

Developing Multiscale Methodologies for Computational Fluid Mechanics

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Contents

Signed Statement	vi
Acknowledgements	vii
Abstract	viii
1 Introduction	1
1.1 Multiscale methods	1
1.2 A new class of multiscale methods	3
1.2.1 The equation-free approach	3
1.2.2 The gap-tooth scheme	5
1.2.3 Patch scheme	7
1.3 Atomistic simulations	8
1.4 Centre manifold theory	10
1.5 Overview and contributions	10
2 A periodic patch scheme in atomistic simulations	12
2.1 An isolated triply-periodic patch	16
2.2 Equations of motion	17
2.2.1 The inter-atomic potential energy	17
2.2.2 Non-dimensionalisation of the variables	19
2.2.3 Numerical integration of the equations of motion	20
2.2.4 Periodic boundary conditions	21
2.3 Couple patches with a proportional controller	22
2.3.1 Coupling atomistic simulations	25
2.3.2 Numerical simulations verify the validity of the proportional control	27
2.4 Analyse optimal control for a single patch	29
2.4.1 An eigenproblem of the controlled patch scheme	31
2.4.2 Symmetric eigenfunctions	31
2.4.3 Antisymmetric eigenfunctions	36

2.5	A spectral gap generally exists	41
2.5.1	Numerical eigenvalue analysis of a controlled patch verifies derived exact eigenvalues	46
2.5.2	Approximation to the eigenvalue of macroscale interest	48
2.5.3	Determining optimal forcing control for a single patch .	50
2.6	Estimate the diffusivity	51
2.7	Conclusion	60
3	One patch scheme for diffusion with time-varying boundary forcing	62
3.1	Patch boundary conditions	63
3.2	Solving the homogeneous equation	65
3.2.1	The spectrum	65
3.3	Non-homogeneous problem	66
3.3.1	The biorthogonal eigenfunction expansion	67
3.3.2	Determining the spectral sine coefficients	68
3.3.3	Determining the spectral cosine coefficients	69
3.4	Eigenfunctions of the adjoint operator	71
3.4.1	Case in which n is even	72
3.4.2	Case in which n is odd	73
3.4.3	The spectral coefficients d_n	73
3.4.4	Finding the coefficients for $r = 1$	76
3.5	Constructing the formal solution	79
3.5.1	The eigenvalue of macroscale interest	80
3.5.2	Analyse the long-time behaviour of the patch dynamics solutions	82
3.6	Patch dynamics with time-delayed communications	87
3.6.1	Parabolic interpolation provides patch boundary values	89
3.6.2	Homogeneous boundary conditions	90
3.6.3	Analyse the forced patch dynamics	91
3.7	Conclusion	93
4	Multiple patches for diffusion with time-varying boundary forcing	95
4.1	Divide the macroscale domain into small patches	96
4.1.1	Couple multiple patches across the whole domain	97
4.1.2	Existence of slow manifold and initial approximation .	103
4.1.3	Computer algebra constructs the slow manifold	106
4.1.4	Model physical boundary conditions at a grid point . .	107
4.1.5	Time-varying boundary values	110

4.2	Comparison between slow manifold predictions and analytical solutions to diffusion dynamics	111
4.2.1	Evolution equations with constant and varying boundary forcing	111
4.2.2	Analytical solution for diffusion equation	112
4.3	Conclusion	118
5	Multiscale modeling couples patches of advection-diffusion equations	120
5.1	One patch boundary conditions	122
5.2	Real homogeneous eigenfunctions	123
5.3	Complicated eigenspectrum	124
5.3.1	Complex eigenvalues of faster advection	129
5.4	A spectral representation of the solution within a patch	132
5.4.1	Determining the spectral coefficients	133
5.4.2	Eigenfunctions of the adjoint operator	134
5.4.3	Case n is even	136
5.4.4	Case n is odd	138
5.4.5	The spectral coefficients a_n	138
5.4.6	The spectral coefficients b_n	142
5.5	Constructing the formal solution	145
5.6	Multiple patches across the whole domain	151
5.6.1	The microscale simulator	152
5.6.2	Coupling microscale patches across gaps	152
5.6.3	Centre manifold theory supports multiscale models	154
5.6.4	Computer algebra constructs the slow manifold	160
5.7	Numerical validation of analytical computation of the eigenvalues	161
5.8	Nonlinear reaction-diffusion equations	166
5.8.1	Existence of slow manifold and initial approximation	168
5.8.2	The first approximation of the slow manifold	169
5.8.3	Varying boundary values with time	171
5.8.4	Method of lines	171
5.8.5	Comparison of the long time behaviour	173
5.8.6	Evaluation of quantitative error	177
5.9	Conclusion	178
6	Conclusion	180
6.1	Summary of the periodic atomistic patch simulations	180
6.2	Summary of analysed patch dynamics scheme for different classes of PDEs	181

6.3	Future directions	183
A	Ancillary material	185
A.1	Code for 3D atom simulation	185
A.1.1	Main driver code	185
A.1.2	Interpose periodicity on positions	186
A.1.3	Time derivatives of position and velocity	187
A.2	Code to compute many realisations	188
A.2.1	Main driver code	189
A.2.2	Interpose periodicity on positions	190
A.2.3	Time derivative	191
A.3	Results of 58 computational simulations	192
B	Reduce programs	194
B.1	Computer algebra code constructs the slow manifold of the diffusion PDEs	194
B.1.1	Construct the slow manifold model with physical boundary conditions	197
B.2	Construct the slow manifold of advection-diffusion and reaction-diffusion equations	199
	Bibliography	202

Signed Statement

I certify that this work contains no material which has been accepted for the award of any other degree or diploma in my name, in any university or other tertiary institution and, to the best of my knowledge and belief, contains no material previously published or written by another person, except where due reference has been made in the text. In addition, I certify that no part of this work will, in the future, be used in a submission in my name, for any other degree or diploma in any university or other tertiary institution without the prior approval of the University of Adelaide and where applicable, any partner institution responsible for the joint-award of this degree. I give consent to this copy of my thesis, when deposited in the University Library, being made available for loan and photocopying, subject to the provisions of the Copyright Act 1968. I also give permission for the digital version of my thesis to be made available on the web, via the Universitys digital research repository, the Library Search and also through web search engines, unless permission has been granted by the University to restrict access for a period of time.

Signed: Hammad Alotaibi

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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 Kevrekidis 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.