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ANALYSIS OF MULTISCALE METHODS *[1)]

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Dedicated to Professor Zhong-ci Shi on the occasion of his 70th birthday

Abstract

The heterogeneous multiscale method gives a general framework for the analysis of multiscale methods. In this paper, we demonstrate this by applying this framework to two canonical problems: The elliptic problem with multiscale coefficients and the quasicontinuum method.

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1. Introduction

In recent years we have seen a tremendous growth of activity on multiscale modelling and computation. Many of these problems and numerical algorithms involve multi-physics [16], i.e. the models at different scales are of very different nature, for example, molecular dynamics at the microscale and continuum mechanics at the macroscale. By coupling the macro-scale and micro-scale models, one hopes to obtain numerical algorithms that have the accuracy of microscale models at a cost comparable to the macroscale models. Many methods have been developed along these lines, including the Car-Parrinello method [12], the quasicontinuum method [39, 27] and more recently the heterogeneous multiscale method (HMM) [15].

The analysis of multiscale methods presents new challenges in numerical analysis. This is particularly true when multi-physics is involved. First of all, there is the issue of what one should take as the "exact solution" that the numerical solution should be compared with. Since multiscale methods typically involve several different components, the error also has several different contributions. Therefore one important point in the analysis of these methods is to be able to separate out these different contributions.

The framework of the heterogeneous multiscale method provides a general strategy both for the design and the analysis of multiscale methods. In this article we will discuss the application of HMM to two different problems. The first is the elliptic PDE with multiscale coefficients. The second is the quasicontinuum method for crystalline solids. We will focus on the analysis of these methods. For other applications and analysis of HMM, we refer to [32].

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2. General Strategy for the Analysis of Multiscale Methods

A general principle for analyzing HMM has been established in [15] and later elaborated in [17, 19, 34] on a variety of homogenization problems, ODEs [14] and stochastic ODEs [18, 41], and on quasicontinuum methods [21]. The common feature of all these problems is that there exists a closed macroscopic model, which may not be explicitly available or are very inefficient to use directly in numerical computations. We can then design multiscale methods using the microscale model and known qualitative features of the macroscale process in order to capture efficiently the macroscale behavior.

There are two main ingredients in HMM: An overall macroscopic scheme for the macroscopic state variable U, and estimating the missing macroscopic data by the microscopic model. Even though the HMM procedure is far more general, rigorous error estimates can only be expected in cases for which a lot is known about the macroscale model, even though it is not explicitly used in the numerical methods.

To analyze HMM, we begin by defining a macroscopic approximation method with the same macroscopic solver as that in HMM. The error between this approximate solution and the macroscopic solution can be analyzed using standard numerical analysis techniques (see [13] for finite element methods, [37] for finite difference methods, [24] for finite volume methods, and [1] for discontinuous Galerkin methods). Next we estimate the error between the HMM solution and the approximate solution of the macroscopic model, due to the fact some of the macroscopic data are estimated using the microscopic model, instead of being given by the macroscopic model itself, this gives us a general statement of the following type:

$$\|U - U_{\mathrm{HMM}}\| \leq C\big(H^k + e(\mathrm{HMM})\big), \tag{2.1}$$

where U_{HMM} is the HMM solution, U is the exact solution of the macroscopic model, k is the order of the macroscopic solver, and H is the step size of the macroscale numerical grid. The norm $\|\cdot\|$ should be chosen according to the specific problem at hand. The second term $e(\mathrm{HMM})$ is the new source of error due to the data estimation. Typically, the error $e(\mathrm{HMM})$ depends on the rate of relaxation of the microscopic state to the local equilibrium, the accuracy of the microscopic solver, and the accuracy of the data-processing step.

Observe that (2.1) bears some similarity to *Strang's Lemma* in finite element methods [13].

3. Application to the Elliptic Homogenization Problem

Consider the classical elliptic problem

$$\begin{cases} -\operatorname{div}\big(a^\varepsilon(x)\nabla u^\varepsilon(x)\big) = f(x) & x \in D \subset \mathbb{R}^d, \\ u^\varepsilon(x) = 0 & x \in \partial D. \end{cases} \tag{3.1}$$

Here ε is a small parameter that signifies the multiscale nature of the coefficient $a^\varepsilon(x)$. Several classical multiscale methodologies have been developed for the numerical solution of (3.1), the most well-known among which is the multigrid technique [10]. These classical multiscale methods are designed to resolve the details of the fine scale problem and are applicable for general problems, i.e., no special assumptions are required for the coefficient $a^\varepsilon(x)$. In contrast modern multiscale methods are designed specifically for recovering partial information about u^ε at a sublinear cost, i.e. the total cost grows sublinearly with the cost of solving the fine scale problem [16]. This is only possible by exploring the special features that $a^\varepsilon(x)$ might have, such as scale separation or self-similarity. The simplest example is when $a^\varepsilon(x) = a(x, x/\varepsilon)$, where $a(x, y)$ can either be periodic in y, in which case we assume the period to be $I = [-1/2, 1/2]^d$, or random but stationary under shifts in y, for each fixed $x \in D$. In both cases, it has been shown that [5, 36]

$$\|u^\varepsilon(x) - U(x)\|_{L^2(D)} \to 0, \tag{3.2}$$