# 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.

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# 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 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.

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