromechanics and their analogs, but certain classes such as boundary value problems for Laplace's equation and bi-harmonic two-dimensional (2D) elasticity equations can be solved in analytical form.

At least for an arbitrary 2D multiply connected domain with circular inclusions our methods yield analytical formulae for most of the important effective properties, such as conductivity, permeability, effective shear modulus and effective viscosity. Randomness in such problems is introduced through random locations of non-overlapping disks. It is worth noting that any domain can be approximated by special configurations of packed circular disks.

Many respectful authors apply various self-consistent methods (SCM) such as effective medium approximation, differential scheme, Mori–Tanaka approach, etc. [2]. They claim that such methods give general analytical formula for the effective properties. Careful analysis though shows their restriction to the first- or second- order approximations in concentration.

Actually SCM perform elaborated variations on the theme of the celebrated Maxwell formula, Clausius–Mossotti approximation, and so forth [3]. All of them are justified

[1]The complete answer on the question is yet to be found, and most likely after many experiments. But the mathematical answer is given on 268.

rigorously only for a dilute composites when interactions among inclusions are neglected. In the same time, exact and high-order formulae for special regular composites which go beyond SCM were derived.

Despite a considerable progress made in the theory of disordered media, the main tools for studying such systems remain numerical simulations and questionable designs to extend SCM to high concentrations. These approaches are sustained by unlimited belief in numerics and equal underestimation of constructive analytical and asymptotic methods. They have to be drastically reconsidered and refined. In our opinion there are three major developments which warrant such radical change of view.

1. Recent mathematical results devoted to explicit solution to the Riemann–Hilbert and $\mathbb{R}-$linear problems for multiply connected domains, see Chapter 1, [4].[2]

2. Significant progress in symbolic computations (see MATHEMATICA®, MAPLE®, MATLAB® and others) greatly extends our computational capacities. Symbolic computations operate on the meta-level of numerical computing. They transform pure analytical constructive formulae into computable objects. Such an approach results in symbolic algorithms which often require optimization and detailed analysis from the computational point of view. Moreover, symbolic and numeric computations do integrate harmoniously [1].

But we can not declare a victory just yet, because even long power series in concentration and contrast parameters are not sufficient because they won't allow to cover the high-concentration regime. Sometimes the series are short, in other cases they do not converge fast enough, or even diverge in the most interesting regime. Your typical answer to the challenges is to apply an additional methods powerful enough to extract information from the series. But in addition to a traditional Padé approximants applied in such cases, we would need a

3. New post-Padé approximants for analysis of the divergent or poorly convergent series, including different asymptotic regimes discussed in Chapter 5.

In the present book, we demonstrate that the theoretical results [4] can be effectively implemented in symbolic form that yields long power series. Accurate analytical formulae 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 where the problems we encounter are characterized by power laws.

As to the engineering needs we recognize the need for an additional fourth step. The engineer would like to have a convenient formula but also to incorporate in it all available information on the system, with a particular attention to the results of numerical simulations or known experimental values.

[2]Poisson's type formula for an arbitrary circular multiply connected domain is one of its particular cases.

Method of "regression on approximants" consists in applying different multivariate regression techniques to the results of interpolation and (or) extrapolation with various approximants within the framework of supervised learning paradigm. In this case approximants by themselves are treated as new variables and experimental, exact or numerically "exact" data, or else training data set, are used to construct regression on approximants. Some statistical learning procedure should be included in order to select the best regression and to make sure it is better indeed than choosing the best performer among the approximants.

Consider a non-dimensional effective property $\vartheta(f)$. Here f stands for the concentration of particles. Let the asymptotic expansion of $\vartheta(f)$ in the weak-coupling limit be

$$\vartheta(f) \simeq a_0 + a_1 f + a_2 f^2 + a_3 f^3 + a_4 f^4 + \cdots, \quad \text{as } f \to 0. \tag{0.0.1}$$

In addition to the expansion, let us consider as available to us, "exact" numerical values $\vartheta(f_i)$ (or "labels"), for the effective property for some typical values of $f = f_i$, $i = 1, 2, \ldots, K$.

This information to be incorporated into the algorithm:

(a) construct all possible approximants for such expansion, such as $Ap_j^*(f)$, $j = 1, 2, \ldots, M$. The approximants are also assumed to incorporate the information from the high-concentration regime whenever such information is available.

(b) make "predictions", i.e., calculate with all constructed approximants for all f_i the values of $Ap_j^*(f_i)$.

Let us consider all predictions as a j-dimensional vector $\mathbf{Ap}^*(f_i)$ and organize $\mathbf{Ap}^*(f_i)$ and $\vartheta(f_i)$ into pairs $\{\mathbf{Ap}^*(f_i), \vartheta(f_i)\}, i = 1, 2, \ldots, K$, thus creating a training data set.

(c) based on information contained in the training data set, we attempt to learn the (multivariate) mapping $\vartheta^* = F(\mathbf{Ap}^*)$ (regression model), allowing to make predictions for arbitrary f (since $\mathbf{Ap}^*$ depends on f);

(d) most simple regression models, such as multivariate linear regression and k-Nearest Neighbors could be used.

(e) for learning, i.e., selection of the best regression based on prediction error incurred by particular regression within a given training data set, one can use, e.g., a jackknife (or leave-one-out cross-validation) error estimates. Starting from the whole training data set, the jackknife begins with throwing away the first label, leaving a resampled data set, which is used to construct regression and " prediction" is made for the " missing " label. In turn, such obtained prediction is compared with the true label. Resampling is continued till predictions and comparison are performed for each and every label from the training data set.

(f) as a cumulative measure for the prediction error one can take mean absolute percentage error calculated over all labels.

Such approach is amenable to automation and true predictions of the sought physical quantity for any f can be generated.

REFERENCE

1. Czapla R, Nawalaniec W, Mityushev V, Effective conductivity of random two-dimensional composites with circular non-overlapping inclusions, Comput. Mat. Sci. 2012; 63: 118–126.
2. Kanaun SK, Levin VM, Self-consistent methods for composites. Dordrecht: Springer-Verlag; 2008.
3. Landauer R, Electrical conductivity in inhomogeneous media. ed. Garland JC, Tanner DB, Electrical Transport and Optical Properties of Inhomogeneous Media, 1978.
4. Mityushev VV, Rogosin SV, Constructive methods to linear and non-linear boundary value problems of the analytic function. Theory and applications. Boca Raton etc: Chapman & Hall / CRC; 1999/2000. [Chapter 4].
5. Zohdi TI, Wriggers P, An introduction to Computational mechanics. Berlin etc: Springer-Verlag; 2008. [Chapter 1].

Simon Gluzman, Vladimir Mityushev, and Wojciech Nawalaniec
Kraków, Poland
April 2017