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Examples of computational approaches for elliptic, possibly multiscale PDEs with random inputs

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ABSTRACT

We overview a series of recent works addressing numerical simulations of partial differential equations in the presence of some elements of randomness. The specific equations manipulated are linear elliptic, and arise in the context of multiscale problems, but the purpose is more general. On a set of prototypical situations, we investigate two critical issues present in many settings: variance reduction techniques to obtain sufficiently accurate results at a limited computational cost when solving PDEs with random coefficients, and finite element techniques that are sufficiently flexible to carry over to geometries with random fluctuations. Some elements of theoretical analysis and numerical analysis are briefly mentioned. Numerical experiments, although simple, provide convincing evidence of the efficiency of the approaches.

1. Introduction

We consider in this review article a series of works [8,9,19,33–35,37,41,42,45], completed in collaboration with some colleagues of ours, that all share the following common denominator. The task to perform is, possibly repeatedly, to approximate numerically the solution to a partial differential equation that has some random character. In most of our works, the equation has the simplest possible form: it is scalar-valued, elliptic, linear, non-degenerate, in divergence form. Typically, and with self-explanatory notations, it reads as

$$-\mathrm{div}\,(a\,\nabla u) = f \tag{1}$$

on a domain $\mathcal{D}$, and for a certain right hand side f. The random character of the problem can be encoded in the coefficient a, and/or in the right-hand side f, and/or in the domain $\mathcal{D}$ itself.

Needless to say, there exist a number of successful approaches to explicitly treat randomness in such partial differential equations. Recent years have witnessed an explosion of the number of methods invented in this extremely lively topic, in particular motivated by the field of *uncertainty quantification*. Stochastic finite elements, spectral methods, sparse tensor products methods, reduced basis techniques, quantization, all methods based one way or another on Karhunen–Loeve, Polynomial Chaos, or other types of similar – or not – economical decompositions of the random functions present in the equation, both as parameters and unknown functions, have been increasingly studied and considerably improved lately. Some accessible general references in the field are the textbooks [25,40]. Review articles on each of the many categories of approaches, such as [49], are also available. The *rationale* behind all these methods is the reduction of the dimension of the

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problem, considered as a problem in a high-dimensional space consisting of the ambient physical space where the original problem is posed *augmented* by the space of approximation for the random dependency. A simplification of the random dependency follows, and the problem becomes amenable to efficient computational techniques. We ourselves have used, in [15], and reviewed, in [14], some of these methods (specifically, reduced basis type methods) in the context of equations with random parameters.

In the present review article, we would like to concentrate on a somewhat alternate strategy: *not attempt to simplify the dependency upon randomness, but embrace the difficulty arising from it*. Of course, this may only be achieved in some specific situations, sufficiently general to be of broad interest, but certainly not covering the immense spectrum of applications in the engineering and life sciences, and perhaps not with the same generic character as the above mentioned general purpose methods. To some extent, the cases we consider must be slightly simpler than, and not as general as, the cases targeted by the above methods. Our ambition and our achievements are more modest. On the other hand, it turns out that the cases we consider arise from a context that brings an additional level of complexity: they originate from multiscale modeling. In that respect, the mix between the presence of randomness, the multiscale feature, and the wish to compute accurately and efficiently lead to an essentially unsolved difficulty (despite the many efforts of outstanding contributors). In multiscale computational science, a number of techniques exist, and are improved constantly. But, most of the times, and despite some overly optimistic claims, they do not marry so well with randomness when it comes to practical computations. Conversely, the extremely efficient toolbox available for random problems has essentially no intersection with multiscale science. Well beyond the somewhat limited purpose of this review article, our intention is thus to attract the attention of the community to the state of the art: *efficiently computing when randomness and many scales are simultaneously present is still an essentially open, considerably challenging, issue*.

1.1. The two situations considered: similarities and differences

We will consider below two prototypical situations. As we mentioned, we encountered both situations in our research efforts devoted to multiscale science, and more precisely in our endeavor to study and improve computational approaches in materials science: (i) the approximation of the homogenized tensor in the context of stochastic numerical homogenization, and (ii) the multiscale finite element computation of the solution to an (harmless) equation posed on a randomly perforated domain.

In both situations, randomness originates from geometry. But, in either situation, geometry is encoded differently in the equation. In (i), it is encoded in the heterogeneities of the coefficient. In contrast, in (ii) it is encoded in the computational domain itself. The similarity of the two problematics is evident. By penalization, the second problem may even be viewed as a particular case of the first problem. However, the techniques we employ are different in nature, and have a different purpose.

The former problem (approximation of the homogenized tensor) consists in the repeated resolution of an elliptic equation (the celebrated "corrector equation") on an as large as possible bounded domain, truncation of the whole space $\mathbb{R}^d$, typically for $d = 2$, or $d = 3$, in practice. The equation is of the above type (1) and will be made explicit below, see (9). The purpose of that repeated solution procedure is to compute an expectation (thus, in practice an empirical mean) from the solutions obtained for various realizations of the local environment (mathematically encoded in the coefficient a of (1)). The reader may think of different microstructures of the material, different inclusions in the medium, etc. The task of computing an average, that is a single, deterministic output, sounds simple. In particular, the very process of averaging, performed here in the context of a stationary ergodic problem (see the details below), is essentially of the same nature as the law of large numbers. This suggests that the random character of the problem progressively vanishes when the number of realizations considered increases. However, the practical Monte Carlo approach (generate random environments and average out an outcome based on the computed solutions) is plagued by variance issues. The rate of convergence of the approximation, in terms of the size of the truncated computational domain asymptotically covering the whole ambient space, is universal. It is dictated by the central limit theorem. The prefactor appearing in the error estimate is related to the variance of the problem. Efficient computational approaches consist in designing tools to reduce that variance, thus the statistical error in the approximation. That error largely dominates the bias (the deterministic part of the error), and thus is the critical quantity that governs the overall quality of the numerical approach. Our series of works addresses various techniques to reduce the variance: antithetic variables, control variate, selection approach, the latter being somewhat in the spirit of stratified sampling. They are imported from several different contexts and are adjusted to the specific context of numerical homogenization.

The latter problem (multiscale finite element computations on randomly perforated domains) differs from the former problem in several respects. As mentioned above, the randomness of the geometry is now encoded not in the coefficients of the equations (which are constant, for simplicity), but in the domain where the equation is posed. We deal with perforations of that domain that are randomly located. Note however that, as briefly mentioned above, the perforations of the domain can be, in the numerical discretization, treated by penalization, in which case the two situations we consider become closer to one another. Another, more substantial, difference is that this second example is a representative case of modern multiscale techniques. In contrast with classical techniques which (i) aim at computing an equivalent "homogenized" medium, and (ii) achieve this in the asymptotic limit of vanishing length scales of the oscillations originally present (this is the case of our former situation), modern techniques attack the multiscale problem (i) directly and (ii) at the actual length scales.