Multiscale modelling of continuum and discrete dynamics in materials with complicated microstructure

PhD Thesis

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Abstract

Homogenization and other multiscale modelling techniques empower scientist and engineers to build efficient macroscale mathematical models for simulating materials with complicated microstructure. But the modelling methodology rarely systematically derives the boundary conditions for macroscale model. This thesis aims to systematically derive boundary conditions for macroscale models without heuristic arguments.

I start by building a smooth macroscale model for a one-dimensional discrete diffusion system with rapidly varying microscale diffusivity, finite scale separation, and Dirichlet boundary conditions. I apply both centre manifold theory and homogenization theory to build the macroscale model. Both theories find same macroscale model. I then apply modern dynamical system theory to derive macroscopic boundary conditions for this class of diffusion problems. The results suggest a specific Robin boundary condition is a good choice for the macroscale model.

I extend my methodology to a linear two-strand diffusion problem. My method finds macroscale boundary conditions for the microscale two-strand problem with different classes of microscale boundary conditions such as specified flux and mixed microscale boundary conditions. The two-strand problem has a more complicated eigen structure than the single strand problems but my method performs well. I also show this method is suitable for continuous problems, such as a class of continuous heterogeneous wave partial differential equations. Furthermore, I apply this technique to wave equations with periodic elasticities and densities and with arbitrary periodicity and number of strands. The algebra in these problem is tedious so I extensively implement computer algebra to find the corresponding macroscale models and boundary conditions. Finally, I consider nonlinearity by analysing the macroscale modelling and the derivation of macroscale boundary conditions for a nonlinear heat exchanger.

The proposed technique provides a systematic tool for deriving macroscale boundary conditions for multiscale models. In comparison with heuristically proposed boundary conditions, my derived boundary conditions improve the accuracy of multiscale models in physical science and engineering.

Plagiarism declaration

This work contains no material which has been accepted for the award of any other degree or diploma 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.

I consent to this copy of my thesis, when deposited in the University Library, being available for loan and photocopying.

SIGNED: .... DATE: ....

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Dedication

This thesis is dedicated to my parents who always encourage me to seek higher education when possible. Without them standing behind me, I would not consider a career as a mathematician and then I would not have a chance to spend these wonderful three years with Prof Tony Roberts and Dr Judith Bunder in the University of Adelaide.

这篇论文献给我的爸爸妈妈—支持我静心探索科学之美的人，没有他们的鼎力支持和暖心鼓励，我可能不会选择在这条路上追求至今，更不会拥有和Prof Tony Roberts以及Dr Judith Bunder在阿德莱德大学共同度过的绚烂三年。

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