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The choice of representative volumes for random materials

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The most widely employed method for determining the effective large-scale properties of materials with random heterogeneities on a small scale is the *representative volume element* (RVE) method: It basically proceeds by choosing a sample of the random material – the *representative volume element* – and computing its properties. To obtain an accurate approximation for the effective material properties, the sample should reflect the statistical properties of the material well. As a consequence, it is desirable to choose a large sample of the random material. However, an increased size of the sample comes with an increased computation cost; for this reason, there have been attempts in material science [6] and mechanics [5] towards capturing the statistical properties of the material in a better way in a sample of a fixed size.

Inspired by these attempts, in the context of diffusion in a random medium Le Bris, Legoll, and Minvielle [4] have devised a method capable of significantly increasing the accuracy of the RVE method for a given size of the sample. Their idea is to select among many samples of the random medium the one that captures certain statistical properties of the random medium best, i. e. the one that is "most representative" of the material. For example, for a composite of two constituent materials, in the simplest setting of their method they propose to select the material sample in which the volume fractions of the constituent materials match best with the volume fractions of the constituents in the overall material; see Figure 1 for an illustration of this approach.

In numerical examples with moderate ellipticity contrast, the method of Le Bris, Legoll, and Minvielle [4] has provided an increase in accuracy by a factor of about $3-10$ or equivalently a reduction in computational cost by a factor of about $10-50$. However, the analysis of the approach has essentially been limited to the one-dimensional setting, in which an explicit formula for the homogenization corrector is available, as well as a purely qualitative convergence result in the multidimensional setting in the limit of infinite size of the RVE.

In the recent work [3], we establish a rigorous mathematical justification of the approach of Le Bris, Legoll, and Minvielle. In particular, we quantify the gain in accuracy of the ansatz of Le Bris, Legoll, and Minvielle and prove that the method does never worse than a random selection of samples. Furthermore, we show that it fails to increase the accuracy for some (rather artificial) counterexamples of random media.

The diffusion in a random medium is described by the stationary or time-dependent diffusion equation

$$-\nabla\cdot(a\nabla u)=f \qquad \text{or} \qquad \partial_t u=\nabla\cdot(a\nabla u)$$

with a random diffusion coefficient field a. Assuming spatial homogeneity, ellipticity, and a finite range of dependence $\varepsilon\ll 1$ for the probability distribution of a (i. e. in particular fast decorrelation of the material properties on scales larger than ε), the theory of stochastic homogenization predicts that the diffusion in the random medium behaves on large scales like a diffusion with a constant effective diffusion

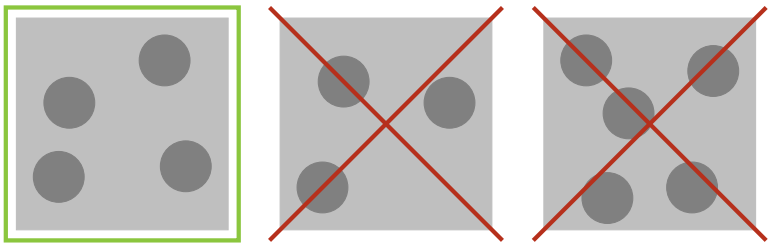

FIGURE 1. Among the three depicted material samples, the method of Le Bris, Legoll, and Minvielle would choose the first sample as the representative volume element and discard the other two, as the volume fraction of the inclusions in the first sample is closest to the overall material average. For a better illustration of the method, exaggeratedly small material samples are depicted.

coefficient a_{hom}: One may approximate the solution u by the solution u_{hom} of an effective diffusion equation

$$-\nabla \cdot (a_{\mathrm{hom}} \nabla u_{\mathrm{hom}}) = f \qquad \text{or} \qquad \partial_t u_{\mathrm{hom}} = \nabla \cdot (a_{\mathrm{hom}} \nabla u_{\mathrm{hom}})$$

with a constant diffusion coefficient a_{hom}. In this context of diffusion in a random medium, the representative volume element method is employed to obtain an approximation a^{RVE} for the effective coefficient a_{hom}. Roughly speaking, the approximation a^{RVE} is computed by choosing a sample $a|_{[0,L\varepsilon]^d}$ of the random medium (where ε is the length of correlations in the medium and where $L \gg 1$), solving the equation for the homogenization corrector $-\nabla \cdot (a(e_i + \nabla \phi_i)) = 0$ on this sample, and averaging the fluxes

$$a^{\mathrm{RVE}} e_i := \fint_{[0,L\varepsilon]^d} a(e_i + \nabla \phi_i)\, dx.$$

This approximation a^{RVE} is a random quantity, as it depends on the sample $a|_{[0,L\varepsilon]^d}$ of the random medium. In contrast, the macroscopic effective diffusion coefficient a_{hom} is deterministic. In fact, as shown by Gloria and Otto [1, 2] the leading-order contribution to the error $a^{\mathrm{RVE}} - a_{\mathrm{hom}}$ consists of random fluctuations: The order of the fluctuations of a^{RVE} is given by

$$\sqrt{\operatorname{Var} a^{\mathrm{RVE}}} \leq C L^{-d/2},$$

while the systematic error is of higher order in the size L of the sample

$$\left| \mathbb{E}[a^{\mathrm{RVE}}] - a_{\mathrm{hom}} \right| \leq C L^{-d} |\log L|^d.$$

As observed numerically by Le Bris, Legoll, and Minvielle [4], their method of selecting the material sample to obtain a "particularly representative sample" of the material increases the accuracy of approximations for a_{hom} by reducing the fluctuations. They also observed numerically that this strategy maintains the order of the systematic error. In the simplest case of their method, they select the sample $a|_{[0,L\varepsilon]^d}$ according to the following criterion on the spatial average of the coefficient field

$$\left| \fint_{[0,L\varepsilon]^d} a\, dx - \mathbb{E}\left[\fint_{[0,L\varepsilon]^d} a\, dx \right] \right| \leq \delta L^{-d/2} \ll \sqrt{\operatorname{Var} \fint_{[0,L\varepsilon]^d} a\, dx} \tag{1}$$

for some $0 < \delta \ll 1$. In a numerical example with moderate ellipticity contrast, this selection criterion achieves a numerical variance reduction by a factor of ≈ 10. By additionally considering a second statistical quantity derived from an expansion of

a_{hom} in the case of small ellipticity contrast $a \approx \mathrm{Id}$, in the same setting of moderate contrast they even achieve a variance reduction by a factor of ≈ 50.

In the recent work [3] we prove that the approach of Le Bris, Legoll, and Minvielle [4] indeed leads to a reduction of the fluctuations of the approximations a^{RVE}: Denoting the approximation obtained by the selection criterion (1) by a^{SQS}, we derive the estimate

$$\frac{\operatorname{Var} a^{\mathrm{SQS}}}{\operatorname{Var} a^{\mathrm{RVE}}} \leq 1 - (1-\delta^2)|\rho|^2 + \frac{C}{\delta} L^{-d/2} |\log L|^p$$

where ρ denotes the Pearson correlation coefficient

$$\rho := \frac{\operatorname{Cov}\left[a^{\mathrm{RVE}}, \fint_{[0,L\varepsilon]^d} a\,dx\right]}{\sqrt{\operatorname{Var}[a^{\mathrm{RVE}}]}\sqrt{\operatorname{Var} \fint_{[0,L\varepsilon]^d} a\,dx}}.$$

Note that we also construct a counterexample for which this correlation is zero [3], in which case the method is shown to fail to give an advantage over random sampling. We also show in [3] that the method of Le Bris, Legoll, and Minvielle essentially preserves the order of the systematic error in the sense

$$\left|\mathbb{E}[a^{\mathrm{SQS}}] - a_{\mathrm{hom}}\right| \leq \frac{C}{\delta} L^{-d} |\log L|^p$$

and that the tails (more precisely, the moderate deviations) of the probability distribution are reduced just as suggested by the variance reduction. Similar results are proven for the enhanced methods proposed by Le Bris, Legoll, and Minvielle.

References

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