INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING (ICME) FOR METALS

Using Multiscale Modeling to Invigorate Engineering Design with Science

MARK F. HORSTEMEYER

TMS

WILEY

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FOREWORD

This book by Dr. Mark F. Horstemeyer lays the foundations to develop the field of computational materials science further into a robust simulation-based design strategy for understanding, improving, and optimizing materials, parts, and engineering structures.

The great progress that is inherent in this novel Integrated Computational Materials Engineering (ICME) approach is its practical perspective toward solving engineering design tasks in a holistic way by combining exact ab initio simulations with finite element analysis of complex microstructures and failure prediction.

These three columns of the author's novel hierarchical approach are the essence of modern computational materials engineering. First, ab initio simulations can provide exact intrinsic thermodynamic and structure information that cannot be obtained by any other theory. This part of the approach follows the tenet that simulations should be as simple as possible but not simpler. Second, such generic first-principle predictions enter into mesoscopic models that capture the interaction of the different phases and defects. This modeling level is essential as modern engineering materials are often characterized by complex multiphase, multidefect, and multimechanism microstructures. Third, these microstructure models are combined with adequate structure–property relationships, placing particular attention on defect initiation and growth. This is essential as reliable failure prediction is one the main ultimate goals in structural design. In real engineering parts, it is particularly the lifetime that matters for final products such as engines, planes structures, or power plant structures.

This excellent book is an absolute must for everyone active or interested in computational materials and design engineering, written by the leader of the exiting new field of ICME.

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PREFACE

This book is designed as a textbook for a course on Integrated Computational Materials Engineering (ICME) in which hierarchical multiscale modeling focused on metal alloys that have structural applications is the center of attention. As such, there are lecture notes in Powerpoint form, a questions and solutions manual, and tutorials to use the models and codes that one can access related to this instructional book (found on the ftp site for the book at ftp://ftp.wiley.com/public/sci_tech_med/icme_metals). If an instructor would like to add modifications/corrections to the lectures, questions/solutions manual, or tutorials, I would be very interested in the updates. Also, to any instructor who would like to employ this course at his or her institution, I am available to discuss any aspect of the course from the information to the management of it. The intended audience is senior-level undergraduates and graduate students who have an interest in computational methods.

The book was borne out of research that I conducted starting at Sandia National Laboratories and have continued at Mississippi State University over the past 15 years. The examples are mostly related to aluminum to help the reader follow the logical patterns without the confusion of different atomic structures, different deformation mechanisms, or different mechanical responses. After seeing the benefits of the methodology in design optimization and analysis, I realized that the greatest impact of transforming the trial-and-error design methods in practice to a simulation-based design ("do it right the first time") method was to train the next generation of designers. Thus, this book is for those instructors "in the know" to teach and train their students to use such techniques.

While working at Sandia National Laboratories in the mid-1990s, there was a meeting of an engineering mechanic, physicist, and materials scientist, and they were talking about stress. At the end of the meeting, they had all agreed that they understood each other's position. After the meeting, I interviewed each person separate from the others and asked what he or she thought about when the stress discussion came about. The physicist talked about pressure, pressure, pressure. The materials scientist talked about strain, strain, strain. And the engineering mechanics researcher talked about second-rank tensor, second-rank tensor, second-rank tensor. They had thought that they communicated, but they really did not because the paradigm of each one's discipline skewed his or her semantical communication. This is often the case for interdisciplinary researchers, so one has to be careful when discussing multiscale modeling or history modeling from process to performance using the ICME tools with others who were trained under a different paradigm.

Because of these different paradigms, I decided shortly after those interviews to perform simulations at all the different length scales and to try to understand the pertinent cause–effect relationships with the hope that I could understand the bridging concepts. This book is a result of conducting what is called hierarchical multiscale modeling over the years in trying to relate the history effects of a material through its processing to performance life cycle.

Because of constraints of space, I could not include all of the good ICME examples that have been demonstrated, so I will mention some of them here, mostly automotive in nature from which the phrase "From Atoms to Autos" was coined. One project that I was involved in included the development of a Corvette cradle, which had been aluminum; we changed it to a cast magnesium alloy using an ICME approach starting at the atomic level. Since 2006, it has been used in all Corvettes. Another ICME project was the design optimization of a steel powder metal bearing cap for an engine. Here, the multiscale modeling method was used for the process of compaction, springback during unloading, and sintering, and then the results were used for analysis of performance and fatigue life prediction. Weight savings, strength, and fatigue life were all improved. Greg Olson at Northwestern University has also employed the ICME idea in generating new metal alloys for structural applications and was a spiritual leader in a large DARPA project called AIM for tool integration to accelerate development and insertion of new materials. John Allison, while at Ford Motor Company, led an ICME effort within the company to analyze the fatigue life of cast engine products. Hence, others have been working on the ICME methodologies as well. It is hoped that other books will be published that include different perspectives. The term "ICME," although borne out of the multiscale modeling endeavors in the 1990s, was coined by Allison in a 2007 USAMP Lightweight Metals program of which I was (and am) a member. I am sure that there exist other projects that I have not mentioned here that have operated under the spirit of the ICME and multiscale materials modeling, but clearly the trend is that ICME is catching on as a new paradigm for design, development, and manufacturing of structural products.

A recent National Academy of Engineering (NAE) report (2008) defines ICME as the following: "an emerging discipline that aims to integrate computational materials science tools into a holistic system that can accelerate materials development, transform the engineering design optimization process, and unify design and manufacturing." The report stated the following regarding education:

> Implementing cultural change in the materials discipline will require the integration of ICME into the MSE curriculum if ICME is to become part of the identity of an MSE professional. With the recent reforms in engineering accreditation, the role of materials in design and the importance of computation in materials engineering undergraduate curricula are now recognized, and graduates must demonstrate the following:
>
> - An integrated understanding of the scientific and engineering principles underlying the four main elements of the field: structure, properties, processing, and performance.
> - The ability to apply and integrate knowledge from each of the above four elements of the field to solve materials selection and design problems.
> - The ability to utilize experimental, statistical, and computational methods consistent with the program educational objectives.

The objectives of this textbook are in line with these three areas from the NAE report.

I would like to thank some people who have influenced my thinking, guided my research, helped me learn the many aspects of ICME-related ideas, and helped me put this book together: Firas Akeshah, Doug Bammann, Mike Baskes, Rose Mary Dill, Youssef Hammi, Barbara Horstemeyer (my wife), Brian Jordon, Seong Gon Kim, Sungho Kim, Alan Kushner, Esteban Marin, Dave McDowell, Quenceng Ma, Amitava Moitra, Alan Needleman, Dean Norman, Kiran Solanki, Don Trotter, Paul Wang, and Hussein Zbib. Anita Lekhwani has been a great editor, helping me put this together and being a great cheerleader. My son, Christopher, and daughter, Nicole, have been a great source of inspiration for me. Finally, to all the students who have studied with me at Sandia and Mississippi State University: I want to thank you so much, because it is you who have allowed me to fulfill my destiny as a teacher, mentor, and coach.

Color figures and supplementary materials for this title may be found at ftp://ftp.wiley.com/public/sci_tech_med/icme_metals.

MARK F. HORSTEMEYER

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When trying to write such a book, the different collaborators come to mind, who helped me understand and appreciate the type of work required with those particular simulations at a particular length. Actually, I am overwhelmed with all of the helpers who guided me over the years in helping me formulate my thinking regarding multiscale modeling. The phrase from Isaac Newton arises: "I am here today, because I have stood on the shoulders of giants." Multiscale modeling really is a systems engineering approach, and it took a system of scientists and engineers to not only shape my thinking but also help in putting the appropriate information into this book.

I learned plasticity and damage mechanics from Doug Bammann, crystal plasticity and fatigue from Dave McDowell, dislocation dynamics from Hussein Zbib and Sebastien Groh, atomistic modeling from Mike Baskes, and quantum theory from Seong Gon Kim. Others who strongly influenced my thinking include Alan Needleman, Mike Ortiz, Wing Kam Liu, Greg Olson, and Tony Chen. My systems level thinking however was a reluctant gift that I received while working on a design team under Mim John, who taught me systems thinking and that everything should be viewed from a systems perspective. She and Mike Birnbaum were really the first managers to believe in my research capabilities. Without the influences from these individuals, this book would not be written.

Of course, my students, postdocs, and colleagues at Mississippi State University also helped me work on these Integrated Computational Materials Engineering (ICME) ideas since 2002. Special recognition goes to Amitava Moitra for helping me write Chapters 5 and 6 on the electronics structures and atomistic simulations models/codes, respectively. Firas Akasheh helped

CHAPTER 1

AN INTRODUCTION TO INTEGRATED COMPUTATIONAL MATERIALS ENGINEERING (ICME)

The concept of Integrated Computational Materials Engineering (ICME) arises from the new simulation-based design paradigm that employs a hierarchical multiscale modeling methodology for optimizing load-bearing structures. The methodology integrates material models, structure–property relationships that are observed from experiments, and simulations starting at the quantum level. At the structural level, heterogeneous microstructures are embedded in the finite element analysis. Because these microstructures are included, the paradigm shift from safety factors to predicting failure is fundamental.

ICME's opportunity has emerged because of the recent confluence of smaller desktop computers with enhanced computing power coupled with the advent of physically based material models. Furthermore, the clear trend in modeling and simulation is to integrate more knowledge into materials processing and product performance. I propose that ICME is the appropriate means to garner the required accuracy for a simulation-based design and manufacturing paradigm, and this book is a means for engineers to realize that goal. This first chapter includes Horstemeyer's [1] review of the various multiscale methodologies related to solid materials and the associated experimental influences, the various influences of multiscale modeling on different disciplines, and some examples of multiscale modeling in design of structural components.

1.1 BACKGROUND

Although computational multiscale modeling methodologies were developed in the very late 20th century, the fundamental notions of multiscale modeling have been around since da Vinci studied different sizes of ropes. The recent rapid growth in multiscale modeling arose from the confluence of parallel computing power, experimental capabilities that characterize structure–property relations down to the atomic level, and theories that admit multiple length scales. The ubiquitous research focused on multiscale modeling has since broached different disciplines (solid mechanics, fluid mechanics, materials science, physics, mathematics, biological, and chemistry), different regions of the world (most continents), and different length scales (from atoms to autos).

With the advent of accurate modeling and simulation and significant increases in economical computing power, virtual design and manufacturing provides the means to reduce product development time and cost while improving overall quality and manufacturing efficiency. However, the quality of the end product depends on the quality of the modeling with respect to the particular conditions involved and the computational efficiency of the simulations (e.g., plasticity and fracture of specific materials under extremely rapid stress conditions). Several case studies are later shown to demonstrate the important benefits of such analysis and design. The knowledge gained and the computational tools developed in these illustrations can then be rapidly applied to other product designs for structural components. Design optimization with different quality standards and uncertainty can then be achieved using virtual simulations with rapid turnaround—even more important in the context of optimizing the "system" with various subsystem and component trade-offs. The foundation for these results is built on the accuracy of the modeling and computational accuracy and efficiency. Accordingly, ICME offers the ideal venue for the simulation-based design and manufacturing paradigm that will be presented in this book.

1.2 THE APPLICATION OF MULTISCALE MATERIALS MODELING VIA ICME

Although this book is dedicated primarily to the application of ICME principles to the design and manufacture of structural materials with nonlinear behavior, the integrated circuits industry provides an analogy of the progress achieved in modeling components and systems with different modeling accuracies and utilizing multilevel simulation tools. Even with the huge advancements in parallel computing power, it is simply impractical to model a complete system that accommodates all possible application conditions (e.g., test conditions) with the highest-accuracy physics. However, these highly accurate physics models are able to capture the phenomena under various extreme

conditions and thereby provide the basis for more abstract models (e.g., current-voltage model of transistors), which are more computationally efficient. These transistor models become the basis for an even higher level of abstraction (e.g., switch level or logic gate level), which in turn becomes the basis for simulating logic blocks or subsystems over the greater range of test conditions with the environmental conditions already being validated by the lower level modeling. Often the systems are simulated using simply input–output logic signals with various degrees of timing delays determined from lower level simulations. Tools have evolved which support concurrent multi-level simulations (e.g., different logic blocks are simulated with different levels of accuracy and with appropriate interfaces between the simulation blocks in order to focus the computing power on particular issues).

These multilevel modeling and simulation tools support rapid virtual design without resorting to the time-consuming physical prototyping until there is sufficient confidence in the design. This virtual simulation capability further supports design optimization because it allows far more iterations than can be achieved utilizing physical prototyping and supports the evolution of more sophisticated and "tuned" design optimization tools, which become the basis of perhaps "automatically generated" subsystem design optimization. In turn, these simulation capabilities become the basis for designing for manufacturability and quality (e.g., selecting test vector conditions for physical testing to minimize expensive test time and correlating product test results to manufacturing variations to assure quality). It simply is not practical to consider designing modern electronic systems with several hundred million transistors on a "chip" without using these virtual computational tools. For such system complexity, a more rapid time-to-market provides a competitive advantage as well as saving costs.

The semiconductor and computer industries have been the leaders in developing these methodologies, representing a **significant paradigm shift** and providing a means for sustaining their phenomenal growth over so many years, illustrated by Gordon Moore's infamous laws of complexity doubling every 2 years and performance doubling every 18 months while maintaining equivalent costs. With such industrial productivity exemplified by the culture of "Silicon Valley," the competition drives new product development with rapid time-to-market being vital.

With the currently available computing power, the question remains: can a similar philosophy of multilevel modeling and simulation be utilized in material-based mechanical systems in order to achieve rapid time-to-market in product design and manufacturing? If so, what is the current state of knowledge and practice? What can one expect in the future? Clearly, the primary underlying issue relates to the multilevel material modeling (multiscale) involved in order to achieve the required accuracy and computational efficiency under the **associated conditions**.

Several detailed case studies are presented in this book to help the paradigm shift for employing multiscale modeling methods for structural and

mechanical designed components. In each example case, this book considers an aluminum alloy for instructional purposes and consistency, but the ICME methodology of multiscale modeling has been used for magnesium, steel, and other alloys.

Whether designing an automobile, airplane, building, or any structural system for that matter, large-scale systems tests are both expensive and time-consuming. However, the cost models for using virtual design methodologies that are physics based show significant reduction in the time-to-market and costs. The advantages include the following:

1. ICME can reduce the product development time by alleviating costly trial-and-error physical design iterations (design cycles) and facilitate far more cost-effective virtual design optimization.
2. ICME can reduce product costs through innovations in material, product, and process designs.
3. ICME can reduce the number of costly large systems scale experiments.
4. ICME can increase product quality and performance by providing more accurate predictions of response to design loads.
5. ICME can help develop new materials.
6. ICME can help medical practice in making diagnostic and prognostic evaluations related to the human body.

These benefits, which are now being realized, are the market drivers for such an explosion of multiscale modeling into various industrial sectors.

1.3   HISTORY OF MULTISCALE MODELING

The recent surge in multiscale modeling, from the smallest scale (atoms) to full system level (e.g., autos) related to solid mechanics, that has now grown into an international multidisciplinary activity, was birthed from an unlikely source. Since the U.S. Department of Energy (DOE) national labs (Los Alamos National Laboratory (LANL), Lawrence Livermore National Laboratory (LLNL), Sandia National Laboratories (SNL), and Oak Ridge National Laboratory (ORNL)) started to reduce nuclear underground tests in the mid-1980s, with the last one in 1992, the idea of simulation-based design and analysis concepts emerged. After the Comprehensive Test Ban Treaty of 1996 in which many countries pledged to discontinue all systems level nuclear testing, programs like the Advanced Strategic Computing Initiative (ASCI) were initiated within the U.S. DOE and managed by the labs. The basic premise of ASCI was to provide more accurate and precise simulation-based design and analysis tools. In essence, the numerous, large-scale systems level tests that were previ-

ously used to validate a design were no longer acceptable, thus warranting the tremendous increase in reliance upon simulation results of complex systems for design verification and validation purposes.

Because of the requirement for greater complexity in these simulations, advancing parallel computing and multiscale modeling became top priorities. With this perspective, experimental paradigms shifted from the large-scale, complex tests to multiscale experiments that provided material models with validation at different length scales. If the modeling and simulations were physically based and less empirical, then a predictive capability could be realized for other conditions. As such, various multiscale modeling methodologies were independently but concurrently created at the U.S. DOE national labs. In addition, personnel from these national labs encouraged, funded, and managed academic research related to multiscale modeling. Hence, the creation of different methodologies and computational algorithms for parallel environments gave rise to different emphases regarding multiscale modeling and the associated multiscale experiments.

Significant advances in parallel computing capabilities further contributed to the development of multiscale modeling. Since more degrees of freedom could be resolved by parallel computing environments, more accurate and precise algorithmic formulations could be admitted. This thought also drove political leaders to encourage the simulation-based design concepts.

At LANL, LLNL, and ORNL, the multiscale modeling efforts were driven from the materials science and physics communities with a bottom-up approach. Each had different programs that tried to unify computational efforts, materials science information, and applied mechanics algorithms with different levels of success. Multiple scientific articles were written, and the multiscale activities took different lives of their own. At SNL, the multiscale modeling effort was an engineering top-down approach starting from a continuum mechanics perspective, which was already rich with a computational paradigm. SNL tried to merge the materials science community into the continuum mechanics community to address the lower length scale issues that could help solve engineering problems in practice.

Once this management infrastructure and associated funding were in place at the various U.S. DOE institutions, different academic research projects started, initiating various satellite networks of multiscale modeling research. Technological transfer also arose into other labs within the Department of Defense and industrial research communities.

The growth of multiscale modeling in the industrial sector was primarily due to financial motivations. From the U.S. DOE national labs' perspective, the shift from large-scale systems experiments mentality occurred because of the 1996 Nuclear Ban Treaty. Once industry realized that the notions of multiscale modeling and simulation-based design were invariant to the type of product and that effective multiscale simulations could in fact lead to design optimization, a paradigm shift began to occur, in various measures within

different industries, as cost savings and accuracy in product warranty estimates were rationalized.

1.3.1 Bridging between Scales: A Difference of Disciplines

Synergistic systems thinking and interdisciplinary thinking bring about the concept of the whole being greater than the sum of the parts. This relates to the "integrated" part of ICME. Multiscale modeling requires that several disciplines interact, which has led to miscommunications and misunderstandings between communities, particularly about core multiscale modeling and the bridging methodologies between length scales.

Clearly, a key issue in multiscale modeling is how to handle the bridging. Without officially stating the bridging methodology, each discipline has its own methods. Before we discuss each discipline's bridging paradigm, let us consider an analogy of the Brooklyn Bridge in New York versus the Golden Gate Bridge in San Francisco. If one were to just translate the Brooklyn Bridge to San Francisco and call it the Golden Gate Bridge, one would find that the old adage of a "square peg in a round hole" applies. The Golden Gate Bridge required a design different from that of the Brooklyn Bridge because of what was required on each side of the bridge and the environments that must be sustained. In other words, the boundary conditions played a major role in the design of the bridge. The same notion needs to be considered when developing bridges for multiscale modeling between different length scales. However, the different research disciplines (materials science, applied mechanics, atmospheric sciences, etc.) tend to focus on the research at each pertinent length scale and not so much on the bridge. In fact, modern computational tools at each length scale were just recently published in Yip's [2] *Handbook of Materials Modeling*, which provides a thorough review of a wide variety of current tools; however, this work did not really deal with bridging methodologies.

In the next sections, the multiscale modeling methods are presented from the different disciplines' perspectives. Clearly, one could argue that overlaps occur, but differences in the multiscale methods arise based on the paradigm from which they originated. For example, the solid mechanics internal state variable (ISV) theory includes mathematics, materials science, and numerical methods. However, it clearly started from a solid mechanics perspective, and the starting points for mathematics, materials science, and numerical methods has led to other different multiscale methods. ICME starts from the materials perspective, but it is worth noting the context of other disciplines in this textbook.

Some general guidelines about length scale bridging include the following list. Keep in mind that terminology is often an issue when bringing different disciplines together. In the context of this writing, the term "upscaling" means basically a bottom-up approach in which the simulations are performed at a particular scale and the results are averaged in some sense to pass to the next

higher scale. Alternatively, "downscaling" is a top-down approach, like the ISV continuum theory that is defined at the continuum level but allows lower length scale features via the ISVs:

1. For both downscaling and upscaling, only use the minimum required degrees of freedom necessary for that particular length scale for the type of structural problem being produced (e.g., the ISV may need to have the grain size in some cases but maybe does not need it in other cases).

2. For both downscaling and upscaling, be consistent with the energy within the pertinent volume between length scales; note that the geometric effects will most likely not be the same between length scales within a volume.

3. For both downscaling and upscaling, verify the numerical model's implementation and usage before starting a sequence of calculations that might otherwise lead to erroneous results.

4. For downscaling, start with downscaling before upscaling to help make clear the final goal, requirements, and constraints at the highest length scale.

5. For downscaling, find the pertinent variable and associated equation(s) to be the repository of the structure–property relationship from subscale information.

6. For upscaling, find the pertinent "effect" for the next higher scale. Different methods can be used: analysis of variation (ANOVA) methods, computations, experiments, and so on.

7. For upscaling, validate the "effect" by an experiment at the particular length scale before using it in the next higher length scale.

8. For upscaling, quantify the uncertainty (error) bands (upper and lower values) of the particular "effect" before using it in the next higher length scale and then use those limits to help determine the "effects" at the next higher level scale.

1.3.1.1 Solid Mechanics Bridging (Hierarchical Methods). Inherent within the idea of multiscale modeling is the bridging methodology and the associated length scale of the feature that is necessary to gain the accurate physics required for the engineering problem [3]. To decide on the pertinent length scale for the feature of importance, one must consider that in modern solid mechanics, continuum theories are driven by the conservation laws (mass, momentum, and energy); however, there are more unknowns than the number of equations, so constitutive relations (sometimes erroneously called "laws") are required to solve the set of differential equations for finite element or finite difference analysis. Most modern solid mechanics tools employ finite element analysis. When developing a multiscale modeling methodology for the

constitutive relations, the kinetics, kinematics, and thermodynamics need to be consistent in the formulation. There are also certain classical postulates in continuum theory that guide the development of the constitutive theory (objectivity, physical admissibility, equipresence, and locality). Objectivity means that the equations must operate in a consistent manner no matter what frame of reference is used. Physical admissibility means that what is true to the material's behavior must be considered in the equations. Equipresence means that when using a variable in one equation, it must be used in all of the equations. Locality means that the observable variables, such as stress and strain, are related to each other just at the local point in space. Multiscale modeling has been driven by the physical admissibility postulate, and rightly so, at the expense of the postulates of equipresence and locality. In terms of multiscale modeling, physical admissibility means to identify the physical mechanism or discrete microstructural feature at the particular length scale that is a root source of the phenomenological behavior.

Two different general multiscale methodologies exist starting from the solid mechanics continuum theory paradigm: hierarchical and concurrent. The key difference is the bridging methodology. In concurrent methods, the bridging methodology is numerical or computational in nature, with the different length scale algorithms performed (essentially) concurrently. In the hierarchical methods, numerical techniques are independently run at disparate length scales. Then, a bridging methodology utilizing one of several methods (e.g., statistical analysis methods, homogenization techniques, or optimization methods) can be used to distinguish the pertinent cause–effect relations at the lower scale to determine the relevant effects for the next higher scale.

One effective hierarchical method for multiscale bridging is the use of thermodynamically constrained ISVs that can be physically based on microstructure–property relations. It is a top-down approach, meaning the ISVs exist at the macroscale but reach down to various subscales to receive pertinent information. The ISV theory owes much of its development to the state variable thermodynamics constructed by Helmholtz [4] and Maxwell [5]. The notion of ISV was introduced into thermodynamics by Onsager [6] and was applied to continuum mechanics by Eckart [7–8].

The basic idea behind the ISV theory is that, in order to uniquely define the Helmholtz free energy [4] of a system undergoing an irreversible process, one has to expand the dimensions of the state space of deformation and temperature (state variables commonly employed in classical thermodynamics to study elastic materials) by introducing a sufficient number of additional state variables that are considered essential for the description of the internal structure with the associated length scales of the material in question. The number of these ISVs is related to the material structure as well as to the degree of accuracy with which one wishes to represent the material response.

The ISV formulation is a means to capture the effects of a representative volume element (RVE) and not all of the complex causes at the local level;