



Practical Multiscaling

Jacob Fish



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PRACTICAL MULTISCALING

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Jacob Fish

Columbia University, USA

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This edition first published 2014
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John Wiley & Sons, Ltd, The Atrium, Southern Gate, Chichester, West Sussex, PO19 8SQ,
United Kingdom

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Library of Congress Cataloging-in-Publication Data

Fish, J. (Jacob)

Practical multiscale modeling / Jacob Fish.

pages cm

Includes bibliographical references and index.

ISBN 978-1-118-41068-4 (hardback)

1. Mechanical engineering--Mathematical models. 2. Continuum mechanics--Mathematical models. 3. Materials--Mathematical models. 4. Multiscale modeling. 5. Scaling laws (Statistical physics) 6. Mechanical engineering--Computer simulation. 7. Continuum mechanics--Computer simulation. 8. Materials--Computer simulation. I. Title.

TJ153.F455 2013

620.001'51--dc23

2013027948

A catalogue record for this book is available from the British Library.

Set in 10/12pt Times by SPi Publisher Services, Pondicherry, India

To my wife Ora and to my children Adam and Effie

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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).

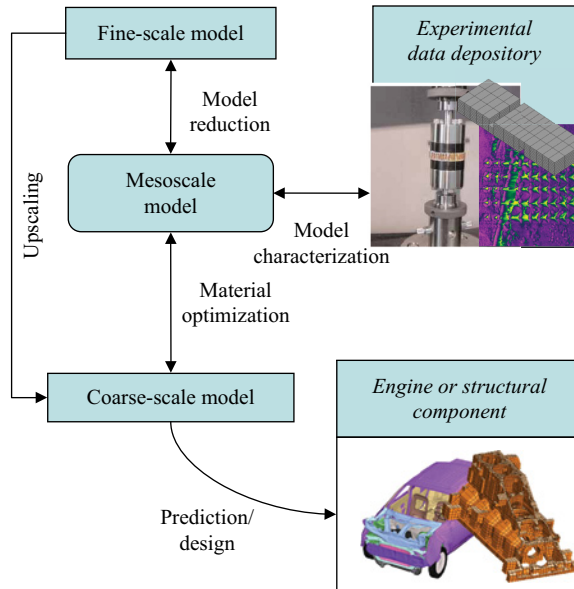


Figure 1 Building blocks of multiscale design. *Upscaling*: derivation of coarse-scale equations from fine-scale equations using homogenization-like theories. *Model reduction*: reducing the complexity of solving fine-scale problems. *Model characterization*: solving an inverse problem for reduced model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

I have many people to thank. I am grateful to Ted Belytschko for his constructive suggestions, which aided me in writing the text. I also appreciate the support of Zheng Yuan, my outstanding former PhD student and the current Chief Technological Officer of MDS, for “MDS-izing” the text and making it useful to both the academic community and practitioners. I received valuable assistance from Vasilina Filonova, an outstanding Research Associate at Columbia University, and a multitude of my PhD students including Sergey Kuznetsov, Nan Hu, Zifeng Yuan, Dimitrios Fafalis and Mahesh Bailakanavar. I express my deepest appreciation to Wendy Bickel for her assistance in editing the text. Finally, I wish to express my gratitude and apologies to my family, Adam, Effie, and Ora, to whom this book is dedicated, for enduring this past year when much of my time and energy should have been devoted to them rather than to this book.



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.

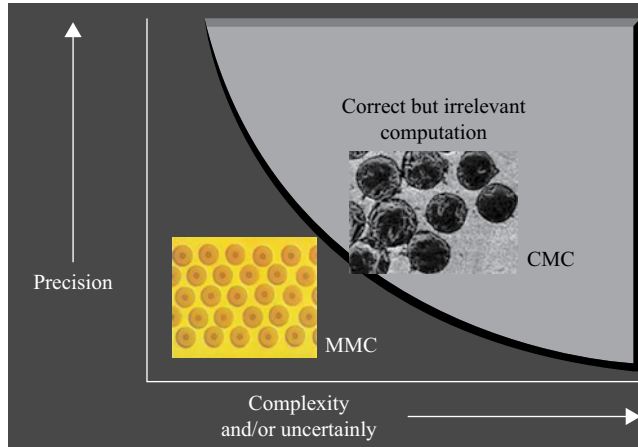


Figure 1.1 Reduced precision due to increase in uncertainty and/or complexity. CMC, ceramic matrix composite; MMC, metal matrix composite

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 *naïve 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

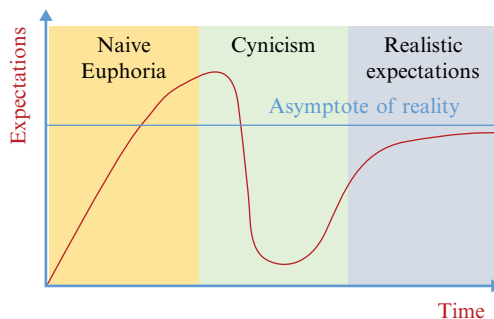


Figure 1.2 Evolution of new technology

a maturity that was nowhere evident.” Interestingly, today you can purchase the hardcover AI handbook [11] for as little as US\$0.73 on Amazon. Multiscale computations also had their share of overpromise, such as inflated claims of designing drugs atom by atom [12] or reliably designing the Boeing 787 from first principles, just to mention a few.

Following this naive euphoria (Figure 1.2), there is almost always an overreaction to ideas that are not fully developed, and this inevitably leads to a crash, followed by a period of wallowing in the depths of cynicism. Many new technologies evolve to this point and then fade away. The ones that survive do so because industry (or perhaps someone else) finds a “good use” (a true user benefit) for this new technology.

The author of this book believes that the state of the art today in multiscale science and engineering is sufficiently mature to take on the more than 50-year-old challenge [13] posed by Nobel Prize Laureate Richard Feynman: “What would the properties of materials be if we could really arrange the atoms the way we want them?” However, progress toward fulfilling the promise of multiscale science and engineering hinges not only on its development as a discipline concerned with the understanding and integration of mathematical, computational, and domain expertise sciences, but more so with its ability to meet broader societal needs beyond those of interest to the academic community. After all, as compelling as a finite element theory is, the future of that field might have been in doubt if practitioners had not embraced it.

Thus, the primary objective of this book is to focus not only on theory but also on practical utilization of multiscale methods.

1.3 Examples and Qualification of Multiscale Methods

Nature and man-made products are replete with multiple scales. Consider, for instance, the Airbus A380 depicted in Figure 1.3. It is 53 m long with a wingspan of 80 m and height of 24 m. The A380 consists of hundreds of thousands of structural components and many more structural details. Just in the fuselage alone there are more than 750,000 holes and cutouts. In addition to various structural scales, there are numerous material scales. At the coarsest material scales, the composites portion of the fuselage consists of laminate and woven/textile composite scales; at the intermediate scale is a tow or yarn, which consists of a bundle of fibers; and finally, there are one or more discrete scales, including atomistic and ab initio (quantum) scales. The metal portion of the airplane consists of a polycrystalline scale, a single crystal scale that considers dislocation density, a discrete dislocation scale, and finally, atomistic and ab initio scales.

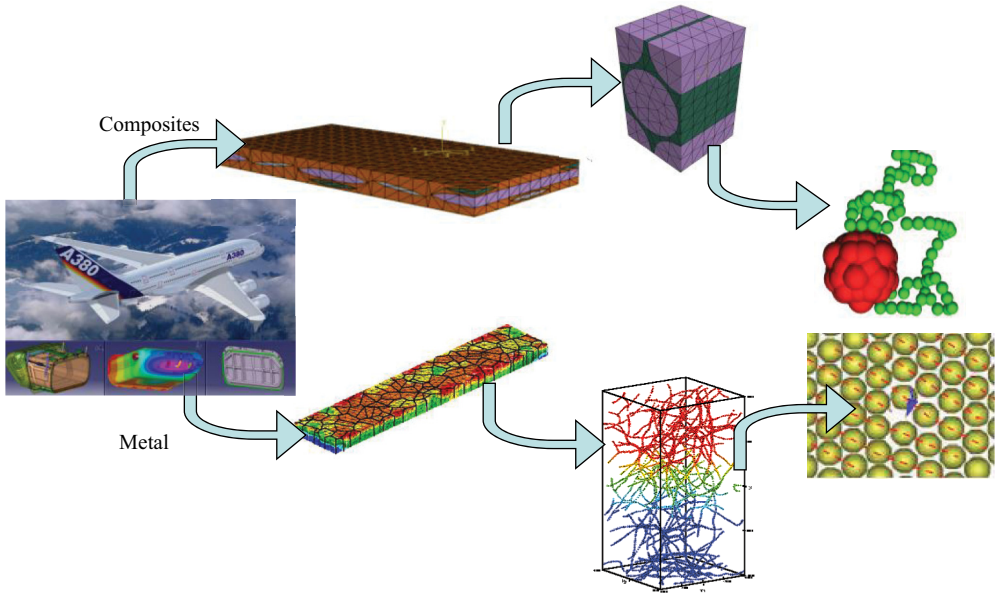


Figure 1.3 Multiple scales in the Airbus A380

It is tempting to start at the *ab initio* scale and to upscale, scale after scale, all the way to the product scale. This, unfortunately, is neither a realistic undertaking nor the goal of the present book. Our goal here is much more modest. We will focus on modeling and simulation approaches that can predict certain quantities of interest with significantly lower computational cost than solving the corresponding fine-scale system. The starting point for the fine-scale system of choice is not necessarily the *ab initio* scale; instead, the computational resources available and the accuracy requirement determine the starting point.

A modeling and simulation approach will be considered multiscale if it is capable of resolving certain quantities of interest with significantly lower cost than solving the corresponding fine-scale system. Schematically, a multiscale method has to satisfy the so-called Accuracy and Cost Requirements (ACR) test:

$$\begin{array}{l} \text{Error in quantities of interest} < \text{tol} \\ \frac{\text{Cost of multiscale solver}}{\text{Cost of fine scale solver}} \ll 1 \end{array}$$

In general, multiscale approaches fall into one of two categories: information-passing (or hierarchical) or concurrent. In the information-passing multiscale approach, which is the main focus of this book, the fine-scale response is idealized (approximated or unresolved) and its overall (average) response is infused into the coarse scale. In the concurrent approaches, fine- and coarse-scale resolutions are simultaneously employed in different portions of the problem domain, and the exchange of information occurs through the interface. The subdomains where different scale resolutions are employed can be either disjoint or overlapping.

Information-passing multiscale methods are typically used to model the overall response of the fine scale, except for the hot spots in the vicinity of cutouts and boundary layers where concurrent multiscale methods are more appropriate.

To this end, we will focus on the qualification of multiscale methods. Loosely speaking, the information-passing multiscale approach is likely to pass the ACR test provided that:

- (i) quantities of interest are limited to or defined only on the coarse scale (provided that these quantities are computable from the fine scale); and
- (ii) special features of the fine-scale problem, such as scale separation and self-similarity, are taken advantage of.

On the other hand, for the concurrent multiscale approach to pass the ACR test, the following conditions must be satisfied:

- (i) the interface (or interphase) between the fine and coarse scales should be properly engineered;
- (ii) the fine-scale model should be limited to a small portion of the computational domain; and
- (iii) the precise material microstructure should be known in the subdomain where the fine-scale model is considered.

It is important to note that even though the concurrent approach may pass the first two criteria in the ACR test, its computational cost will typically exceed that of the information-passing methods. Furthermore, the main hurdle to successful utilization of concurrent methods in practice is a lack of knowledge of precise material microstructure in the hot spots. In these locations, fine-scale resolution is required, as opposed to the information-passing multiscale methods where material microstructure in small representative windows is reconstructed from various test coupons.

1.4 Nomenclature and Definitions

Since various multiscale methods were conceived in different scientific communities, there has been a proliferation of definitions, some of which are contradictory or overlapping. For instance, various information-passing multiscale methods have been labeled by different names, including upscaling methods, coarse-graining methods, homogenization methods, or simply multiscale methods. There are also subcategories of the above definitions, such as systematic upscaling (with obvious implications), operator upscaling, variational multiscale, computational homogenization, multigrid homogenization, numerical homogenization, numerical upscaling, and computational coarse-graining, just to mention a few.

Some authors draw a distinction between upscaling and multiscale methods. According to one such definition, upscaling forms a coarse-scale model with an a priori defined mathematical structure; once the model is conceived, the fine-scale information is discarded, whereas in multiscale methods, the fine-scale information is retained throughout the simulation and the coarse-scale structure is generally not expressed analytically. However, there is no consensus on the above definition. For instance, the variational multiscale method (VMS) [14] is considered to fall into the category of (operator) upscaling methods. Yet, for nonlinear problems, fine-scale

information is not discarded in VMS, suggesting that it belongs to the category of multiscale methods. Likewise, the homogenization method for linear problems provides effective properties, and this is obviously an upscaling method based on the aforementioned definition; and yet, for nonlinear problems, fine- and coarse-scale problems are fully coupled throughout the analysis. Another misconception is the supposition that upscaling is a form of homogenization that is free of the periodicity assumption. Homogenization, like most of the upscaling methods, assumes some form of scale separation, but it can be used to homogenize random heterogeneous media with either periodic, weakly periodic, essential, natural, or hybrid boundary conditions.

Hereafter, upscaling and downscaling will be understood as two building blocks of the information-passing multiscale method. For nonlinear processes, upscaling is a history-dependent process of constructing coarse-scale equations from well-defined fine-scale equations. *History dependence* means that the fine-scale information is retained and used throughout the simulation to update the coarse-scale problem. Downscaling, often called localization, is the second building block of the information-passing multiscale approach. Downscaling is a history-dependent process by which fine-scale information is continuously reconstructed in small windows using the information from the coarse-scale problem. The information-passing multiscale approach is a continuous process of upscaling and downscaling. The window in this information-passing process can be a point in the coarse-scale domain, in which case the information-passing multiscale approach is synonymous with nonlinear (computational) homogenization, a single coarse-scale element [14], or a patch of coarse-scale elements. In the former case, this small window is often referred to as a unit cell or representative volume element. For linear problems, the fine- and coarse-scale problems are one-way coupled, where upscaling provides coarse-scale (effective) properties, while downscaling plays the role of postprocessing of the fine-scale solution. Hereafter, the nested process of upscaling and downscaling will be termed as *upscaling/downscaling*.

Coarse-graining is a subclass of upscaling methods where a coarse-scale (or coarse-grained) model is constructed from the fine-scale information in the preprocessing stage prior to nonlinear analysis. Coarse-grained molecular dynamics is a typical example of such coarse-graining. The fact that fine-scale information is not revisited in these methods offers considerable computational advantages, but often at the expense of accuracy.

Different terminologies are used to indicate various scales. In the case of two scales, the fine scale is often referred to as a microscale, unresolvable scale, atomistic scale, or discrete scale; the coarse scale is often labeled as a macroscale, resolvable scale, component scale, or continuum scale. Here we will simply refer to the two scales as fine and coarse scales. For more than two scales, we will refer to the additional scales as mesoscales.

1.5 Notation

1.5.1 Index and Matrix Notation

Two types of notation will be used: (i) indicial notation; and (ii) matrix notation. All the derivations will be made in the indicial notation. The equations pertaining to the finite element implementation will be given in indicial or matrix notation.

In the indicial notation, the components of tensors or matrices are explicitly specified. Thus a vector, which is a first-order tensor, is denoted in indicial notation by a_i where the range of the index is the number of spatial dimensions n_{sd} . Indices repeated twice in a term

are summed, in conformance with the rules of Einstein notation. Spatial tensor components are denoted by lowercase Latin subscripts, which are always on the right of the tensor. Spatial components of a second-order tensor are indicated by two Latin subscripts, and they always refer to the Cartesian coordinate system. For example, small strain tensor components are denoted by ε_{ij} .

We will alternate between two notations for finite element nodes and degrees of freedom. Nodal indices will always be indicated by uppercase Latin letters positioned at the bottom right of the tensor, vector, or matrix. For example, v_{iA} is the velocity of node A in the direction i . Indices representing finite element degrees of freedom will always be indicated by lowercase Greek letters positioned at the bottom right of the tensor or vector. For example, v_α is the velocity of degree-of-freedom α . The degrees of freedom are related to nodes by

$$\alpha = (A - 1)n_{sd} + i$$

where n_{sd} denotes the number of spatial dimensions.

When nodal and degrees-of-freedom indices are repeated twice, they will be summed over their range, which depends on the context. When dealing with an element, the range is over the nodes or degrees of freedom of the element, whereas when dealing with a mesh, the range is over the nodes or degrees of freedom of the mesh.

In the finite element implementation, we will often use matrix notation. We will indicate matrices and vectors, which are the first-order matrices, in boldface. Second-order tensor components will often be converted to Voigt notation in the implementation phase. In Voigt notation, kinetic symmetric tensors, such as Cauchy stress σ_{ij} , and kinematic symmetric tensors, such as small strain ε_{ij} , are written as column matrices:

$$\sigma_{ij} \rightarrow \boldsymbol{\sigma} = \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix}; \quad \varepsilon_{ij} \rightarrow \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{bmatrix}$$

Note that kinematic tensor components for which indices are not equal are multiplied by 2 in Voigt notation. The Voigt rule is particularly useful for converting fourth-order tensors. For example, the linear elastic constitutive tensor components L_{ijkl} are written in Voigt notation as

$$L_{ijkl} \rightarrow \mathbf{L} = \begin{bmatrix} L_{1111} & L_{1122} & L_{1133} & L_{1123} & L_{1113} & L_{1112} \\ L_{2211} & L_{2222} & L_{2233} & L_{2223} & L_{2213} & L_{2212} \\ L_{3311} & L_{3322} & L_{3333} & L_{3323} & L_{3313} & L_{3312} \\ L_{2311} & L_{2322} & L_{2333} & L_{2323} & L_{2313} & L_{2312} \\ L_{1311} & L_{1322} & L_{1333} & L_{1323} & L_{1313} & L_{1312} \\ L_{1211} & L_{1222} & L_{1233} & L_{1223} & L_{1213} & L_{1212} \end{bmatrix}$$

such that $\boldsymbol{\sigma} = \mathbf{L}\boldsymbol{\varepsilon}$ in matrix notation.

The fourth-order identity tensor in the indicial notation is given as

$$I_{ijkl} = \frac{1}{2} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})$$

where δ_{ik} is the Kronecker delta, which is equal to zero for $i \neq j$ and one for $i = j$. The nonzero components of I_{ijkl} are

$$\begin{aligned} I_{1111} &= I_{2222} = I_{3333} = 1 \\ I_{1212} &= I_{1313} = I_{2323} = I_{2121} = I_{3131} = I_{3232} = \frac{1}{2} \\ I_{2112} &= I_{3113} = I_{3223} = I_{1221} = I_{1331} = I_{2332} = \frac{1}{2} \end{aligned}$$

Let \mathbf{I} be a 6×6 diagonal matrix and \mathbf{H} be any $6 \times n$ matrix. The identity matrix \mathbf{I} is defined so that $\mathbf{IH} = \mathbf{H}$, which requires diagonal terms with unequal indices to be multiplied by two.

$$\mathbf{I} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

1.5.2 Multiple Spatial Scale Coordinates

The coordinates in the coarse-scale deformed (or current) and undeformed (initial) configurations will be denoted by \mathbf{x} and \mathbf{X} , respectively. For small deformation problems, a single coarse-scale coordinate \mathbf{x} will be used.

The focus of this book is on two-scale analysis. The fine-scale problems will be considered in a small representative window often referred to as a unit cell. The unit cell will be generally assumed to be much smaller than the coarse-scale domain, and therefore its deformed and undeformed coordinates, denoted by \mathbf{y} and \mathbf{Y} , respectively, will be rescaled by a small positive parameter ζ as

$$\mathbf{y} = \mathbf{x}/\zeta; \quad \mathbf{Y} = \mathbf{X}/\zeta \quad 0 < \zeta \ll 1$$

For three-scale problems, \mathbf{y} and \mathbf{Y} will denote the intermediate scale (or mesoscale) configuration, whereas \mathbf{z} and \mathbf{Z} will denote the finest scale configuration, such that

$$\mathbf{z} = \mathbf{y}/\zeta; \quad \mathbf{Z} = \mathbf{Y}/\zeta$$

For the general case of n_{sc} scales, the left uppercase superscript in the brackets will denote the scale, with 0 denoting the coarsest scale and $n_{sc} - 1$ the finest scale. The position vector at scale I , $^{(I)}\mathbf{x}$, will be related to the position vector at scale $I-1$, $^{(I-1)}\mathbf{x}$, by

$$\begin{aligned} ^{(I)}\mathbf{X} &= ^{(I-1)}\mathbf{X}/\zeta \\ ^{(I)}\mathbf{x} &= ^{(I-1)}\mathbf{x}/\zeta \end{aligned} \quad \text{for } I = 1, \dots, n_{sc} - 1$$

1.5.3 Domains and Boundaries

For two-scale problems, we will consider three types of problem domains: (i) the composite domain denoted by Ω^ζ ; (ii) the coarse-scale domain denoted by Ω ; and (iii) the unit cell domain denoted by Θ . The corresponding boundaries are denoted by $\partial\Omega^\zeta$, $\partial\Omega$, and $\partial\Theta$, respectively. \mathbf{n}^ζ , \mathbf{n}^c , and \mathbf{n}^Θ denote unit normals to the boundaries $\partial\Omega^\zeta$, $\partial\Omega$, and $\partial\Theta$, respectively. The volumes of the three domains are denoted by $|\Omega^\zeta|$, $|\Omega|$, and $|\Theta|$.

Throughout this book, the right superscript ζ will denote the existence of fine-scale features. The source problem will be always stated on a domain that, in addition to heterogeneities, may include microstructural voids. The composite domain Ω^ζ is defined as a solid part of the coarse-scale domain that does not contain voids in the material microstructure. Furthermore, the boundary of the composite domain $\partial\Omega^\zeta$ may be rough due to the intersection of voids with the external boundary. On the other hand, the coarse-scale domain Ω and its boundary $\partial\Omega$ are free of fine-scale material features. In the absence of information about surface roughness, we will often assume that $\partial\Omega^\zeta = \partial\Omega$ and $\mathbf{n}^\zeta = \mathbf{n}^c$.

$\partial\Omega^{\prime\zeta}$, $\partial\Omega^{\prime\zeta}$ and $\partial\Omega''$, $\partial\Omega'$ denote the essential (displacement) and natural (traction) boundaries of the composite and coarse-scale domains, respectively, related by

$$\begin{aligned}\partial\Omega^{\prime\zeta} \cup \partial\Omega^{\prime\prime\zeta} &= \partial\Omega^\zeta \quad \text{and} \quad \partial\Omega^{\prime\zeta} \cap \partial\Omega^{\prime\prime\zeta} = 0 \\ \partial\Omega' \cup \partial\Omega'' &= \partial\Omega \quad \text{and} \quad \partial\Omega' \cap \partial\Omega'' = 0\end{aligned}$$

A unit cell may consist of two or more fine-scale phases. The internal boundary between the fine-scale phases will be denoted by S , with $\tilde{\mathbf{n}}$ being the unit normal to the boundary.

For three-scale problems, Θ_z will denote the unit cell domain at the finest scale, and $\partial\Theta_z$ will denote its boundary. For more than three scales, ${}^{(I)}\Theta$ and $\partial^{(I)}\Theta$ will be the unit cell domain and its boundary at scale I , with indices $I = 1$ and $I = n_{sc} - 1$ denoting the coarsest and finest scale unit cell domains, respectively.

For large deformation problems, we will distinguish between deformed and undeformed configurations. Ω_X^ζ and Ω_X will denote initial (undeformed) composite and coarse-scale domains, whereas Ω_x^ζ and Ω_x are the corresponding current (deformed) configurations. $\partial\Omega_X^{\prime\zeta}$, $\partial\Omega_X^{\prime\prime\zeta}$ and $\partial\Omega_x^{\prime\zeta}$, $\partial\Omega_x^{\prime\prime\zeta}$ will denote the essential and natural boundaries of the initial and current composite domains. Similarly, $\partial\Omega_X''$, $\partial\Omega_X'$ and $\partial\Omega_x''$, $\partial\Omega_x'$ are the essential and natural boundaries of the initial and current coarse-scale domains, respectively. Unit normals to the initial and current composite, coarse-scale, and unit cell domains will be denoted by $(\mathbf{N}^\zeta, \mathbf{N}^c, \mathbf{N}^\Theta)$ and $(\mathbf{n}^\zeta, \mathbf{n}^c, \mathbf{n}^\Theta)$, respectively.

The unit cell domains Θ_y and Θ_y will denote initial and current configurations, with $\partial\Theta_y$ and $\partial\Theta_y$ being the corresponding boundaries.

1.5.4 Spatial and Temporal Derivatives

Upscaling methods will be predominantly derived from either the Hill–Mandel macrohomogeneity condition [15] or by using multiple-scale asymptotic methods. For two-scale problems, the various response fields $f^\zeta(\mathbf{x})$ will be assumed to depend on the fine- and coarse-scale coordinates

$$f^\zeta(\mathbf{x}) = f(\mathbf{x}, \mathbf{y})$$

Spatial derivatives of the response function $f^\zeta(\mathbf{x})$ can be calculated by the chain rule as

$$f_{,i}^\zeta = \frac{\partial f(\mathbf{x}, \mathbf{y})}{\partial x_i} + \frac{1}{\zeta} \frac{\partial f(\mathbf{x}, \mathbf{y})}{\partial y_i} = f_{,x_i} + \frac{1}{\zeta} f_{,y_i}$$

where a comma followed by a subscript variable denotes a partial derivative with respect to the subscript variable. Symmetric spatial derivatives are denoted as

$$f_{(i,x_j)} = \frac{1}{2} \left(\frac{\partial f_i}{\partial x_j} + \frac{\partial f_j}{\partial x_i} \right) \quad \text{and} \quad f_{(i,y_j)} = \frac{1}{2} \left(\frac{\partial f_i}{\partial y_j} + \frac{\partial f_j}{\partial y_i} \right)$$

For problems involving multiple temporal scales, such as fatigue in Chapter 4 and lattice vibration in Chapter 3, various response fields $f^\zeta(\mathbf{x}, t)$ will be assumed to depend on multiple spatial and temporal coordinates

$$f^\zeta(\mathbf{x}, t) = f(\mathbf{x}, \mathbf{y}, t, \tau)$$

where τ is the fast time coordinate related to the slow time coordinate t by

$$\tau = \frac{t}{\eta} \quad 0 < \eta \ll 1$$

Time differentiation of response fields with respect to multiple temporal scales is given by the chain rule

$$\frac{df^\zeta(\mathbf{x}, t)}{dt} = \frac{\partial f(\mathbf{x}, \mathbf{y}, t, \tau)}{\partial t} + \frac{1}{\eta} \frac{\partial f(\mathbf{x}, \mathbf{y}, t, \tau)}{\partial \tau} = \dot{f}(\mathbf{x}, \mathbf{y}, t, \tau) + \frac{1}{\eta} f'(\mathbf{x}, \mathbf{y}, t, \tau)$$

Most often, it will be assumed that spatial and temporal scaling parameters are identical, that is, $\zeta = \eta$.

1.5.5 Special Symbols

Throughout this book, special notations will denote certain attributes, as follows:

- $\hat{\mathbf{x}}, \hat{\mathbf{X}}$ – coordinates of the unit cell centroid
- $\bar{\mathbf{u}}, \bar{\mathbf{t}}$ – prescribed fields (displacements and tractions)
- χ – local Cartesian coordinate in the physical domain placed at the unit cell centroid
- $()^{(k)}$ – right Latin superscript in parentheses denotes k th term in asymptotic expansion
- $()^f$ – right superscript f denotes fine-scale fields and properties
- $()^c$ – right superscript c denotes coarse-scale fields and properties
- $()^M$ – right superscript M denotes master (independent) nodes on the unit cell boundary
- $()^S$ – right superscript S denotes slave (dependent) nodes on the unit cell boundary

- $()^T$ – right superscript T denotes transpose
- $()^{-1}$ – right superscript -1 denotes inverse
- $^i()$ – left superscript denotes iteration count
- $_k()$ – left subscript denotes time increment or load parameter
- $()^{(\alpha)}$ – right Greek superscript in parentheses denotes phase or interface partition in the unit cell

References

- [1] Curtin, W.A. and Miller, R.E. Atomistic/continuum coupling in computational materials science. *Modeling and Simulation in Materials Science and Engineering* 2003, 11(3), R33–R68.
- [2] Fish, J. Bridging the scales in nano engineering and science. *Journal of Nanoparticle Research* 2006, 8, 577–594.
- [3] Fish, J., ed. *Bridging the Scales in Science and Engineering*. Oxford University Press, 2007.
- [4] Ghoniem, N.M. and Cho, K. The emerging role of multiscale modeling in nano- and micro-mechanics of materials. *Modeling in Engineering and Sciences* 2002, 3(2), 147–173.
- [5] Liu, W.K., Karpov, E.G., Zhang, S. and Park, H.S. An introduction to computational nanomechanics and materials. *Computer Methods in Applied Mechanics and Engineering* 2004, 193, 1529–1578.
- [6] Khare, R., Mielke, S.L., Paci, J.T., Zhang, S.L., Ballarini, R., Schatz, G.C. and Belytschko, T. Coupled quantum mechanical/molecular mechanical modeling of the fracture of defective carbon nanotubes and graphene sheets. *Physical Review B* 2007, 75(7), 075412.
- [7] National Nanotechnology Initiative. Supplement to the President's FY 2004 Budget. National Science and Technology Council Committee on Technology, 2004.
- [8] Horstemeyer, M.F. Multiscale modeling: a review. In *Practical Aspects of Computational Chemistry*, eds J. Leszczynski and M.K. Shukla. Springer Science Business Media, 2009, pp. 87–135.
- [9] Belytschko, T. and de Borst, R. Multiscale methods in computational mechanics. *International Journal for Numerical Methods in Engineering* 2010, 89(8–9), 939–1271.
- [10] Bezdek, J. Fuzzy models—what are they, and why? *IEEE Transactions on Fuzzy Systems* 1993, 1, 1–5.
- [11] Barr, A., Cohen, P.R. and Feigenbaum, E.A., ed. *The Handbook of Artificial Intelligence*, Volume IV. Addison-Wesley, 1990.
- [12] The Next Industrial Revolution: designing drugs by computer at Merck. *Fortune Magazine*, October 5, 1981.
- [13] Feynman, R.P. There's plenty of room at the bottom. 29th Annual Meeting of the American Physical Society. California Institute of Technology, 1959.
- [14] Hughes, T.J.R. Multiscale phenomena: Greens functions, the Dirichlet to Neumann formulation, subgrid scale models, bubbles and the origin of stabilized methods. *Computer Methods in Applied Mechanics and Engineering* 1995, 127, 387–401.
- [15] Hill, R. Elastic properties of reinforced solids: some theoretical principles. *Journal of the Mechanics and Physics of Solids* 1963, 11, 357–372.

