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Universal material property in conductivity of planar random microstructures

M. Ostoja-Starzewski [*†]

Abstract

We study scatter involved in finite size scaling of the conductivity and resistivity tensors resulting, respectively, from uniform essential and natural boundary conditions applied to domains that are finite relative to the size of a heterogeneity. For various types of planar microstructures generated from Poisson processes (multi-phase Voronoi mosaics, composites with circular or needle-like inclusions, etc.) we report a universal property: the coefficient of variation of the second invariant stays practically constant at about 0.55 ± 0.1, irrespective of: the domain size, the boundary conditions applied to it, the contrast, and the volume fraction of either phase.

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Scale-dependent bounds on effective, macroscopic response tensors in conductivity and elasticity of random media have been studied for one decade now [1-3]. While analyzing the statistical character of these bounds for various types of microstructures - two-phase Poisson-Voronoi mosaics [4, 5], composites with soft needle-like inclusions [6], and disk-inclusion composites [7] - we have recently observed an interesting property: the coefficient of variation of the second invariant stays almost constant at about 0.55$\pm$0.1 irrespective of: the window size, the boundary conditions applied to the window (uniform Dirichlet or uniform Neumann type), the mismatch in stiffness between the inclusions and the matrix, and the inclusions shape, providing the inclusions aspect ratio is moderate (does not exceed 10 : 1). In this paper we report that several other and more general microstructures possess the same property. They are: multi-phase Poisson-Voronoi mosaics, matrix-disk composites with circular or elliptical disks, matrix-needle composites (with stiff needles), and superpositions of these such as matrix-disk-needle composites.

The fundamental concept is that of a random microstructure; it is an ensemble $\mathcal{B} = \{B(\omega); \omega \in \Omega\}$ of deterministic media $B(\omega)$, where ω is an indicator of a given realization, and Ω is an underlying sample space. We consider two-dimensional microstructures of spatially homogeneous, isotropic and ergodic statistics, that are generated from planar Poisson point fields. In particular, we consider two special cases: (i) Voronoi tessellations (mosaics) and (ii) several Boolean models, e.g. [8, 9]. The important thing to note is that hard-core point processes are excluded from this model, and so, we do see partial overlaps of the inclusions in Fig. 1(b).

In the first case, the material of each Voronoi cell is sampled at random from either two, three, or four types of phases; $p = 1, ..., 4$, depending on the actual choice of a p-phase random microstructure. The sampling is done sequentially, independent of the states of other cells of the mosaic. An example of a mosaic with four phases present is shown in Fig. 1(a).

In the case of Boolean models, we generate inclusions sampled at random from any one of two (or three, or four) types of phases; matrix is phase $p = 1$, and inclusions are or $p = 2, 3$, or 4. Also here, the sampling is done sequentially - one inclusion after another - independent of the states of other cells of the composite.

In the language of Boolean models [9], inclusions are so-called *grains* generated from *germs* (Poisson points) in the *germ-grain process*. Our inclusions are either circular disks (Fig. 1(b)), or elliptical disks, or needles (Fig. 1(c)). In the latter two cases, the aspect ratio is kept moderate (i.e., under 10:1). A more complex Boolean model is shown in Fig. 1(d): a superposition of a field of disks with a field of needles. Each phase is locally homogeneous and isotropic, and it is characterized by its volume fraction $f^{(p)}$ and conductivity $C^{(p)}$. Thus, the contrast for a phase $p \neq 1$ is $\alpha^{(p)} = C^{(p)}/C^{(1)}$.

The material is governed locally by a Laplace equation $C^{(p)}\nabla^2 T = 0$. We are interested in the material response on scales L (window size) larger than the heterogeneity size d (Voronoi cell size or inclusion size), see Fig. 1 of [3]. To that end, we employ a dimensionless scale parameter $\delta = L/d$, and compute boundary value problems on any given random microstructure under uniform essential (Dirichlet) and natural (Neumann) boundary conditions. That is, the essential condition

$$T = \overrightarrow{\nabla T} \cdot \overrightarrow{x}, \quad \forall \overrightarrow{x} \in \partial B \tag{1}$$

yields a tensor $\mathbf{C}_\delta^e$ (e stands for essential boundary conditions), where T is the temperature, $\overrightarrow{\nabla T}$ is the spatial average temperature gradient, $\overrightarrow{x}$ is the position vector, and ∂B is the window's boundary of B. On the other hand,

$$\overrightarrow{q} \cdot \overrightarrow{n} = \overrightarrow{\overline{q}} \cdot \overrightarrow{n}, \quad \forall \overrightarrow{x} \in \partial B \tag{2}$$

yields $\mathbf{C}_\delta^n = (\mathbf{S}_\delta^n)^{-1}$ (n stands for natural boundary conditions), where $\overrightarrow{q}$ is the heat flux, $\overrightarrow{\overline{q}}$ is the spatial average heat flux, and $\overrightarrow{n}$ is the outer unit normal to ∂B. In the above we employ boldface for a second-rank tensor, and an overbar for a spatial average over the window domain. As discussed in [1-7], these boundary conditions bound the effective macroscopic conductivity tensor $\mathbf{C}^{eff}$, and the latter may be interpreted as $\lim_{\delta\to\infty} \mathbf{C}_\delta^n = \lim_{\delta\to\infty} (\mathbf{S}_\delta^n)^{-1}$ in the sense of homogenization theory [2].

For each of these second-rank tensors - conductivity $\mathbf{C}_\delta^e$ and resistivity $\mathbf{S}_\delta^n$, respectively - for any specific configuration $B(\omega)$ of $\mathcal{B}$ we can compute the second invariants

$$R_\delta^e = \sqrt{(C_{11} - C_{22})^2/4 + C_{12}^2}, \quad R_\delta^n = \sqrt{(S_{11} - S_{22})^2/4 + S_{12}^2} \tag{3}$$

Thus, in the ensemble sense, for any scale δ and any type of boundary conditions (e or n), we have two random invariants: $\{R_\delta^e; \omega \in \Omega\}$ or $\{R_\delta^n; \omega \in \Omega\}$. We next consider the coefficient of variation of each of these invariants

$$CV_\delta^e = \frac{\sigma(R_\delta^e)}{\mu(R_\delta^e)}, \quad CV_\delta^n = \frac{\sigma(R_\delta^n)}{\mu(R_\delta^n)} \tag{4}$$

In the above, μ stands for the ensemble average and σ stands for the standard deviation of the given invariant.

We carry out a range of numerical experiments on microstructures of Voronoi mosaic type and Boolean type to determine CV_δ^e and CV_δ^n. We employ a very fine spring network (avoiding mesh dependence) for the resolution of the microstructure and solution of both types of boundary value problems; in select cases we also use finite element and boundary element programs.

Our parameter space (window size δ, contrast $\alpha^{(p)}$, and volume fraction of either phase $p = 1, ..., 4$) is continuous valued. Now, for each and every choice of parameters we need to perform a sufficiently large number of generations of the microstructure, and then compute $\mathbf{C}_\delta^e$ (and $\mathbf{S}_\delta^n$) under essential (respectively, natural) boundary condition. Note that at small scales δ, and especially for strong contrasts, the scatter in $\mathbf{C}_\delta^e$ and $\mathbf{S}_\delta^n$ is very strong, and, therefore, very large numbers of realizations of random fields need to be studied in order to get reliable estimates of CV_δ^e and CV_δ^n. As the scale δ increases, the scatter goes down and, consequently, smaller numbers are needed; but then the computation of the Dirichlet, and especially Neumann, boundary value problem tends to be much more time consuming.

All this would result in an impossibly large number of computations that would be limited by any computer resources. Thus, one can investigate the parameter space only spotwise - i.e., for a small subset of parameters - and this is exactly what we do. Indeed, we have tried some 200 cases selected randomly from the following ranges of values:

$$\begin{aligned} \alpha^{(p)} &= 10, \quad n = 1, ..., 5, \quad p = 2, ..., 4 \\ f^{(p)} &= 0.1m, \quad m = 1, ..., 9, \quad p = 1, ..., 4 \\ \delta &= 2, 4, 10, 20, 50, 100 \end{aligned} \tag{5}$$

It has turned out that, whatever the spot in the parameter space, the coefficients of variation of the two invariants (i.e., CV_δ^e and CV_δ^n), at $\delta > 1$, are equal about 0.55 ± 0.1 irrespective of:

(a) the window size δ;

(b) the boundary conditions applied to the window (uniform Dirichlet or uniform Neumann type);

(c) the contrasts $\alpha^{(p)}$ ($p = 2, ..., 4$), and the inclusion's shape;

(d) the volume fraction $f^{(p)}$ of any phase $p = 1, ..., 4$, providing its conductivity is not 0 or ∞. This result indicates a universal nature of CV_δ^e and CV_δ^n for planar random media generated from Poisson point patterns.

The fluctuations of up to ± 0.1 around 0.55 appear to be due to the finite number of realizations of the random microstructure (generated by a Monte Carlo method) in any given parameter case. As the number of these realizations is increased, the fluctuations tend to go down and the CV_δ^e and CV_δ^n stabilize around 0.55.

An exact mathematical analysis and proof of the constancy of these coefficients of variation does not appear possible at the present stage of theories of random media. However, we offer some observations which may prove vital to such a proof in the future:

(i) The Poisson point process does not possess any intrinsic length scale, which fact seems consistent with CV_δ^e and CV_δ^n being independent of the window size δ.

(ii) If our microstructures are generated from hard-core point processes (i.e. non-Poisson point fields), then CV_δ^e and CV_δ^n are usually lower than 0.55 for window sizes on the order of several grains (about 5 times larger), and then rise and stabilize around 0.55 at higher δ [7].

(iii) While there are no explicit formulas for the conductivity or resistivity tensors for heterogeneous domains of finite size, we can argue that these tensors are continuous in three parameters: window size δ, contrast $\alpha^{(p)}$, and volume fraction

$f^{(p)}$ of either phase. The extreme cases of $\alpha^{(p)} = 0$ or ∞ need to be excluded in order to avoid discontinuous dependence at percolation points.

(iv) The second invariant of the conductivity tensor $\mathbf{C}_\delta^e$ (as well as the resistivity tensor $\mathbf{S}_\delta^n$) of the material possessing isotropic statistics goes to zero as the window size $\delta \to \infty$. Thus, the mean $\mu(R_\delta^e)$ and standard deviation $\sigma(R_\delta^e)$ of this invariant also go to zero as $\delta \to \infty$. In view of (4), the constancy of CV_δ^e (and CV_δ^n) with δ implies that the mean and standard deviation remain in the same ratio as they both go to zero.

We end with a conjecture that the property found here also holds for any multi-phase material microstructures generated from Poisson point fields such as, for example, p-phase Poisson-Voronoi mosaics with $p \geqslant 5$.

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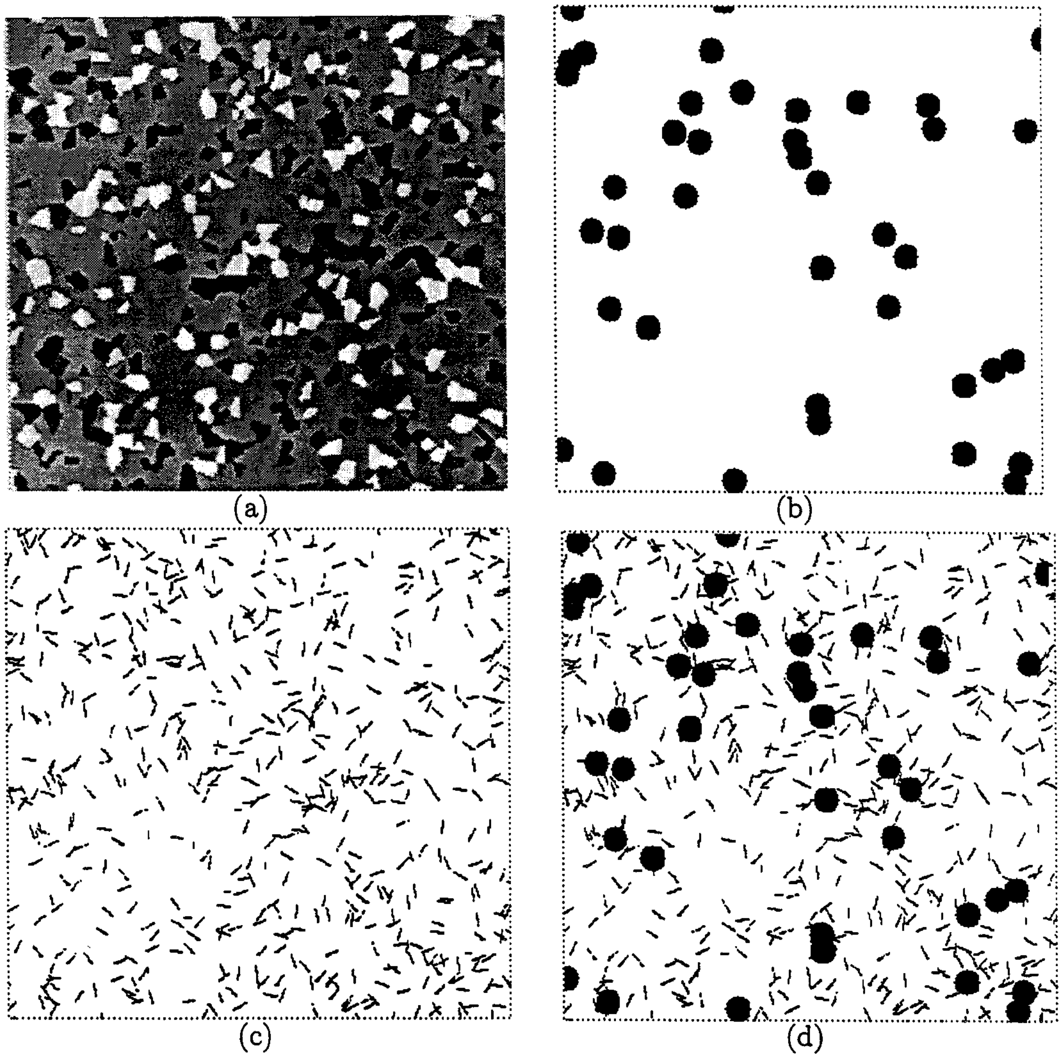

Figure 1: Examples of planar random microstructures studied in this paper: (a) four-phase Poisson-Voronoi mosaics; (b) matrix-disk composite; (c) matrix-needle composite; (d) matrix-disk-needle composite, which is a superposition of (b) and (c).