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Editor's Choice

A model-to-model interface for concurrent multiscale simulations

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ABSTRACT

We present a low-level model-to-model interface that will enable independent models to be linked into an integrated system of models. The interface is based on a standard set of functions that contain appropriate export and import schemas that enable models to be linked with no changes to the models themselves. These ideas are presented in the context of a specific multiscale materials problem that couples atomistic-based molecular dynamics calculations to continuum calculations of fluid flow to examine the influence of interactions of the fluid with an adjacent solid on the fluid flow.

1. Introduction

Multiscale modeling is ubiquitous in science and engineering, arising in many and quite divergent domains, from the design of materials to simulations of power plants. All of these systems are governed by important features that control their behavior at multiple scales of length and time. Describing such systems often depends on having independent models based on differing physics for each scale [1,2].

Integrated modeling [3,4], which can be defined as modeling that "includes a set of interdependent science-based components (models, data, and assessment methods) that together form the basis for constructing an appropriate modeling system" [3], provides a structure to develop and organize the relevant information about a multiscale system and to apply that information to model the behavior of that system in response to external forces. The challenges of creating such integrated modeling systems are common to many disciplines. The environmental modeling community, for example, has been very active in this area, driven by their need to coordinate between various disciplines and to integrate a wide range of models that are often developed autonomously and independently from the integrated modeling efforts, and generally by experts who may not be tightly connected to the overall effort [3,4]. Inclusion of new models and codes into an integrated modeling system thus often requires coordination between disparate groups, which can inhibit addition of new capabilities into the integrated scheme. As discussed in more detail below, we have similar challenges in multiscale materials modeling.

In this paper we present an approach to integrated modeling based on the development of a model-to-model interface that enables independent models to be more readily linked into an integrated system with no changes to the models themselves. We examined a number of existing technologies for linking models, all from environmental modeling. While these systems have not been applied to systems with the range of scales found in materials, their basic structures provide an excellent starting point for creating integrated multiscale materials models. The models we examined include the Bespoke Framework Generator [5], Earth System Modeling Framework - Flexible Modeling System [6], OASIS (Ocean Atmosphere Sea Ice Soil) [7], and CSDMS (Community Surface Dynamics Modeling System) [8]. All of these systems require models to have *initialize*, *run*, *finalize*, *get*, and *set* functions (examples are described below) for basic control over models. Also generally required by these couplers is a description of how the models are connected together, which is done in the form of an XML file or some other type of configuration file. OASIS and CSDMS have an additional advantage of having GUI's that allow placing the models and their connections into the interface for visualization and automated configuration file generation. CSDMS also uses Babel [9] to allow model writing in different languages (C++, C, Fortran, XML, Python, and Java are supported) whereas the other couplers are limited to models all being in the same language.

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After consideration of the attributes of the various approaches, we have chosen to adapt the basic methodology of the CSDMS approach, which is based on the use of a low-level model-to-model interface, for linking materials models together. The purpose of this paper is to give an example of how to construct such an interface within a multiscale problem, with a focus on the types of information that must be passed from one model to another.

The biggest challenge for computational materials science is the extreme range of length and time scales that govern materials behavior, ranging from the Å and sub-picoseconds of atomistic behavior to the meters and years of materials in engineered applications. In between those extremes lie complex sets of physical phenomena that depend on the overall material behavior of interest and the type of material. We show a simple example of this range of mechanisms in Fig. 1, highlighting the various scales that govern the mechanical behavior of metallic materials [10]. Consideration of other types of materials or other properties would lead to a similar, but not identical, figure.

Looking more closely at Fig. 1, we see that at each scale there is a structural "unit" that dominates the physical processes at the given length and timescales. These units are the entities whose dynamics define the physics of interest at each scale. Typically, a set of models of materials behavior is created for each of the various scales [2,11]. These models are generally developed and used by different groups. In the traditional view of computational materials science, this hierarchy of models and simulations, each describing a specific scale and its associated phenomena, are linked to create a multiscale description of materials behavior. Typically, information is passed sequentially from scale to scale, an approach that is often referred to as information passing or sequential multiscale [1]. Inherent in the information-passing paradigm is the lack of inverse models that would allow us to predict the needed structures and properties at the small scale from desired properties at a larger scale – information flows only one way. It is common that information passing is done be separate groups of researchers, using codes specific to the scales of their particular interests.

While the information-passing approach has proved useful for many systems and properties, it is, at its core, suspect in a number of ways. Information passing assumes that there is a separation of scales, which is not always clear. It is inherently a coarse-graining procedure, which loses information at each step, especially about the distribution of properties other than their mean. Indeed, this latter statement reflects the fundamental flaw of this approach – it assumes that we can start from fundamental laws and build up to a description of a macroscopic system, which is not obviously true [12].

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

Fig. 1. Length and time scales in materials science adapted from Ashby [10]. 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. We note that the approaches used at each scale are generally distinct to that scale and, most often, are developed and used by different research groups.

Another approach, which is often referred to as "concurrent multiscale" [1], links simulations at differing scales directly within a single integrated framework. This approach has the advantage of enabling the flow of information between scales, which eliminates many of the uncertainties inherent in the information-passing paradigm. For recent examples, see [13–15]. As in sequential multiscale simulations, models must be developed and applied at multiple scales, with the added complication of developing appropriate interfaces between the models that enable them to be used concurrently. As we will discuss in detail below, the integrated approach described here provides for an efficient construction of integrated multiscale materials models.

We will present these ideas in the context of a specific problem, involving the interaction between an atomistic scale and a continuum scale, to serve as an example of the types of problems inherent in multiscale modeling of materials. Specifically, we use molecular dynamics to examine the interactions between a fluid and an underlying solid to set the boundary condition between a continuum fluid (described using the Lattice Boltzmann method) and the solid. Our focus is not on fluid properties, per se, but rather on how one connects an atomistic scale to a continuum scale in the context of creating a model-to-model interface to link together independent multiscale models.

We describe the basic methodologies in Section 2, followed by a description of our implementation of a basic model-to-model interface in Section 3, in which we discuss modifications to the CSDMS approach necessary for our test problem. Section 4 is a summary of results from an application of model, with comments about the efficiency with the model interface. Concluding remarks are given in Section 5.

2. Coupled multiscale model of surface-fluid interactions in couette flow

The goal of this work is to provide a method for coupling multiscale simulations using a low-level model-to-model interface. We focus on an example problem in which we examine the role of surface interactions on Couette flow, which is the laminar flow of a viscous fluid held between two plates, with one plate moving at some velocity relative to the other, fixed, plate. In traditional computational solutions to Couette flow, the velocity of the fluid at the stationary plate (which we will refer to as the slip velocity) is assumed to be zero and a linear increase of velocity is seen between the two plates. In this sample problem, our goal is to examine the role of fluid-surface interactions on determining the slip velocity by incorporating realistic descriptions of the interactions between atoms in the fluid and those on the surface of the solid. We model the system using a lattice Boltzmann method for the continuum fluid flow coupled to a molecular dynamics simulation of the interaction between the atoms of the fluid and the underlying surface. The models operate at different scales and are based on different physics so provide a good case for understanding information mediation in multiscale simulations. We note that this problem has been used previously as an example of coupled multiscale simulations, though without the model integration strategy introduced here [e.g., [16]].

2.1. Lattice Boltzmann (LB) method

The lattice Boltzmann (LB) method [17] was introduced in the 1990 s to address deficiencies in the lattice-gas cellular automaton