

PRINCIPLES OF MULTISCALE MODELING

Physical phenomena can be modeled at varying degrees of complexity and at different scales. Multiscale modeling provides a framework, based on fundamental principles, for constructing mathematical and computational models of such phenomena, by examining the connection between models at different scales.

This book, by one of the leading contributors to the field, is the first to provide a unified treatment of the subject, covering, in a systematic way, the general principles of multiscale models, algorithms, and analysis. The book begins with a discussion of the analytical techniques in multiscale analysis, including matched asymptotics, averaging, homogenization, renormalization group methods, and the Mori–Zwanzig formalism. A summary of the classical numerical techniques that use multiscale ideas is also provided. This is followed by a discussion of the physical principles and physical laws at different scales. The author then focuses on the two most typical applications of multiscale modeling: capturing macroscale behavior and resolving local events. The treatment is complemented by chapters that deal with more specific problems, ranging from differential equations with multiscale coefficients to time scale problems and rare events. Each chapter ends with an extensive list of references to which the reader can refer for further details.

Throughout, the author strikes a balance between precision and accessibility, providing sufficient detail to enable the reader to understand the underlying principles without allowing technicalities to get in the way. Whenever possible, simple examples are used to illustrate the underlying ideas.

WEINAN E's research is concerned with developing and exploring the mathematical framework and computational algorithms needed to address problems that arise in the study of various scientific and engineering disciplines, ranging from mechanics to materials science to chemistry. He has held positions at New York University, the Institute for Advanced Study in Princeton, Peking University, and Princeton University, where he currently is Professor in the Department of Mathematics and in the Program in Applied and Computational Mathematics. His research has been recognized by numerous awards, including the 2003 Collatz Prize of ICIAM, and the 2009 Ralph E. Kleinman Prize, from SIAM.

Cambridge University Press
978-1-107-09654-7 - Principles of Multiscale Modeling
Weinan E
Frontmatter
[More information](#)

PRINCIPLES OF MULTISCALE MODELING

WEINAN E
Princeton University



Cambridge University Press
978-1-107-09654-7 - Principles of Multiscale Modeling
Weinan E
Frontmatter
[More information](#)

CAMBRIDGE UNIVERSITY PRESS
Cambridge, New York, Melbourne, Madrid, Cape Town,
Singapore, São Paulo, Delhi, Tokyo, Mexico City

Cambridge University Press
The Edinburgh Building, Cambridge CB2 8RU, UK

Published in the United States of America by Cambridge University Press, New York

www.cambridge.org
Information on this title: www.cambridge.org/9781107096547

© Weinan E 2011

This publication is in copyright. Subject to statutory exception
and to the provisions of relevant collective licensing agreements,
no reproduction of any part may take place without the written
permission of Cambridge University Press.

First published 2011

Printed in the United Kingdom at the University Press, Cambridge

A catalogue record for this publication is available from the British Library

ISBN 978-1-107-09654-7 Hardback

Cambridge University Press has no responsibility for the persistence or
accuracy of URLs for external or third-party internet websites referred to
in this publication, and does not guarantee that any content on such
websites is, or will remain, accurate or appropriate.

Contents

<i>Preface</i>	<i>page</i> xii
1 Introduction	1
1.1 Examples of multiscale problems	1
1.1.1 Multiscale data and their representation	2
1.1.2 Differential equations with multiscale data	2
1.1.3 Differential equations with small parameters	4
1.2 Multi-physics problems	5
1.2.1 Examples of scale-dependent phenomena	5
1.2.2 Deficiencies of the traditional approaches to modeling	7
1.2.3 The multi-physics modeling hierarchy	10
1.3 Analytical methods	12
1.4 Numerical methods	13
1.4.1 Linear scaling algorithms	13
1.4.2 Sublinear scaling algorithms	13
1.4.3 Type A and type B multiscale problems	14
1.4.4 Concurrent versus sequential coupling	15
1.5 What are the main challenges?	17
1.6 Notes	19
References for Chapter 1	21
2 Analytical methods	25
2.1 Matched asymptotics	26
2.1.1 A simple advection–diffusion equation	26
2.1.2 Boundary layers in incompressible flows	28

vi	<i>Contents</i>	
	2.1.3 Structure and dynamics of shocks	30
	2.1.4 Transition layers in the Allen–Cahn equation	32
2.2	The WKB method	35
2.3	Averaging methods	37
	2.3.1 Oscillatory problems	38
	2.3.2 Stochastic ordinary differential equations	41
	2.3.3 Stochastic simulation algorithms	46
2.4	Multiscale expansions	54
	2.4.1 Removing secular terms	54
	2.4.2 Homogenization of elliptic equations	56
	2.4.3 Homogenization of the Hamilton–Jacobi equations	60
	2.4.4 Flows in porous media	63
2.5	Scaling and self-similar solutions	64
	2.5.1 Dimensional analysis	65
	2.5.2 Self-similar solutions of PDEs	66
2.6	Renormalization group analysis	70
	2.6.1 The Ising model and critical exponents	70
	2.6.2 An illustration of the renormalization transformation	74
	2.6.3 Renormalization group analysis of the two-dimensional Ising model	76
	2.6.4 A PDE example	80
2.7	The Mori–Zwanzig formalism	82
2.8	Notes	86
	References for Chapter 2	87
3	Classical multiscale algorithms	90
	3.1 Multigrid method	90
	3.2 Fast summation methods	99
	3.2.1 Low-rank kernels	100
	3.2.2 Hierarchical algorithms	103
	3.2.3 The fast multipole method	107
	3.3 Adaptive mesh refinement	110
	3.3.1 <i>A posteriori</i> error estimates and local error indicators	111
	3.3.2 The moving mesh method	113

	<i>Contents</i>	vii
3.4	Domain decomposition methods	115
3.4.1	Nonoverlapping domain decomposition methods	115
3.4.2	Overlapping domain decomposition methods	118
3.5	Multiscale representation	119
3.5.1	Hierarchical bases	120
3.5.2	Multi-resolution analysis and wavelet bases	122
3.5.3	Examples	124
3.6	Notes	129
	References for Chapter 3	129
4	The hierarchy of physical models	132
4.1	Continuum mechanics	133
4.1.1	Stress and strain in solids	136
4.1.2	Variational principles in elasticity theory	138
4.1.3	Conservation laws	141
4.1.4	Dynamic theory of solids and thermoelasticity	144
4.1.5	Dynamics of fluids	147
4.2	Molecular dynamics	150
4.2.1	Empirical potentials	151
4.2.2	Equilibrium states and ensembles	156
4.2.3	The elastic continuum limit; the Cauchy–Born rule	158
4.2.4	Nonequilibrium theory	163
4.2.5	Linear response theory and the Green–Kubo formula	166
4.3	Kinetic theory	167
4.3.1	The BBGKY hierarchy	168
4.3.2	The Boltzmann equation	170
4.3.3	The equilibrium states	173
4.3.4	Macroscopic conservation laws	176
4.3.5	The hydrodynamic regime	178
4.3.6	Other kinetic models	181
4.4	Electronic structure models	181
4.4.1	The quantum many-body problem	182
4.4.2	Hartree and Hartree–Fock approximations	185
4.4.3	Density functional theory	187
4.4.4	Tight-binding models	193

4.5	Notes	198
	References for Chapter 4	198
5	Examples of multi-physics models	201
5.1	Brownian dynamics models of polymer fluids	202
5.2	Extensions of the Cauchy–Born rule	210
5.2.1	High-order, exponential and local Cauchy–Born rules	211
5.2.2	An example of a one-dimensional chain	211
5.2.3	Sheets and nanotubes	213
5.3	The moving contact line problem	216
5.3.1	Classical continuum theory	217
5.3.2	Improved continuum models	219
5.3.3	Measuring the boundary conditions using molecular dynamics	224
5.4	Notes	227
	References for Chapter 5	228
6	Capturing the macroscale behavior	232
6.1	Some classical examples	235
6.1.1	Car–Parrinello molecular dynamics	235
6.1.2	The quasicontinuum method	237
6.1.3	Kinetic schemes	239
6.1.4	Cloud-resolving convection parametrization	242
6.2	The multigrid and equation-free approaches	243
6.2.1	Extended multigrid method	243
6.2.2	The equation-free approach	245
6.3	The heterogeneous multiscale method	248
6.3.1	The main components of the method	248
6.3.2	Simulating gas dynamics using molecular dynamics	252
6.3.3	The classical examples from the HMM viewpoint	255
6.3.4	Modifying traditional algorithms to handle multiscale problems	257
6.4	Some general remarks	258
6.4.1	Similarities and differences	258
6.4.2	Difficulties with the three approaches	260
6.5	Seamless coupling	262

	<i>Contents</i>	ix
6.6	Application to fluids	269
6.7	Stability, accuracy and efficiency	278
6.7.1	The heterogeneous multiscale method	279
6.7.2	The boosting algorithm	282
6.7.3	The equation-free approach	284
6.8	Notes	287
	References for Chapter 6	291
7	Resolving local events or singularities	296
7.1	Domain decomposition method for type A problems	297
7.1.1	Energy-based formulation	298
7.1.2	Dynamic atomistic and continuum methods for solids	301
7.1.3	Coupled atomistic and continuum methods for fluids	302
7.2	Adaptive model refinement or model reduction	305
7.2.1	The nonlocal quasicontinuum method	306
7.2.2	Coupled gas-dynamic-kinetic models	310
7.3	The heterogeneous multiscale method	312
7.4	Stability issues	315
7.5	Consistency questions illustrated using nonlocal QC	320
7.5.1	The appearance of the ghost force	322
7.5.2	Removing the ghost force	323
7.5.3	Truncation error analysis	324
7.6	Notes	327
	References for Chapter 7	329
8	Elliptic equations with multiscale coefficients	334
8.1	Introduction	334
8.2	Multiscale finite element methods	337
8.2.1	The generalized finite element method	337
8.2.2	Residual-free bubbles	338
8.2.3	Variational multiscale method	340
8.2.4	Multiscale basis functions	342
8.2.5	Relations between the various methods	344
8.3	Upscaling via successive elimination of fine-scale components	345
8.4	Sublinear scaling algorithms	349
8.4.1	Finite element HMM	350

8.4.2	The local microscale problem	352
8.4.3	Error estimates	355
8.4.4	Information about the gradients	356
8.5	Notes	357
	References for Chapter 8	363
9	Problems that have multiple time scales	368
9.1	ODEs with disparate time scales	368
9.1.1	General setup for limit theorems	368
9.1.2	Implicit methods	371
9.1.3	Stabilized Runge–Kutta methods	372
9.1.4	Heterogeneous multiscale method	378
9.2	Application of HMM to stochastic simulation algorithms	379
9.3	Coarse-grained molecular dynamics	386
9.4	Notes	393
	References for Chapter 9	393
10	Rare events	397
10.1	Introduction	397
10.2	Theoretical background	402
10.2.1	Metastable states and reduction to Markov chains	402
10.2.2	Transition state theory	403
10.2.3	Large-deviation theory	405
10.2.4	First-exit times	409
10.2.5	Transition path theory	415
10.3	Numerical algorithms	425
10.3.1	Finding transition states	425
10.3.2	Finding the minimal energy path	427
10.3.3	Finding the transition path ensemble or the transition tubes	433
10.4	Accelerated dynamics and sampling methods	438
10.4.1	TST-based acceleration techniques	438
10.4.2	Metadynamics	440
10.4.3	Temperature-accelerated molecular dynamics	441
10.5	Notes	442
	References for Chapter 10	443

	<i>Contents</i>	xi
11	Other perspectives	448
11.1	Open problems	448
11.1.1	Variational model reduction	450
11.1.2	Modeling memory effects	455
	References for Chapter 11	459
	<i>Subject index</i>	461

Preface

Traditional approaches to modeling focus on one scale. If our interest is the macroscale behavior of a system in an engineering application, we model the effect of the smaller scales by some constitutive relations. If our interest is in the detailed microscopic mechanism of a process, we assume that there is nothing interesting happening at the larger scales, for example, that the process is homogeneous at larger scales.

Take the example of solids. Engineers have long been interested in the macroscale behavior of solids. They use continuum models and represent atomistic effects by constitutive relations. Solid state physicists, however, are more interested in the behavior of solids at the atomic or electronic level, often working under the assumption that the relevant processes are homogeneous at the macroscopic scale. As a result, engineers are able to design structures and bridges without acquiring much understanding about the origins of the cohesion between the atoms in the material. Solid state physicists can provide such an understanding at a fundamental level. But they are often quite helpless when faced with a real engineering problem.

The relevant constitutive relations, which play a key role in modeling, are often obtained empirically, on the basis of very simple ideas such as linearization, Taylor expansion and symmetry. It is remarkable that such a simple-minded approach has had so much success: most of what we know in the applied sciences and virtually all of what we know in engineering is obtained using such an approach. Indeed the hallmark of deep physical insight has been the ability to describe complex phenomena using simple ideas. When successful, we hail such a work as “a stroke of genius,” as we often describe Landau’s work, say.

A very good example of a constitutive relation is that for simple or Newtonian fluids, which is obtained using only linearization and symmetry and gives rise to the well-known Navier–Stokes equations. It is quite amazing that such a linear constitutive relation can describe almost all the phenomena of simple fluids, which are often very nonlinear, with remarkable accuracy.

However, extending these simple empirical approaches to more complex systems has proven to be a difficult task. A good example is complex fluids or non-Newtonian fluids – that is, fluids whose molecular structure has a non-trivial effect on its macroscopic behavior. After many years of effort, the results of trying to obtain the constitutive relations for such fluids by guesswork or by fitting a small set of experimental data are quite mixed. In many cases, either the functional form becomes too complicated or there are too many parameters to fit. Overall, empirical approaches have had limited success for complex systems or for small-scale systems in which the discrete or finite-size effects are important.

The other extreme is to start from first principles. As was recognized by Dirac immediately after the birth of quantum mechanics, almost all the physical processes that arise in applied sciences and engineering can be modeled accurately using the principles of quantum mechanics. Dirac also recognized the difficulty of such an approach, namely, the mathematical complexity of quantum mechanics principles is so great that it is quite impossible to use them directly to study realistic chemistry or, more generally, engineering problems. This is true not just for the true first principle, the quantum many-body problem, but also for other microscopic models such as those in molecular dynamics.

This is where multiscale modeling comes in. By considering simultaneously models at different scales we hope to develop an approach that shares the efficiency of the macroscopic models as well as the accuracy of the microscopic models. This idea is far from new. After all, there have been considerable efforts to try to understand the relations between microscopic and macroscopic models; for example, computing from molecular dynamics models the transport coefficients needed in continuum models. There have also been several classical success stories of combining physical models at different levels of detail for the efficient and accurate modeling of complex processes of interest. Two of the best known examples are the quantum-mechanics–molecular-mechanics (QM–MM) approach in chemistry and the Car–Parrinello molecular

dynamics. The former is a procedure for modeling chemical reactions involving large molecules, by combining quantum mechanics models in the reaction region and classical models elsewhere. The latter is a way of performing molecular dynamics simulations using forces that are calculated from electronic structure models “on-the-fly,” instead of using empirical interatomic potentials. What has prompted the increase in interest in recent years in multiscale modeling is the recognition that such a philosophy is useful for all areas of science and engineering, not just chemistry and material science. Indeed, compared with the traditional approach of focusing on one scale, looking at a problem simultaneously from several different scales and different levels of detail could be said to be a more mature way of constructing models. It represents a fundamental change in the way we view modeling.

The multiscale multi-physics viewpoint opens up unprecedented opportunities for modeling. It provides the opportunity to put engineering models on a solid footing. It allows us to connect engineering applications with basic science. It offers a more unified view of modeling, by focusing more on the different levels of application of physical laws and the relations between them, with specific applications as examples. In this way we will find that our approaches to solids and fluids are very much parallel to each other, as we explain later in the book.

Despite the exciting opportunities offered by multiscale modeling, one thing we have learned during the past decade is that we should not expect quick results. Many fundamental issues have to be addressed before its expected impact becomes a reality. These issues include:

- (1) a detailed understanding of the relation between the different levels of physical models;
- (2) boundary conditions for atomistic models such as molecular dynamics;
- (3) systematic and accurate coarse-graining procedures.

Without properly addressing these and other fundamental issues, we run the risk of simply replacing one set of ad hoc models by another, or by ad hoc numerical algorithms. This would hardly be a step forward.

This volume is intended to present a systematic discussion of the basic ideas in multiscale modeling. The emphasis is on the fundamental principles and common issues, not on specific applications. Selecting the materials to be covered proved to be a very difficult task since the subject

Preface

xv

is so vast and, at the same time, quickly evolving. When deciding what should be included in this volume, I asked the following question: what are the basics that one has to know in order to get a global picture about multiscale modeling? Since multiscale modeling touches upon almost every aspect of modeling in almost every scientific discipline, it is inevitable that some discussions are very brief and some important aspects are neglected entirely. Nevertheless, we have tried to make sure that the fundamental issues are indeed covered.

The book can be divided into two parts: background materials and general topics. The background materials include:

- (1) an introduction to the fundamental physical models, ranging from continuum mechanics to quantum mechanics (Chapter 4);
- (2) basic analytical techniques for multiscale problems, such as averaging methods, homogenization methods, renormalization group methods, and matched asymptotics (Chapter 2);
- (3) classical numerical techniques that use multiscale ideas (Chapter 3).

For the second part, we chose the following topics.

- (1) Examples of multi-physics models. These are analytical models that use multi-physics coupling explicitly (Chapter 5). *It is important to realize that multiscale modeling is not just about developing algorithms, it is also about developing better physical models.*
- (2) Numerical methods for capturing the macroscopic behavior of complex systems with the help of microscopic models, in cases when empirical macroscopic models are inadequate (Chapter 6).
- (3) Numerical methods for coupling macroscopic and microscopic models locally in order to better resolve localized singularities, defects or other events (Chapter 7).

We have also included three more specific examples: elliptic partial differential equations with multiscale coefficients, problems with both slow and fast dynamics, and rare events. The first was selected to illustrate problems that involve spatial scales. The second and third are selected to illustrate problems that involve time scales.

Some of the background materials mentioned above have been discussed in numerous textbooks. However, each such textbook contains materials that are enough for a one-semester course, and most students and

researchers will not be able to afford the time to go through them all. Therefore, we decided to discuss these topics in a simplified fashion, to extract the longwinded ideas necessary for a basic understanding of the relevant issues.

The book is intended for scientists and engineers who are interested in modeling and doing it right. I have tried to strike a balance between precision, which requires a considerable amount of mathematics and detail, and accessibility, which requires glossing over some details and making compromises on precision. For example, we will discuss asymptotic analysis quite systematically, but we will not discuss the related theorems. We will always try to use the simplest examples to illustrate the underlying ideas, rather than dwelling on particular applications.

Many people helped to shape my views on multiscale modeling. Björn Engquist introduced me to the subject while I was a graduate student, at a time when multiscale modeling was not a fashionable area to work on. I have also benefitted from the other mentors I have had at different stages of my career; they include Alexandre Chorin, Bob Kohn, Andy Majda, Stan Osher, George Papanicolaou, and Tom Spencer. I am very fortunate to have Eric Vanden-Eijnden as a close collaborator. Eric and I discuss and argue about the issues discussed here so often that I am sure his views and ideas are reflected in many parts of this volume. I would like to thank my other collaborators: Assyr Abdulle, Carlos Garcia-Cervera, Shanqin Chen, Shiyi Chen, Li-Tien Cheng, Nick Choly, Tom Hou, Zhongyi Huang, Tiejun Li, Xiantao Li, Chun Liu, Di Liu, Gang Lu, Jianfeng Lu, Paul Maragakis, Pingbing Ming, Cyrill Muratov, Weiqing Ren, Mark Robbins, Tim Schulze, Denis Serre, Chi-Wang Shu, Qi Wang, Yang Xiang, Huanan Yang, Jerry Yang, Xingye Yue, Pingwen Zhang, and more. I have learned a lot from them, and it is my good fortune to have the opportunity to work with them. I am grateful to the many people that I have consulted at one point or another on the issues presented here. They include Achi Brandt, Roberto Car, Emily Carter, Shi Jin, Tim Kaxiras, Yannis Kervrekidis, Mitch Luskin, Felix Otto, Olof Runborg, Zuowei Shen, Andrew Stuart, Richard Tsai, and Chongyu Wang.

My work has been consistently supported by the Office of Naval Research. I am very grateful to Wen Masters and Reza Malek-Madani for their confidence in my work, particularly at the time when multiscale, multi-physics modeling was not quite as popular as it is now.

Preface

xvii

Part of this volume is based on lecture notes taken by my current or former students Dong Li, Lin Lin, Jianfeng Lu, Hao Shen, and Xiang Zhou. Their help is very much appreciated.

Finally, I would like to thank Rebecca Louie and Christina Lipsky for their help in typing the manuscript.