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Reduced basis finite element heterogeneous multiscale method for high-order discretizations of elliptic homogenization problems

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ABSTRACT

A new finite element method for the efficient discretization of elliptic homogenization problems is proposed. These problems, characterized by data varying over a wide range of scales cannot be easily solved by classical numerical methods that need mesh resolution down to the finest scales and multiscale methods capable of capturing the large scale components of the solution on macroscopic meshes are needed. Recently, the finite element heterogeneous multiscale method (FE-HMM) has been proposed for such problems, based on a macroscopic solver with effective data recovered from the solution of micro problems on sampling domains at quadrature points of a macroscopic mesh. Departing from the approach used in the FE-HMM, we show that interpolation techniques based on the reduced basis methodology (an offline-online strategy) allow one to design an efficient numerical method relying only on a small number of accurately computed micro solutions. This new method, called the reduced basis finite element heterogeneous multiscale method (RB-FE-HMM) is significantly more efficient than the FE-HMM for high order macroscopic discretizations and for three-dimensional problems, when the repeated computation of micro problems over the whole computational domain is expensive. A priori error estimates of the RB-FE-HMM are derived. Numerical computations for two and three dimensional problems illustrate the applicability and efficiency of the numerical method.

1. Introduction

The characterization of effective properties of physical processes in heterogeneous media is a basic problem for many applications. We mention for example the study of thermal diffusion or elastic properties in composite materials. As the heterogeneities of the material occur at microscopic scales, usually much smaller than the scale of interest, it is computationally difficult if not impossible to use a standard numerical method (e.g., as the finite element method (FEM), the finite volume method (FVM) or the finite difference method (FDM)) to discretize the physical domain of the composite material going down to the finest scales. A successful theoretical approach for such problems modeled by partial differential equations (PDEs) uses homogenization theory. In this framework, one aims at deriving an effective equation (the homogenized equation) for the PDE under study, where the fine scales have been averaged out [1,2]. However such a strategy cannot be used directly for numerical computations, as the effective parameters are rarely known in explicit form. This has triggered the development of multiscale methods capable of capturing the coarse behavior of the problem without resolving the full fine scale details on the whole computational domain. Among the huge literature available we mention [3–7] and references therein.

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Here we focus on the finite element heterogeneous multiscale method (FE-HMM), a numerical homogenization method developed in the framework of the heterogeneous multiscale method (HMM) proposed in [8]. In a nutshell, these methods rely on a macro partition of the computational domain with effective (homogenized) coefficients recovered (on the fly) from micro problems defined on sampling domains located at quadrature points within each element of the macro partition (see [9] for a recent review of the FE-HMM). As macro and micro meshes have to be refined simultaneously for optimal convergence rates–as shown by the fully discrete error analysis [10]–such methods require a large number of repeated micro computations. This is a common feature shared by any numerical homogenization method. For higher order macro methods (where more sampling domains are required) or three-dimensional problems, these methods can become computationally very expensive (even though order of magnitude cheaper than a full fine scale approach). Attempts to reduce the computational cost have been pursued in [11], where fast micro solvers have been coupled with standard FEM. By selecting a special quadrature formula with integration points on the interfaces of the macro partition, one can also in some situations reduce the computational cost (this does however only reduce the constant in front of the computational cost for the FE-HMM, e.g., a reduction factor of one half is reported in [12] for two dimensional problems with first or second order macro solvers). Finally, by using adaptive strategies, it has been shown in [13,14] that substantial computational savings can be achieved as new micro computations are only required in elements marked for refinement.

In this paper we depart from the classical approach of the FE-HMM which consists in solving a micro problem on a sampling domain at each quadrature point of a macro FEM with numerical integration. In our new approach, a small number of sampling domains located anywhere in the computational domain are computed accurately in an offline stage, following the methodology of reduced basis (RB). A suitable interpolation of these precomputed microsolutions is used in an online stage to compute the macro solution in a cheap and efficient way. We demonstrate that such a strategy allows to design efficient

- numerical homogenization methods with high order macro solvers;
- numerical homogenization methods for three-dimensonal problems.

RB techniques for model reduction, pioneered in [15–17], have seen recently a renewed interest thanks to the development of new sampling techniques and rigorous a posteriori error bounds for outputs of interest [18] (see also [19,20] for additional references on the recent literature). In the context of numerical homogenization, the use of RB was first proposed in [21,22]. We also note that in [23], the RB techniques were used in combination with the multiscale finite element method [3]. While the emphasis in [21,22] was on parametrizing various configurations of cell problems (e.g. inclusion with various shapes, etc.), here, building on [21,22], we focus on integrating the RB methodology in a micro macro FEM such as the FE-HMM. As in the FE-HMM, we compute a macro FEM based on quadrature formula (QF), but do not solve micro FE problems around every integration point of the QF in each macro element. Instead, we select by a greedy procedure a number of representative sampling domains on which we solve accurate micro problems. Their corresponding solutions span the RB space. This procedure is called the offline stage, in the RB terminology, and is usually only done once, as a pre-processing step. In a so-called online stage, the effective solution is obtained from the macro solver of the FE-HMM with effective coefficients recovered from micro problems solved in the RB space. The required data at the macro integration points are now obtained from the solutions of small dimensional linear problems involving suitable interpolations of the precomputed RB space. Unlike the FE-HMM, in the RB-FE-HMM the dimension of the micro linear systems solved in the online stage is *independent* of the macro resolution (e.g., macro meshsize). In turn, there is no need in the RB-FE-HMM to refine simultaneously macro and micro meshes to obtain optimal convergence rates. Thus, expensive micro FE computations as required by the FE-HMM are avoided. High order macroscopic methods can be designed with the same set of RB as used for linear macro FE. As illustrated in numerical experiments, the RB-FE-HMM is particularly suited for high order macro FEM or high dimensional problems for which the cost of the standard FE-HMM justifies (even when a single macroscopic output is required) the overhead of the offline work in the RB methodology.

A priori error analysis including macro error, micro error, resonance error and error coming from the use of the RB is derived. We also show how RB can be used to reconstruct fine scale information on the whole computational domain to approximate the fine scale solution. Such a reconstruction is simpler than the similar procedure for the FE-HMM. Indeed, we do not need to store micro solutions in each sampling domains, nor to implement a periodic extension of the micro solutions in each macro elements, which might be cumbersome, specially for three dimensional problems with simplicial elements.

Our paper is organized as follows. In Section 2, we introduce the homogenization problem and give a short description of the FE-HMM. Section 3 is devoted to our multiscale method, the RB-FE-HMM. The a priori error analysis of the method is presented in Section 4. Finally, various numerical examples in two and three dimensions are presented in Section 5, to illustrate the behavior and the efficiency of the proposed method.

Notation. Let $\Omega \subset \mathbb{R}^d$ be an open set, and $Y = \left(-\frac{1}{2}, \frac{1}{2}\right)^d$. Denote the standard Sobolev Space by $W^{\ell,p}(\Omega)$. For $p = 2$, we sometimes use the notation $W^{\ell,p}(\Omega) = \mathcal{H}^{\ell}(\Omega)$. $\mathcal{H}_0^1(\Omega)$ denotes the closure of $C_0^\infty(\Omega)$ in $\mathcal{H}^1(\Omega)$. We define $\mathcal{H}_{per}^1(Y) := \{g \in \mathcal{H}^1(Y) | g \text{ periodic in } Y\}$. We also have the property that $\mathcal{H}_{per}^1(Y) = \overline{C_{per}^\infty(Y)}$, where $C_{per}^\infty(Y)$ is a subspace of $C^\infty(\mathbb{R}^d)$ of periodic functions in the cube Y. The Frobenius norm of a matrix, denoted by $\|\cdot\|_{\mathcal{F}}$, is defined as $\|A\|_{\mathcal{F}} = \sqrt{\mathrm{trace}(A^T A)}$.