1 Introduction to materials modeling and simulation

With the development of inexpensive, yet very fast, computers and the availability of software for many applications, computational modeling and simulation of materials has moved from being entirely in the hands of specialists to being accessible to those who use modeling not as their principal activity, but as an adjunct to their primary interests. With that change in accessibility of materials modeling and simulation come exciting new opportunities for using computational modeling to greatly advance the development and refinement of materials and materials processing.

The goal of this text is not to make experts – there are entire books on subjects that are treated in a few pages here. The text is, by design, introductory and we leave out many, if not most, details about implementation. We will present the key features and possibilities of computational materials science and engineering and discuss how to use them to advance the discovery, development, and application of materials.

1.1 MODELING AND SIMULATION

Before we start discussing materials modeling and simulation, it is appropriate to consider those words a bit more carefully. What do we mean by a "model" or a "simulation"? How are they different? Not to be overly pedantic, but it may help our discussion if we are a bit more precise in our definitions of these terms.

A *model* is an idealization of real behavior, i.e., an approximate description based on some sort of empirical and/or physical reasoning. A model most often begins life as a set of concepts, and then is usually transcribed into a mathematical form from which one can calculate some quantity or behavior. The distinction between a *theory* and a model is that, in the creation of a model, the attempt is to create an idealization of real behavior to within some accuracy, not a fundamental description that is strictly true.

A *simulation* is a study of the response of a modeled system to external forces and constraints. We perform simulations by subjecting models to inputs and constraints that simulate real events. A key thing to remember about simulations is that they are based on models. Thus, a simulation does not represent reality, rather it is a model of reality.

The accuracy of a simulation relative to the real system it is trying to emulate can depend on many factors, some involving the simulation method itself, for example the accuracy in numerically solving sets of equations. Often, however, the biggest errors in a simulation, at

least with respect to how well it describes a real system, are the inadequacies of the models upon which the simulation is based. Thus, we cannot separate simulations from the underlying models.

In this text, we deal with both models and simulations. We will discuss in some detail how to model specific materials behavior and how to create and understand the models and their limitations. We will also describe in detail many of the commonly used simulation methods, indicating some of the critical issues that must be addressed when developing accurate numerical methods.

1.2 WHAT IS MEANT BY COMPUTATIONAL MATERIALS SCIENCE AND ENGINEERING?

In the most general terms, Computational Materials Science and Engineering (CMSE) is the computer-based employment of modeling and simulation to understand and predict materials behavior. In practice, we generally make a distinction between computational materials science, in which the goals are to better understand and predict materials behavior, and computational materials engineering, which is focused on practical applications of materials, typically with an emphasis on products. We note that this distinction is arbitrary and not well defined, given that the basic methods are generally the same and it is the applications of those methods that have different goals. For this text, our focus is on the methods and we will not be concerned with the distinction between science and engineering.

We can use CMSE for many purposes. We could, for example, take a simple model that incorporates in some way the essential physical behavior of a system and then interrogate that model to describe the phenomenology of a process or property. The goal of such calculations is generally to seek understanding and not to describe the behavior in an accurate way. For example, a modeler could eliminate all the physical processes except one of interest, thus performing a "clean experiment" that sheds light on the role of that process in behavior – sort of an ultimate *gedanken* (thought) experiment. We could also, however, develop more detailed models and methods with the goal of predicting some property or behavior of a specific material, for example the prediction of the thermodynamic behavior of a new alloy or the mechanical properties of a doped ceramic. The models upon which such calculations would be based could be complicated or simple, depending on the actual goals of the study and the desired accuracy of the calculations. Both types of materials modeling are common and will be represented in this text.

CMSE is most powerful when it has a strong tie to experiment. At its simplest, experimental data can serve a validation of the accuracy of the models and the calculations based on them. However, when used together, CMSE can provide a deeper understanding of a materials system than possible by experiment alone by probing phenomena that experiments cannot see. Modeling can also predict behavior, whether under conditions for which we have no experimental data or as a screen for systems with so many parameters that performing all possible experiments is not feasible. Indeed, at its best, CMSE serves as an equal partner with experiment.

Unit	Length scale	Time scale	Mechanics
Complex structure	10^{3} m	10^{6} s	Structural mechanics
Simple structure	10^{1} m	10^{3} s	Fracture mechanics
Component	10^{-1} m	10^{0} s	Continuum mechanics
Grain microstructure	10^{-3} m	10^{-3} s	Crystal plasticity
Dislocation microstructure	10^{-5} m	10^{-6} s	Micro-mechanics
Single dislocation	10^{-7} m	10^{-9} s	Dislocation dynamics
Atomic	10^{-9} m	10^{-12} s	Molecular dynamics
Electron orbitals	10^{-11} m	10^{-15} s	Quantum mechanics

Figure 1.1 Length and time scales in materials science adapted from [12]. On the left, we indicate the important unit structure at each scale, in the middle, the approximate length and time scales, and at the right, the approach used to simulate the material's mechanical behavior.

1.3 SCALES IN MATERIALS STRUCTURE AND BEHAVIOR

The modeling and simulation of materials is challenging, largely because of the extreme range of length and time scales that govern materials response. Length scales that govern a phenomenon may span from the nanometers of atoms to the meters of engineered structures. Similarly, important time scales can range from the femtoseconds of atomic vibrations to the decades of use of materials in products. Given the range of physical processes at each of these scales, it should not be surprising that no single technique will work for all scales. Thus, many methods have been developed, each focused on a specific set of physical phenomena and appropriate for a given range of lengths and times. In this text we will provide a background into some of the most important of these methods.

In Figure 1.1, we show a schematic view of the important length and time scales for just one type of materials behavior – the mechanical behavior of crystalline materials [12]. This figure is just an example – similar tables could be developed for other properties as well.

In the left column of Figure 1.1, we list the fundamental structural "unit" whose behavior dominates the materials response at the given length and time scales.[1] At the smallest scale, that "unit" represents the electrons in the solid, while at the largest scale it is some sort of complex structure (e.g., the wing of an airplane). In between are the other structures that matter for the scales listed: atoms, dislocations, grains, etc.

Consider as an example the general range of 100 microns to 10 millimeters, in which the dominant structural features in a material are the grains (in this schematic view). It is the behavior

[1] If these terms are unfamiliar, please see Appendix B for a brief introduction to materials.

of the ensemble of those grains that dominates the mechanical response of the material at that scale. Of course, the deformation behavior of a grain depends on the dislocations, which depend on the atoms, which depend on the bonding. Thus, the behavior at each scale is dependent on what happens at smaller scales. In a model of the deformation of a set of grains, while we may explicitly include the dislocations (and atoms and electrons), more likely we will develop a model that reflects, in some averaged way, the behavior of the dislocations (and atoms and electrons). That model will describe the mechanical behavior at the grain level (and is usually referred to as "crystal plasticity").

Each scale in Figure 1.1 reflects behavior that is dominated by its structural "unit", which is described by its own set of models. For example, consider the range of length scales from 1 Å to 100 microns (10^{-10} to 10^{-4} m). At the smallest of these scales, the bonding between atoms dominates the behavior. This bonding arises, of course, from the underlying electronic structure and to describe it requires the use of methods that can calculate the distribution of electrons. Such methods require quantum mechanics and are described (briefly) in Chapter 4. At a somewhat larger scale, we need to consider the behavior of many atoms. While we can use electronic structure methods to describe the bonding, in general those methods are so complicated that we must approximate the bonding with some sort of empirical or approximate function. Such functions are called interatomic potentials and are discussed in Chapter 5. The interatomic potentials are thus models of the interactions between atoms. To understand the behavior of the atoms, we must simulate their behavior, which we can do with various atomistic simulation methods, such as molecular dynamics (Chapter 6) or the Monte Carlo method (Chapter 7). As discussed above, if we use a model for the interatomic interactions then we are not simulating the material, but rather a model of the material, and our results will be good only to the extent that the model represents the true interactions.

At still larger scales, there are too many atoms for us to consider, so we must find new approaches that focus on the dominant "units". These units may be dislocations, grain boundaries, or some other defect, and the simulations are based on these defects being the fundamental units. The length scale that is dominated by defects is often called the *mesoscale*.[2] We describe a number of mesoscale modeling methods in Part III of the text.

As we will see, while great strides have been made in extending the *length* scales of many of the simulation methods we will cover here, often the methods are still very restrictive in their ability to describe *time* scales of the order of what we measure in the laboratory. For example, we will see that molecular dynamics methods, used to describe dynamic motions of atoms, have a fundamental time scale in the 10^{-14} seconds range and atomistic simulations of more than a few nanoseconds are challenging.[3] Thus, even for problems for which an approach can describe the length scale, often we must find new approaches to also cover the time scales of interest.

[2] There is no definitive definition of what the "mesoscale" is. For our purposes, it represents the length and time scales between phenomena that can be described by atoms and those that can be described by continuum theories.
[3] Advances have been made in *accelerated dynamics* methods, which will be discussed in Chapter 6.

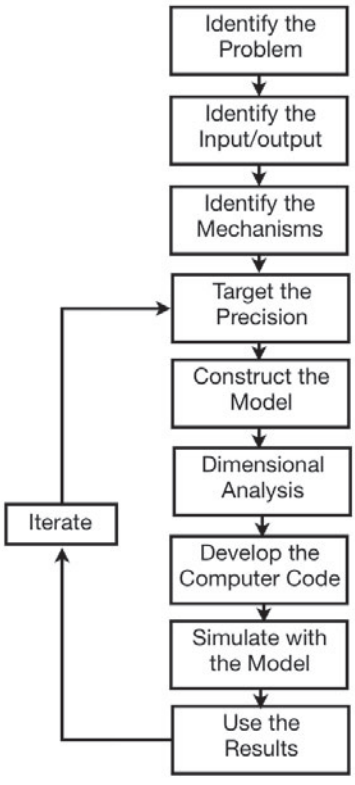

Figure 1.2 The stages in model development, adapted from [12].

1.4 HOW TO DEVELOP MODELS

The first, and most important, step in any computational materials project is the creation of a model that describes the properties of a material at the length and time scales of interest. Here we want to introduce the logical steps one takes to create a model. Our discussion is based on a very useful article by Ashby, in which he describes a process for the systematic development and validation of materials models [12]. He gives a flow chart for the modeling process, which we reproduce in a somewhat streamlined fashion in Figure 1.2.

It may seem obvious, but the first step in model development is to identify the problem (given at the top of Figure 1.2). Often models go astray because the developer does not start with a clear idea of what he or she is actually trying to model. This type of misstep may arise from not understanding the problem well enough or from just not thinking through what the model has to accomplish.

Given the problem, the next step in any model development must be to specify what information the model is going to yield and what information one has at hand to use in that model – in other words, the outputs and inputs. This step is critical, and one that is often not well considered. Ignoring information that may be important can lead to either poor-quality or overly complex models (or both), creating problems for any subsequent simulations.

The next step is the identification of the physical mechanisms, which is often the most challenging part of any modeling effort. We may not have a complete picture of the fundamental phenomenology of a problem. It is in this step that modeling at a smaller scale often comes into play, serving to help identify the underlying physical processes at the larger scale. Close examination of experimental data and trends also can lead to the development of a clearer understanding of the physical mechanisms.

While identifying the problem, the inputs and outputs, and the mechanisms that define the framework for the real work of model development, it is also essential to specify the necessary quality of the model. Models should be no more complicated than needed for a specific problem. Anything more is a waste of effort. Seeking perfection in a model generally leads to high complexity, which may present difficulty when one has to "interrogate" the model, i.e., when one actually calculates something based on the model.

After creating the model, the simple act of doing a dimensional analysis often shows where the model might be incorrect. Dimensional analysis is a way to check relations among physical quantities based on their dimensions. A simple consequence of physics is that any equation must have the same dimensions on the left and right sides. Checking that the dimensions are equal is the basic step of dimensional analysis. We cannot stress enough the value of dimensional analysis as a check of the model as well as a tool to help group variables. Why group variables? As we shall see below, often two models that look very different can be shown to be quite similar when put in the same form. Recognizing such similarities can help avoid much unneeded effort.

Models are useless unless one can do something with them, which generally requires implementation into a computer code of some sort. Often this step has a major influence on the form of the model – if a model cannot be implemented or would require too much computer time to use, then it is not useful. There is thus often a balance between the desired accuracy of a model and the ability to actually use it in a calculation.

After implementation, the next step is the real point of CMSE, namely to calculate something with the model, i.e., to interrogate how the model works. This may be a *validation* step, in which predictions of the model are compared to available experimental data, theory, etc. to assess the quality of the model, the range of its validity, sensitivity to parameters, etc. One often uses this comparison to tune the model to make it more accurate and robust. It is not uncommon to go back to the construction of the model at this point to adjust its form so that it better meets the needs of the calculations. Of course, the reason for model development is to use the model to calculate some material property or function. What that "something" is depends on the problem. We note that a critical component of this step is to display the results in such a way so as to show its important features.

In this text, we shall use the process in Figure 1.2 often as we create models. While we shall rarely show the explicit links to these steps, they underlie all of what we do.

Before closing the discussion of model building, we would like to emphasize the importance of the Verification and Validation process (V&V). While validation is an attempt to assess the quality of the model to describe some behavior, *verification* is the process of ensuring that the computer code actually calculates what was planned. The goal is to model materials response. To ensure that we are doing so accurately requires both a good model and a proper implementation

of that model into code. Too often, one or both of these processes are shortchanged, leading to poor simulations. If one is basing an engineering decision on simulations based on a model, the V&V process may be, quite literally, life-saving.

1.5 SUMMARY

Computational materials science and engineering is a field that is growing in capabilities and importance. The goal of this text is to introduce students to the basics of the most important methods used to simulate materials behavior. We are not intending to create experts, but rather to serve as the first introduction to what is a very exciting field.

Part One

Some basics