Neoclassical theory of composites

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In words of Sergei Prokofiev we define neo-classicism: "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 had 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 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.

The book [2] may be considered as an neo-classical 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? The complete answer on the question is yet to be found, and most likely after many experiments. But the mathematical answer is attempted in the book. Highly accurate computational analysis of structural media allows 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 is expected to tend to infinity as a power-law, as the concentration of inclusions f tends to the maximal value $f_c = \frac{\pi}{4}$ [1]

$$\sigma_e(f) \approx \frac{A}{(f_c - f)^s}. \tag{1}$$

The dependence of s on the shaken-stirred regime of inclusions is displayed in Fig.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 etc.

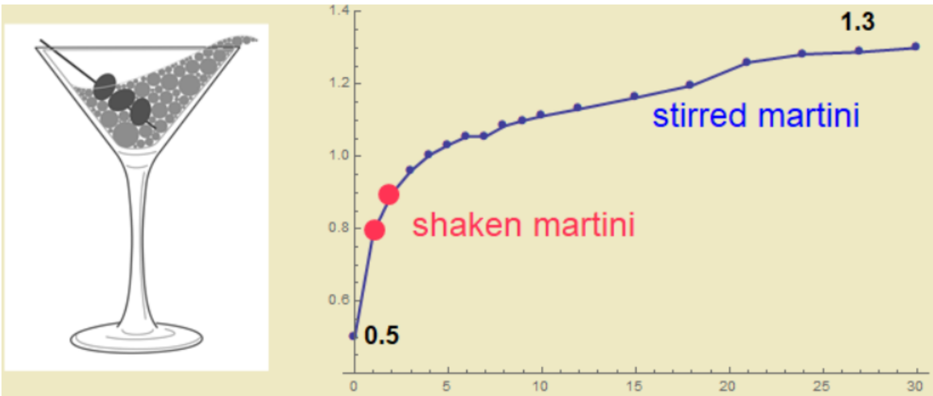

Figure 1: Why did James Bond prefer shaken, not stirred martini with ice? Because he sensed in martini the critical exponent s from formula (1). The dependence of s on the degree of disorder measured in steps of random walk is displayed in the graphics.

We are primarily concerned here with the effective properties of deterministic and random composites and porous media. The analysis is based on accurate analytical solutions to the problems considered by respected specialists as impossible to find their exact solutions.

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.

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.

Discrete numerical solutions such as finite elements and difference methods. are powerful and their application is reasonable when the geometries and the physical parameters are fixed. In this case the researcher can be fully satisfied with numerical solution to various boundary value problems. Various numerical packages sometimes are presented as a universal remedy. But, a sackful of numbers is not as useful as an accurate analytical formulae. Pure numerical procedures fail as a rule for the critical parameters and analytical matching with asymptotic solutions can be useful even for the numerical computations.

Such philosophy is 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 neo-classical 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.

2. Significant progress in symbolic computations (see MATHEMATICA 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.

But 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 book, we demonstrate that the theoretical results 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 by applying the method of "regression on approximants", described in to the book.

Central for our study, series method arises when an unknown element x is expanded into a series $x = \sum_{k=1}^{\infty} c_k x_k$ on the basis $\{x_k\}_{k=1}^{\infty}$ with undetermined constants c_k. Substitution of the series into equation can lead to an infinite system of equations on c_k. In order to get a numerical solution, this system is cut short and a finite system of equations arise, say of order n. Let the solution of the finite system tend to a solution of the infinite system, as $n \to \infty$. Then, the infinite system is called regular and can be solved by the described truncation method. The obtained truncated series are considered as polynomials. They are supposed to "remember their infinite expansions", so that with a help of some additional re-summation procedure one can extrapolate to the whole series.

The book is organized as follows. First, the general term *solution to a problem* is discussed in Introduction since sometimes general methods which are hard to implement numerically, are called "analytical solutions". We have to ensure the Reader that "solved" indeed means "solved", and we deal with exact and approximate analytical solutions. Chapter 2 contains a description of the method of functional equations, the main tool to solve the problems in terms of expansions. A short introduction into complex analysis including the Riemann-Hilbert and R-linear problems for finite multiply connected domains is presented. Chapter 3 is devoted to extension of the results obtained in Chapter 2 to periodic problems (for infinitely connected domains), the principal problems of composites. In statement of the problems, we use Hashin's MMM principle based on the physical intuition and observations. Convergence of the standard cluster and contrast expansions traditionally applied in the theory of composites is demonstrated by treatment of these expansions as the generalized Schwarz alternating method. In Chapter 4, we discuss e-sums and their application to the RVE theory. Chapter 5 contains general description of asymptotic methods of approximation. Chapters 6 and 7 are devoted to computation of the effective conductivity of the square and hexagonal arrays of cylinders. 3D composites are considered in Chapter 8 where we solve a boundary value problem for a finite number of spheres in space and discuss periodic problems for regular locations of inclusions. Analytical formulae for the effective conductivity of random composites are obtained in Chapter 9. Extension to 2D elastic problems are presented in Chapter 10. The most valuable analytical formulae derived in the book are presented in special Table. These formulae are intended for engineers for estimation of the effective properties of composites.

We continue below with a concrete example of classical and neo-classical theories concerning 2D conductivity (thermal, electric etc). Consider a classical problem of the effective conductivity of a 2D regular composite. An accurate approximate formula formula can be deduced for a 2D, two-component composite made from a collection of non-overlapping, identical, ideally conducting circular discs, embedded regularly in an otherwise uniform locally isotropic host. Consider the general situation, when contrast parameter ρ enters the power series for conductivity explicitly. Usually, the conductivity of the matrix is normalized to unity, $\sigma_m = 1$. Let σ denote the conductivity of inclusions, and

$$\rho = \frac{\sigma - 1}{\sigma + 1},$$

so that $|\rho| \leq 1$.

The following expansion in concentration f of the inclusions and contrast parameter ρ was obtained in[2],

$$\sigma_e \approx \frac{1+f\rho}{1-f\rho} + 0.611654 f^5 \rho^3 + 1.22331 f^6 \rho^4 + 1.83496 f^7 \rho^5 + 2.44662 f^8 \rho^6. \tag{2}$$

The coefficients depend only on ρ.

The series (2) are expressed as a correction to the celebrated classical Maxwell's, or Clausius-Mossotti (CM) formula,

$$\sigma_e \approx \frac{1+\rho f}{1-\rho f}.$$

CM is valid for small concentrations but respects the phase interchange symmetry.

Formula (2) respects this symmetry as well. Mind that in 2D one has to respect celebrated Keller's phase-interchange relation [3, 5], valid for the general case of average conductivity of a statistically homogeneous isotropic random distribution of cylinders of one medium in another medium [3]. Since the dependence on the conductivity of inclusions and matrix is hidden within the contrast parameter and depends only on σ, the phase interchange can be expressed as follows,

$$\frac{1}{\sigma_e(\sigma)} = \sigma_e\left(\frac{1}{\sigma}\right),$$

One should check their method's compliance with the symmetry.

The proper steps has to be taken to guarantee corresponding critical properties. Then, we simply modify the solution to move away to a non-critical situations. Such modification can be accomplished from scaling considerations in the vicinity of f_c. For small σ the form of a correction to generic power-law may be also found as a power-law, but with different critical exponent u. In 2D u is always equal to $1/2$ [1]. Although in 2D case there is no exact solution, we are going to look for an approximate analytical solution in the model with two critical exponents. There are two limit-cases. For non-conducting disks, as $\sigma = 0$,

$$\sigma_e \simeq \sqrt{\frac{f_c - f}{f_c}} \tag{3}$$

and for weakly-conducting disks, with $\sigma \neq 0$, as $f = f_c$

$$\sigma_e \approx \sigma^{1/2}, \tag{4}$$

with $f_c = \frac{\pi}{4} \approx 0.7854$.

The simplest solution satisfying both limits can be constructed in additive form

$$\sigma_e \approx \sqrt{\sigma} + \frac{2\sqrt{\frac{\pi}{4} - f}}{\sqrt{\pi}}. \tag{5}$$

In higher orders one can still obtain closed-form expressions and manage them with MATHEMATICA. They are too long to be brought up here. But for concrete parameters their derivation and final form are pretty simple. Assuming the higher-order form $P_{4,4}$ for the correcting Pade approximant, we obtain an accurate formula for $\sigma = 1/50$

$$\sigma_e \approx \frac{0.817042(f(f(f(f-0.13819)-0.034015)+2.33313)-3.22041)\left(\sqrt{0.785398-f}+0.125331\right)}{f(f(f(f+0.226828)+1.01293)-1.70169)-2.66162}. \tag{6}$$

For further comparison we also constructed the Pade approximant for conductivity

$$\sigma_e \approx \frac{(f-0.871396)(f+1.75656)\left(f^2-0.88516f+2.31417\right)}{(f-1.75656)(f+0.871396)\left(f^2+0.88516f+2.31417\right)}. \tag{7}$$

In Fig.3 it is clearly seen a linear behavior of conductivity in the intermediate region. Thus, there are three characteristic parts described by formula (6). For small f there is a diluted situation, also covered by classical CM formula. For intermediate f the conductivity can be approximated by linear behavior well covered also by the Pade approximant. The critical region close to f_c is described only by our formula. Various approximations are compared in In Fig.2. Overall, only neo-classical formula (6) can cover all three situations.

The form (5) is particularly suited to include the critical behavior as $\rho \to -1$, and could be adapted to the case $\rho \to 1$, respectively. The phase-interchange symmetry is preserved when analogous calculations are

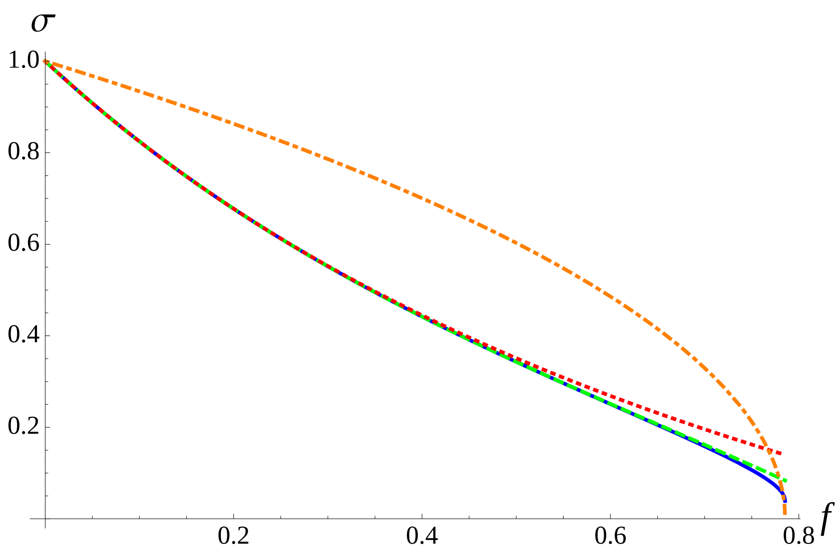

Figure 2: Our suggestion (6) is shown with blue, solid line, and the Pade approximant (7) is shown with green, dashed line. The Clausius-Mossotti (CM) formula is shown with red, dotted line. Naive power-law extrapolation of the formula (3) to the whole region is shown with orange, dot-dashed line. The numerical data are shown with dots.

performed for highly conducting inclusions, $\sigma \gg 1$, with the following "symmetric" choice of the approximation for the critical behavior,

$$\sigma_e \approx \frac{1}{\frac{2\sqrt{\frac{\pi}{4}-f}}{\sqrt{\pi}} + \frac{1}{\sqrt{\sigma}}}. \tag{8}$$

To derive a new formula, valid in the whole range of relevant variables, is not merely a mathematical exercise. 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 arbitrary phenomena. We agree with [4] that power laws are ubiquitous and should be exploited for complete analysis of the system, rather than to imbue them with a vague and mistakenly mystical sense of universality [4].

This note shortly presents the study conducting by the scientific interdisciplinary $Materialica+$, see *www.materialica.plus*. We are cordially invite

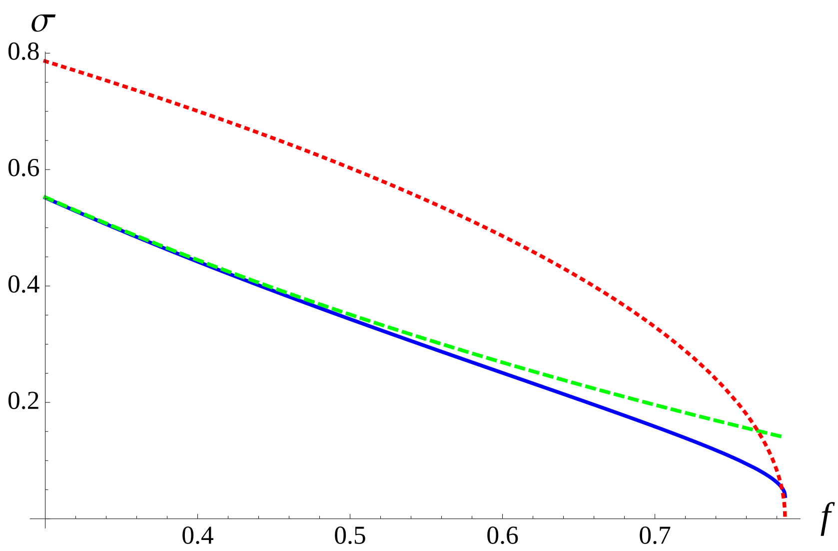

Figure 3: $\sigma = 1/50$. The Clausius-Mossotti (CM) formula is shown with green, dashed line. Our suggestion (6) is shown with blue, solid line. Naive power-law extrapolation of the formula (3) to the whole region is shown with red, dotted line.

engineers to cooperation.

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