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Introduction to Modeling and Simulation (IM/S) – spring 2006
MWF 3-4 PM
Tutorial: MW 7:30 - 9

Lecture Intro1 (2/8/06) Overview of Modeling and Simulation

To get started thinking about this subject we begin with three simple questions.

Why Modeling and Simulation ?

Modeling is a fundamental and quantitative way to understand complex systems and phenomena. Simulation is complementary to the traditional approaches of theory and experiment. Together, they (Mod/Sim) make up an approach that can deal with a wide range of physical problems, and at the same time exploit the power of large-scale computing. This paradigm is becoming increasingly widespread in a number of disciplines in science and technology, giving rise to active fields of studies such as computational physics, chemistry, mechanics, and biology, to name just a few. Through modeling and simulation one can readily cross over from one discipline to another, which is to say that the basic concepts and techniques one learns are applicable to problems seemingly very different at the surface.

Why teach Mod/Sim at the UG level ?

Mod/Sim studies are mostly being carried out at the graduate and postgraduate levels. But there is no reason why the undergraduates cannot participate in a meaningful way and benefit from the physical insights and technical know-how that these activities can provide. We believe that engaging the undergrads broadly across the Institute through a team of multidisciplinary faculty, as instructors and mentors, can succeed at MIT. The students would gain a broader academic exposure than what they would normally encounter within their own departments. Because this is a new way of teaching and networking among the faculty, everyone who participates can contribute to the success of this experiment, and in turn learn a great deal about studying across traditional boundaries. Intro Mod Sim is receiving considerable support from the Dean of Engineering and has the blessings of the department heads of all the participating units. In many ways, a subject like this is an experiment in educational innovation. We hope the students will get into the spirit and work with us to make it a worthwhile experience for all concerned.

What are the aims of Mod/Sim ?

We expect the students will gain a significant appreciation of the broad use of modeling in several fields of science and engineering, acquire hands-on experience with simulation, ranging from basic use of computers to advanced techniques, and develop communication skills by working with practicing professionals. Additional benefits

could come from further interactions with the faculty afterwards, such as mentoring, UROPs, thesis supervision, etc.

This subject will be taught in terms of lectures grouped into two parts, **Continuum Methods (CM)**, and **Particle Methods (PM)**, the latter includes methods that use **quantum mechanics**. These make up the majority of the simulation methods used in implementing and investigating the physical models. Each part spans over several weeks and will have problem sets to go with the lectures. At the end of each part, there will be a quiz. Another significant part of this subject is the **Term Project** with a class presentation towards the end of the semester. This allows the students to develop and pursue in more depth individual interests in modeling and simulation, working with a faculty supervisor from the team of instructors. Basis of grading in the course is: homework (40%), quizzes (20% each) and Term Project (20%). Through it all, the students have an opportunity to learn concepts in thermodynamics, statistical mechanics, quantum mechanics, solid and fluid mechanics, materials science, condensed matter physics, chemical and bio physics, in a modeling and simulation applications context.

In this first part of the Overview, we will consider briefly what we mean by **modeling** and give several examples. In the following introductory lectures we will explain the different **simulation** methods to be introduced in Intro Mod Sim (IM/S), along with illustrations.

We regard a model as a **simplified** description of an actual system, capturing certain essential aspects for use in studying the system behavior. Models are used in every branch of science; they are tools for dealing with complex systems and the interactions of their constituent parts. Scientists and engineers have long used models to better understand the systems they are studying, for analysis and quantification, performance prediction and design.

Quoting M. F. Ashby of Cambridge University who is very well known for his insights and contributions on developing useful models in materials science and engineering [M. F. Ashby, in *J. Computer-Aided Materials Design* **3**, 95 (1996)]:

"A model is an idealization. Its relationship to the real problem is like that of the map of the London tube trains to the real tube systems: a gross simplification, but one that captures certain essentials. The map misrepresents distances and directions, but it elegantly displays the connectivity. So it is with all successful models: they unashamedly distort the inessentials in order to capture the features that really matter. At worst, a model is a concise description of a body of data. At best, it captures the essential physics of the problem, it illuminates the principles that underline the key observations, and it predicts behaviour under conditions which have not yet been studied."

In the monograph, *Modeling and Simulation* (A. K. Peters, Wellesley, MA, 1994), Chap 1, Hartmut Bossel wrote:

"Models and simulations have always been an essential part of the human experience ... Models and simulations of many kinds are tools for dealing with reality: they are as old as humanity itself ... Even thousands of years ago, buildings, boats, and machines were first tested as small models before being constructed on a larger scale ... As scientists identify generalizable principles and processes, they construct models which are used to investigate and simulate new possibilities which lead to new technologies and opportunities ... The fact that computers can process quickly and precisely any mathematical or logical formulation in arbitrary combinations widened the applicability of modeling and simulation to anything -- in any form -- that can be formalized and made computable. This development led to new possibilities in almost all domains of human experience: for representing hitherto hardly accessible complex systems, for simulating their dynamics, and for understanding systems and dealing with them better than before."

Based on these thoughts we propose an all-purpose definition of modeling and simulation:

*“Modeling is the physicalization of a concept,
Simulation its computational realization”*

Types of models we will study in IM/S -- a physical system can be described at different levels:

- (a) a collection of nuclei and electrons (**electronic-structure** level)
- (b) a collection of atoms and molecules (**atomistic** or molecular)
- (c) a set of coupled structural elements (**finite-element**)
- (d) a medium described by fields and distributions (**continuum**)

In terms of details, (a) has the most details (note we are not considering the protons and neutrons that make up a nucleus, that would take us into the domain of nuclear physics). At each level one can construct a model that can be used to analyze the system properties and behavior.

When is a model useful? When a complex system can be simplified (reduced) to a tractable level that makes clear the essential structure of system and how the internal constituents interact with each other.

Key to a good model lies in what and how simplification is introduced; it is very important to understand what aspects of the system the model is intended to describe, and what are the model's limitations as a result of the simplification.

Suppose we are interested in studying a Cu crystal at the atomistic level. This means our model is a collection of N atoms of Cu which interact with each other through a potential energy $U(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$, where $\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N$ denote the positions of atoms 1, 2, ..., N respectively. Suppose U is given (the model is specified). With the knowledge of U and the lattice structure of Cu (this is not considered part of the model because Cu

crystals are known to have the face-centered cubic structure), one can begin to calculate the various properties of Cu crystal. How? There are different ways, some very approximate while others can be quite rigorous and computationally intensive. Each method of calculation that one wants to adopt may be called a **simulation**; in this sense simulation is the process by which one investigates a particular model. One should be aware of this distinction we are making between modeling and simulation is not always followed in the community.

It is not all that surprising that simulations can be performed at different levels of length and time scales. This is because over the years methods of simulation have been developed to focus on certain kinds of properties or phenomena. Since any physical process can be considered at different length scales, it follows that the most appropriate simulation method is determined by the length scale of interest.

To illustrate the multiscale nature of a physical problem, consider the deformation of a piece of material in a compression die, as shown in Fig. 1-1. As the material is deformed into a new shape, one can imagine looking at the material under a microscope at greater magnifications. What may seem to be a structureless material on a large length scale will soon reveal the presence of particulate inclusions. So the material is actually not a single phase. With further increase in resolution one finds that even in a single-phase region the material is made up of many grains of crystals. And if one zooms into one of the crystallites, a single

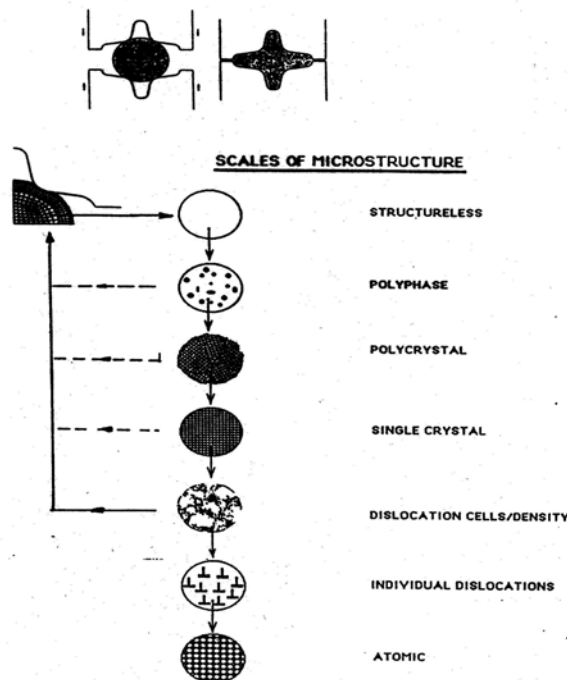


Fig. 1-1. A material, initially in a spherical shape, is being squeezed in a closed-end die into a star shape. Schematic shows the microstructure details on different length scales, illustrating what one would see under a microscope with increasing magnification.

crystal, one sees that instead of being a perfect lattice there are defects such as dislocation lines which form their own patterns in response to the deformation. Going further to still finer scales, the dislocations have core structures which may be studied in terms of the atomic registry (relative to the perfect lattice). In the figure one stops at the individual atoms. If one were to look inside an atom, one would see the electronic orbits and the nucleus, or go inside the nucleus to see the individual nucleons (protons and neutrons), etc.

As the material undergoes deformation in Fig. 1-1, changes will take place at each level. This is nature at work. Whether we see all the changes or only some of them depends on the length scales on which we operate. Some of us operate at the large length scale, the continuum level, and others may work at the atomistic level. It is quite possible that these two groups will see completely different manifestations of the deformation, both are correct and relate to the same process. If the two groups can communicate with each other and share their observations, then there is a greater likelihood of a more complete understanding of the deformation phenomena. Otherwise, the two pieces of puzzle are not connected, resulting in a state of imperfect knowledge and the possibility of erroneous extrapolations in predicting the system response beyond the range of observation.

Because of our limitations in dealing with the complexities of natural phenomena, it is conventional to address only part of the problem by confining the study to a certain length scale where theoretical models and computational methods appropriate only this length scale have been developed. There are four such characteristic length scales in the development of so-called multiscale materials modeling approach; they are illustrated in Fig. 1-2.

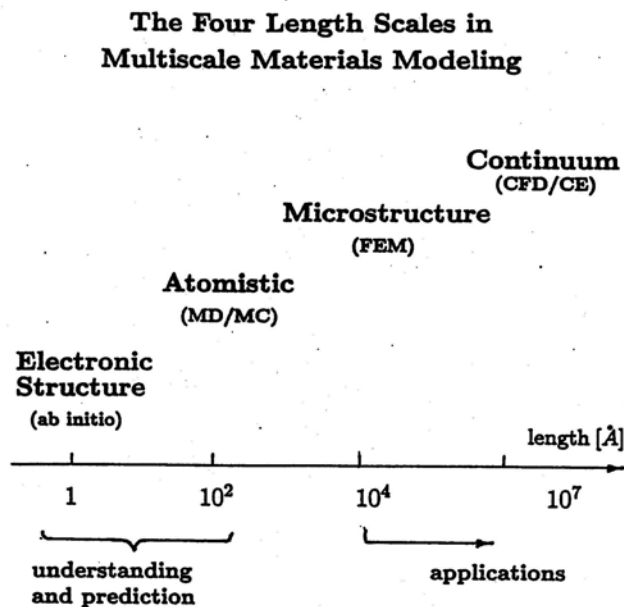


Fig. 1-2. The four characteristic scales of multiscale materials modeling - electronic structure, atomistic, microstructure, and continuum. Different simulation methods have been developed for each scale. Current challenge is to pass information naturally from one level to another.

The concept of multiscale modeling is to link up the different simulation techniques that have been developed for a particular length (and corresponding time) scale. Fig. 1-2 shows the hierarchy of scales typically considered important, each representing an active area of methodology development and application. Together they constitute the multiscale approach. Current challenge is to connect one simulation technique to another in order to be to make use of the fundamental knowledge and prediction developed at the lower scales in applications at the larger scales. In the case of nanotechnology, the information generated at the electronic structure and atomistic scales can be used directly.

The remaining part of the lecture is devoted to showing a few examples of molecular dynamics simulation of mechanical deformation.