Developing Multiscale Methodologies for Computational Fluid Mechanics

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Contents

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Abstract

The development of multiscale computational methods is a key research area in mathematics, physics, engineering and computer science. Engineers and scientists often perform detailed microscale computational simulations of a large scale complicated spatio-temporal system. For most problems of practical interest, there are two major complications in simulating the dynamical behaviour on large macroscopic space-time scales. The first is the often prohibitive computational cost when only a microscopic model is available. The second complication is the memory constraints which often make the simulation over the whole domain of interest infeasible. To overcome these obstacles, the equation-free approach was proposed by Keverkidis and colleagues in 2000. This approach is a multiscale method for capturing the behaviour on large scales of some complicated systems using only relatively small bursts of the microscale models. The patch dynamics scheme was proposed as an essential component of the equation-free framework. The patch scheme promises a great saving in computation time by predicting the macroscopic dynamics using detailed microscopic computation only on relatively small widely distributed patches of the spatial domain. This thesis provides mathematical analysis and computational simulation of some basic atom dynamics on small patches. The most significant novel result of this research is that patches with microscale periodic boundary conditions can be used to efficiently predict macroscale properties of interest. This result is important because microscale computations are often easiest with microscale periodic boundary conditions. As a major test of the approach, we analyse, implement and evaluate such a scheme for a computationally intensive atomistic simulation.

Chapter 1 of this dissertation introduces the challenge of multiscale problems and highlights some recent developments of multiscale methods for complex systems. Chapter 2 explores atomistic simulations in three-dimensional space. The microscale atomistic simulator is used to predict a macroscale temperature field. This is achieved by performing atomistic simulation on a small triply-periodic patch. The method uses locally averaged properties

over small space-time scales to advance and predict relatively large space scale dynamics. Our ultimate aim for this chapter is to explore the macroscopic properties of a system through atomistic simulation in small periodic patches, but as a pilot study this thesis only considers one small patch coupled over the macroscale to boundaries. The computation is implemented only on the periodic patch, while over most of the domain we interpolate in order to predict the macroscale temperature. The thesis develops appropriate control terms to the microscale action regions of the patch. The control is applied to the left and right action regions surrounding a core region. A proportional controller dependent upon the relatively distant boundaries enables reasonably accurate macroscale predictions. The analysis and computational simulations indicate that this innovative patch scheme empowers computation of large scale simulations of microscale systems.

Chapter 3 analyses the case of a one-dimensional microscale diffusion system in a single microscale patch to predict the macroscale dynamics over a comparatively large spatial region. The nature of the solutions of the patch scheme is explored when operating with time-varying boundary conditions that mimic coupling with neighbouring, dynamically varying patches. The patch eigenfunctions and their adjoints form a biorthogonal basis to determine the spectral coefficients in formal series solutions. We also explore this patch scheme with time delays in the communication of boundary values. This models a patch when information from the neighbouring patches is subject to communication delays. The delayed patch scheme prediction is compared with a scheme without delays to delineate when such delays are significant.

Chapter 4 analyses diffusion dynamics on multiple coupled patches. Centre manifold theory supports the patch scheme. The patch coupling conditions are standard Lagrange interpolation from the macroscale values at the centre of surrounding patches to the boundaries of each patch. The results of this chapter demonstrate the feasibility of the microscale patch scheme to model diffusion over large spatial scales.

Chapter 5 extends the analysis to one-dimensional microscale advection-diffusion dynamics in a single patch and for multiple patches. Eigenvalue analysis suggests that a slow manifold exists on the macroscale. Computer algebra constructs the slow manifold model for the advection-diffusion dynamics. The long-time dynamics behaviour of numerical solutions on one patch is compared with the prediction of the slow manifold. Comparisons among the patch dynamics scheme, the microscale model over the complete domain, and published experimental data determines regimes where the patch dynamics accurately predicts the large scale advection-diffusion dynamics.