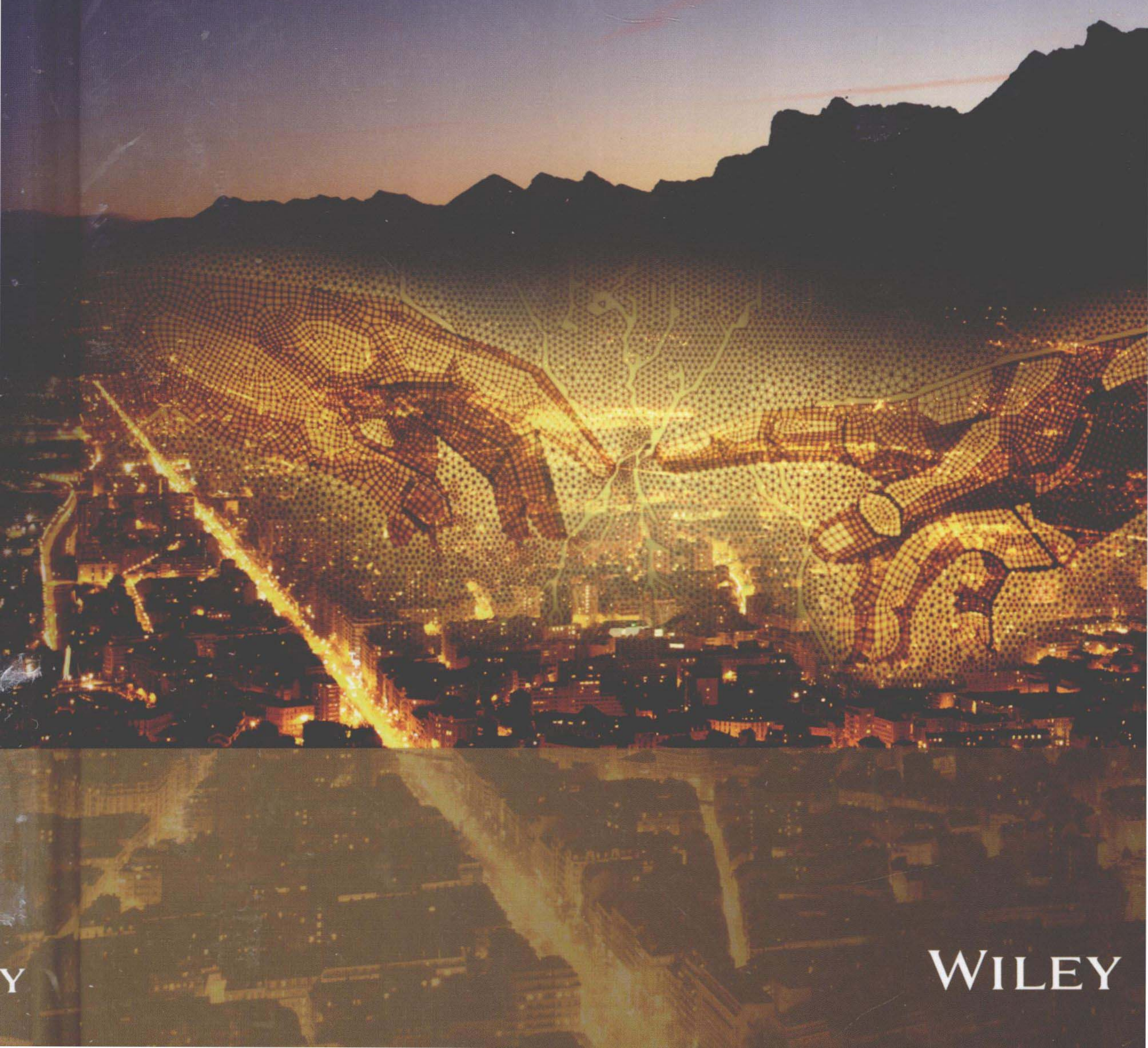
Practical Multiscaling

Jacob Fish



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To my wife Ora and to my children Adam and Effie

Preface

This textbook covers fundamental modeling techniques aimed at bridging diverse temporal and spatial scales ranging from the atomic level to a full-scale product level. The focus is on *practical multiscale methods* that account for fine-scale (material) details but do not require their precise resolution. The text material evolved from over 20 years of teaching experience, which included the development of Multiscale Science and Engineering courses at Rensselaer Polytechnic Institute and Columbia University, as well as from practical experience gained in the application of multiscale software.

Due to a broad spectrum of application areas, this course is intended to be of interest and use to a varied audience, including:

- graduate students and researchers in academia and government laboratories who are interested in acquiring fundamental skills that will enable them to advance the state-of-the-art in the field;
- practitioners in civil, aerospace, pharmaceutical, electronics, and automotive industries who are interested in taking advantage of existing multiscale tools; and
- commercial software vendors who are interested in extending their product portfolios and tapping into new markets.

This textbook is unique in three respects:

- Theory and implementation. The text provides a detailed exposition of the state-of-the-art multiscale theories and their insertion into conventional (single-scale) finite element code architecture.
- Predictability and design. The text emphasizes the *robustness* and *design* aspects of multiscale methods. This is accomplished via four building blocks: *upscaling* of information, *systematic reduction* of information, *characterization* of information utilizing experimental data, and *material optimization* (Figure 1).

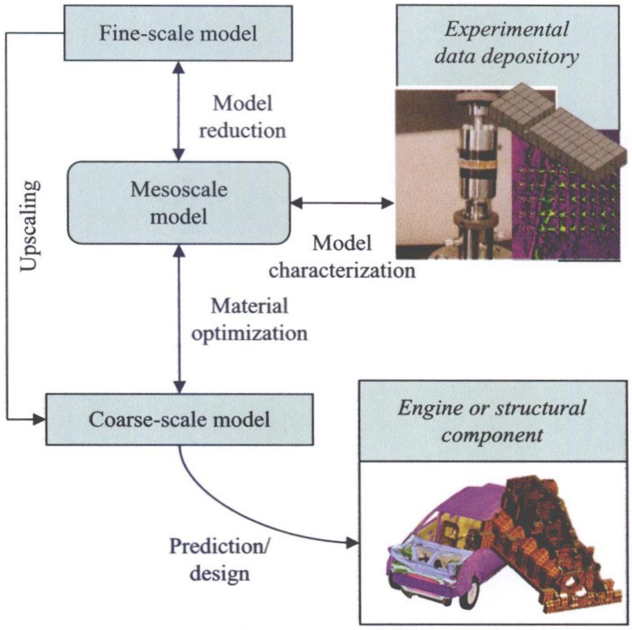

Figure 1 **Building blocks of multiscale design.** ***Upscaling*****: derivation of coarse-scale equations from fine-scale equations using homogenization-like theories.** ***Model reduction*****: reducing the complexity of solving fine-scale problems.** ***Model characterization*****: solving an inverse problem for reduced model parameters.** ***Material optimization*****: optimizing microstructure based on design criteria**

- Hands-on experience. Included with this textbook is an academic version of the multiscale design software (MDS-Lite) [1], which serves as a seamless plug-in to commercial software. A full integration with a built-in coarse-scale solver is also provided.

The material in this book can be covered in a single semester, and a meaningful course can be constructed from a subset of the chapters in this book for a one-quarter course. Following the Introduction to Multiscale Methods (Chapter 1), course material is organized in five chronological chapters: Upscaling/Downscaling of Continua (Chapter 2), Upscaling/Downscaling of Atomistic/Continuum Media (Chapter 3), Reduced Order Homogenization (Chapter 4), Scale-separation-free Upscaling/Downscaling of Continua (Chapter 5), and Multiscale Design Software (Chapter 6). Basic knowledge of continuum mechanics and finite elements is required. Chapters 2–4 focus on multiscale methods that take advantage of the scale separation hypothesis stemming from the infinitesimality of fine-scale features compared with the coarse-scale problem. The issue of how to systematically reduce fine-scale information and to characterize it against available experimental data is detailed in Chapter 4. Multiscale design software, which incorporates the aforementioned building blocks, including continua upscaling, model reduction, experimental characterization, and material optimization, is described in Chapter 6. The software can be used in conjunction with one of the commercial macroscopic solvers, ANSYS, ABAQUS, or LS-DYNA, or, alternatively, with the built-in coarse-scale solver, MDS-Macro. Use of this software provides a valuable hands-on experience to both students and practitioners. Chapters 2, 4, and 6 represent the core course material, which is recommended for one-quarter or full semester courses when supplementary material is used. A link between upscaling methods and the exact solution of the fine-scale problem is provided within the framework of the multigrid methods in Chapters 2 and 3 for continua and discrete media, respectively. Chapter 3, which details upscaling of atomistic media, is self-contained and can be taught independently of the core course material in Chapters 2, 4, and 6. Chapter 5, which is intended for an advanced audience, describes advanced multiscale and model reduction methods that are free of scale separation hypothesis.

Reference

[1] http://multiscale.biz.

Acknowledgments

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Contents

1

Introduction to Multiscale Methods

1.1 The Rationale for Multiscale Computations

Consider a textbook boundary value problem that consists of equilibrium, kinematical, and constitutive equations together with essential and natural boundary conditions. These equations can be classified into two categories: those that directly follow from physical laws and those that do not. A constitutive equation demonstrates a relation between two physical quantities that is specific to a material or substance and does not follow directly from physical laws. It can be combined with other equations (equilibrium and kinematical equations, which do represent physical laws) to solve specific physical problems.

In other words, it is convenient to label all that we do not know about the boundary value problem as a *constitutive law* (a term originally coined by Walter Noll in 1954) and designate an experimentalist to quantify the constitutive law parameters. While this is a trivial exercise for linear elastic materials, this is not the case for anisotropic history-dependent materials well into their nonlinear regime. In theory, if a material response is history-dependent, an infinite number of experiments would be needed to quantify its response. In practice, however, a handful of constitutive law parameters are believed to "capture" the various failure mechanisms that have been observed experimentally. This is known as *phenomenological modeling*, which relates several different empirical observations of phenomena to each other in a way that is consistent with fundamental theory but is not directly derived from it.

An alternative to phenomenological modeling is to derive constitutive equations (or directly, field quantities) from finer scale(s) where established laws of physics are believed to be better understood. The enormous gains that can be accrued by this so-called multiscale approach have been reported in numerous articles [1,2,3,4,5,6]. Multiscale computations have been identified (see page 14 in [7]) as one of the areas critical to future nanotechnology advances.

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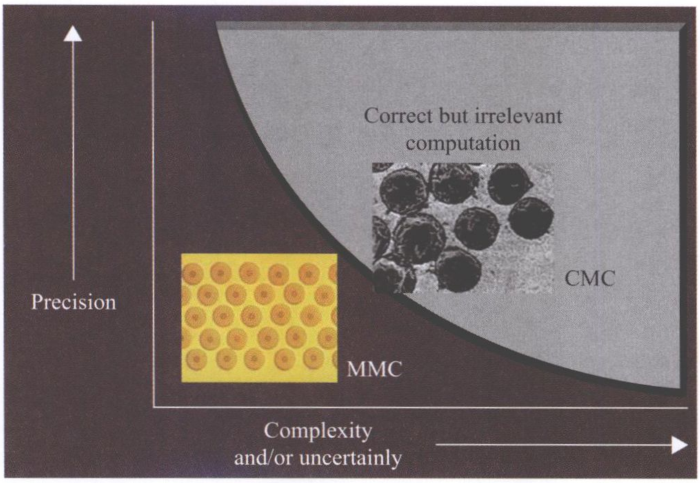

Figure 1.1 Reduced precision due to increase in uncertainty and/or complexity. CMC, ceramic matrix composite; MMC, metal matrix composite

For example, the FY2004 US$3.7 billion National Nanotechnology Bill (page 14 in [7]) states that "approaches that integrate more than one such technique (…molecular simulations, continuum-based models, etc.) will play an important role in this effort."

One of the main barriers to such a multiscale approach is the increased uncertainty and complexity introduced by finer scales, as illustrated in Figure 1.1. As a guiding principle for assessing the need for finer scales, it is appropriate to recall Einstein's statement that "the model used should be the simplest one possible, but not simpler." The use of any multiscale approach has to be carefully weighed on a case-by-case basis. For example, in the case of metal matrix composites (MMCs) with an almost periodic arrangement of fibers, introducing finer scales might be advantageous since the bulk material typically does not follow normality rules, and developing a phenomenological coarse-scale constitutive model might be challenging at best. The behavior of each phase is well understood, and obtaining the overall response of the material from its fine-scale constituents can be obtained using homogenization. On the other hand, in brittle ceramic matrix composites (CMCs), the microcracks are often randomly distributed and characterization of their interface properties is difficult. In this case, the use of a multiscale approach may not be the best choice.

1.2 The Hype and the Reality

Multiscale Science and Engineering is a relatively new field [8,9] and, as with most new technologies, began with a *naive euphoria* (Figure 1.2). During the euphoria stage of technology development, inventors can become immersed in the ideas themselves and may overpromise, in part to generate funds to continue their work. Hype is a natural handmaiden to overpromise, and most technologies build rapidly to a peak of hype [10].

For instance, early success in expert systems led to inflated claims and unrealistic expectations. The field did not grow as rapidly as investors had been led to expect, and this translated into disillusionment. In 1981 Feigenbaum *et al.* [11] reckoned that although artificial intelligence (AI) was already 25 years old, it "was a gangly and arrogant youth, yearning for