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A time dependent approach for removing the cell boundary error in elliptic homogenization problems

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ABSTRACT

This paper concerns the cell-boundary error present in multiscale algorithms for elliptic homogenization problems. Typical multiscale methods have two essential components: a macro and a micro model. The micro model is used to upscale parameter values which are missing in the macro model. To solve the micro model, boundary conditions are required on the boundary of the microscopic domain. Imposing a naive boundary condition leads to $O(\varepsilon/\eta)$ error in the computation, where ε is the size of the microscopic variations in the media and η is the size of the micro-domain. The removal of this error in modern multiscale algorithms still remains an important open problem. In this paper, we present a time-dependent approach which is general in terms of dimension. We provide a theorem which shows that we have arbitrarily high order convergence rates in terms of ε/η in the periodic setting. Additionally, we present numerical evidence showing that the method improves the $O(\varepsilon/\eta)$ error to $O(\varepsilon)$ in general non-periodic media.

1. Introduction

In the present paper, we are interested in developing a multiscale method for the numerical homogenization of multiscale elliptic PDEs in divergence form:

$$\begin{aligned} -\nabla\cdot\left(A^\varepsilon(\boldsymbol{x})\nabla u^\varepsilon(\boldsymbol{x})\right) &= f(\boldsymbol{x}) \quad \text{in} \quad \Omega, \\ u^\varepsilon(\boldsymbol{x}) &= 0 \quad \text{on} \quad \partial\Omega, \end{aligned} \tag{1}$$

where Ω is an open bounded set in $\mathbb{R}^d$ with $|\Omega| = O(1)$, $\varepsilon \ll 1$ and A^ε is a symmetric, uniformly elliptic and bounded, matrix function in $\mathbb{R}^{d\times d}$ such that for every $\zeta \in \mathbb{R}^d$

$$c_1|\zeta|^2 \leq \sup_{\boldsymbol{x}\in\Omega} \zeta^T A^\varepsilon(\boldsymbol{x})\zeta \leq c_2|\zeta|^2. \tag{2}$$

The multiscale method does not assume any knowledge about the exact form of $A^\varepsilon(\boldsymbol{x})$. However, for the sake of comparison with known analytical results, the numerical examples and theoretical claims in this paper are given mainly in two settings: (a) for periodic media where $A^\varepsilon(\boldsymbol{x}) = A(\boldsymbol{x}/\varepsilon)$ and A is a periodic matrix function in the d-dimensional unit cube $Y := (0,1]^d$, and (b) for locally-periodic media where $A^\varepsilon(\boldsymbol{x}) = A(\boldsymbol{x}, \boldsymbol{x}/\varepsilon)$ and $A(x,\cdot)$ is Y-periodic and $A_{ij} \in C^\infty(\overline{\Omega}\times Y)$. The

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smoothness assumptions are only to simplify the analysis and the method performs equally well under weaker assumptions, e.g. $\partial_x^k A_{ij} \in C(\overline{\Omega}; L^\infty(Y))$ at least for all $k \leq 2$.

The term numerical homogenization is used to mean approximating the homogenized solutions of multiscale PDEs without resolving the small scales over the entire domain. Equation (1) models, for instance, steady heat conduction in heterogeneous media, where ε stands for the length-scale of the microscopic variations in the media. A direct numerical simulation of (1) leads to $O(\varepsilon^{-d})$ degrees of freedom which can not be handled even by the best available computers if ε is very small. The aim of homogenization is to describe the macroscopic behavior of the heterogeneous system (1). The idea behind homogenization theory is to mix the heterogeneities of the media infinitely to obtain a homogeneous system which is no more dependent on ε. Traditional numerical techniques will then be amenable for solving the resulting homogenized system.

From a mathematical point of view, the homogenization of equation (1), for purely periodic or a more realistic locally periodic coefficients is well-known, see e.g. [1–3]. In the periodic setting, as $\varepsilon \to 0$, the solution to (1) tends to the homogenized solution $u^0(\boldsymbol{x})$ which satisfies

$$\begin{aligned} &-\nabla \cdot \left(A^0 \nabla u^0(\boldsymbol{x}) \right) = f(\boldsymbol{x}) \quad \text{in} \quad \Omega, \\ &u^0(\boldsymbol{x}) = 0 \quad \text{on} \quad \partial\Omega. \end{aligned} \tag{3}$$

Here the effective conductivity A^0 is a constant matrix given by

$$A^0_{ij} = \int_Y \left(A_{ij}(\boldsymbol{y}) + \sum_{k=1}^{d} A_{ik} \nabla_{\boldsymbol{y}_k} \chi_j(\boldsymbol{y}) \right) d\boldsymbol{y}, \tag{4}$$

where the cell solutions $\boldsymbol{\chi} = \{\chi_i\}_{i=1}^d$ are Y-periodic functions that solve the following periodic problems:

$$\begin{aligned} &-\nabla \cdot (A(\boldsymbol{y}) \nabla \chi_i(\boldsymbol{y})) = \nabla \cdot A(\boldsymbol{y}) \boldsymbol{e}_i \quad \text{in} \quad Y, \\ &\chi_i(\boldsymbol{y}) \text{ is } Y\text{-periodic}, \quad \int_Y \chi_i(\mathbf{s})\, d\mathbf{s} = 0, \end{aligned} \tag{5}$$

where $\{\boldsymbol{e}_i\}_{i=1}^d$ are the canonical basis vectors in $\mathbb{R}^d$. The above formula is valid for periodic and, with a slight modification, for locally-periodic media. In more general settings, on the other hand, finding the limiting behavior of (1) is difficult and often impossible through existing theory of homogenization.

Numerical homogenization is indispensible in cases when homogenization theory is not adequate for finding the effective parameters of the media. From a numerical homogenization point of view, the focus is to develop computationally cheap methods which are potentially applicable to general settings, where the coefficient $A^\varepsilon(\boldsymbol{x})$ is allowed to have more general oscillations/variations in fast and slow scales. Keeping the generality of the main physical model (1) in mind, it is important then to develop a method which does not assume any knowledge about the form of the coefficient $A^\varepsilon(\boldsymbol{x})$, and at the same time performs optimally when applied to periodic and locally-periodic media.

1.1. The heterogeneous multiscale methods

E and Engquist [4], proposed the Heterogeneous Multiscale Methods (HMM) framework as a general methodology for capturing the global/average behavior of multiscale and possibly multi-physics problems. HMM is often very useful when we have a full description of the microscopic model. The idea is to avoid resolving the small scale details all over the domain, at the expense of targeting only an average behavior of the system. Multiscale PDEs such as (1) is within the application areas of HMM. In a typical HMM-based multiscale method, one starts by assuming a macroscopic model with some unknown data. The macroscopic model is discretized through standard finite difference (FD) or finite element methods (FEM) on a coarse mesh. Therefore, one needs the missing data on discrete points of the macro grid. These unknown data have local origin, which in turn is extracted from microscopic simulations performed over boxes of size $\eta = O(\varepsilon)$, where ε represents the size of the small scale in the problem. Already here, we see that HMM exploits the scale separation featured in the main problem (1). In other words, since $\varepsilon \ll 1$, we can set $\eta = O(\varepsilon)$ and therefore the computational cost of the micro simulations will not increase by decreasing ε. It is important to note that the microscopic simulations should be consistent with the current macroscopic data. This is achieved by restricting the microscopic simulations by the coarse-scale information. The overall computational cost of this HMM-based algorithm will then be NC_{micro}, where N is the number of macro grid points and C_{micro} is the cost of performing a single micro simulation, which can be made essentially independent of ε by using high order methods, cf. [5]. For other approaches to decrease the computational burden in linear and quasi-linear elliptic multiscale PDEs see e.g. [6–8].

Now assume that $\Omega = (0,1)^d$. The macro model for a standard HMM-type algorithm for problem (1) is

$$\text{Macro problem:} \quad \begin{aligned} &-\nabla \cdot \boldsymbol{F}(\boldsymbol{x}, \nabla U) = f(\boldsymbol{x}) \text{ in } \Omega \\ &U = 0 \text{ on } \partial\Omega. \end{aligned} \tag{6}$$