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Multiscale Methods for Emerging Technologies

Preface

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The last few years have seen exciting new developments in micro and nanotechnology. For example, advances in nanoelectronics, micro and nanofluidics, micro and nanoelectromechanical systems (MEMS and NEMS), materials and bionanotechnology have led to the development of miniaturized devices and systems with applications ranging from health care to defense to consumer products. The design of these miniaturized devices and systems (also referred to as mixed-technology devices and systems) is at the cutting-edge of interdisciplinary research typically involving the integration of mechanical, materials, electrical, chemical and biological principles. There is now a critical need to develop computational design tools to enable rapid computational prototyping of these mixed-technology micro and nanosystems. The development of accurate and efficient computational design tools is, however, challenging because of the limitations with atomistic simulations and the continuum theories, i.e., atomistic simulations can be accurate, but are inefficient and impractical for large systems and long timescales; similarly continuum theories can be inaccurate for miniaturized devices with atomistic features. As a result, computational design tools, that can bridge the various length and time scales, are central for further advances in micro and nanotechnology.

An exciting and challenging area of research in Computational Science and Engineering is the development of efficient and accurate multiscale methods to bridge the length- and timescales encountered in various applications. For example, the design of nanoelectromechanical systems could be critically dependant on the bond-breaking phenomena that occur at sub-nanometer scales and sub-nanosecond timescales. The transport of water through nanochannels depends strongly on the interfacial water properties (e.g., hydrogen bonding dynamics), which need to be resolved at the Angstrom/pico-second level, though the overall flow phenomena occurs at a length scale of 1 nm ~ 100 nm and a timescale of 1 ns ~ 1 sec. Similarly, the functional behavior of a cell (which is several micrometers in size) depends critically on the selective ion transport through the nanometer scale pores embedded in the cell membrane, whose function can only be described by studying the channel structure with

sub-Angstrom resolution. A variety of multiscale methods combining density functional, tight-binding, molecular dynamics, Monte Carlo, and continuum theories have been reported in the literature. However, many of the existing multiscale techniques are not very general and the development of efficient and accurate multiscale methods is still an open problem. This special issue contains several papers that address the development of multiscale methods for emerging technologies.

Sastry, Johnson, Goldberg, and Bellon report on the use of genetic programming—a genetic algorithm that evolves computer programs—for bridging simulation methods across multiple scales of time and/or length. They demonstrate the effectiveness of the genetic programming in multiscale simulations by using two case studies: multi-timescale materials kinetic modeling and the development of constitutive relation between macroscopic variables using measured data.

Guo, Datta, Lundstrom and Anantram report on multiscale modeling of carbon nanotube transistors. Specifically, they report on the simulation of carbon nanotube field-effect transistors (CNTFETs) by self-consistently solving the Poisson and Schrödinger equations using the non-equilibrium Green's function (NEGF) formalism. The paper also provides a discussion of how semi-empirical device level simulations can be connected with ab initio, continuum, and circuit level simulations in the multi-scale hierarchy.

Drews, Braatz, and Alkire report on the development of a (2+1)D kinetic Monte Carlo (KMC) code for coarse-grained as well as atomic-scale simulation of copper electrodeposition with additives. The physical system used in this paper is similar to that used by the microelectronics industry to fabricate on-chip interconnects, where additives are used to tailor shape evolution. The authors report that the surface roughness at a specified length scale can be accurately simulated by using the coarse-grained KMC code with lattice spacing of 1/10 or smaller of that the specified length scale. This result is particularly useful for comparing experimental data on surface roughness with numerical simulations.

Deshmukh, Mhadeshwar, Lebedeva, and Vlachos discuss hierarchical multiscale simulation of microchemical devices that exhibit a wide spectrum of length- and timescales. The authors use semiempirical models in conjunction with density functional theory to develop quantitative microkinetic models. Three examples of model reduction have been discussed as a means of reducing the degrees of freedom of lower length scale models for passing filtered information to larger length scale models as one moves up on the multiscale ladder of tools. Using the multiscale simulation tools, the authors show that the catalyst surface area is crucial for enhancing the microreactor performance.

Rudd describes concurrent multiscale modeling of nanomechanical systems using two techniques. The first technique, the Coarse-Grained Molecular Dynamics (CGMD) approach, describes the dynamics on a mesh of elements, but the equations of motion are built up from the underlying atomistic physics to ensure a smooth coupling between regions governed by different length scales. The second technique is a hybrid Coupling of Length Scales (CLS) methodology, where molecular dynamics is combined with conventional finite element modeling to greatly reduce the computational cost. The author discusses the two techniques in detail and presents results on the size effects in the elasticity and dissipation of nanomechanical systems.

Qian and Gondhalekar report on a Virtual Atom Cluster (VAC) approach for the mechanics of nanostructures. The VAC model is proposed as an effective representation of the interaction at atomic scale and can be linked to coarse scale simulation methods based on meshfree or finite element methods. In contrast to the crystal elasticity model, continuum concepts,

such as strain and stress, are completely removed from the VAC model. However, the VAC model is built on the underlying interatomic mechanics, and this link guarantees the accuracy in describing the mechanics of the nanostructure.

Ayton and Voth report on a multiscale methodology that is capable of modeling complex biomolecular systems across disparate length- and timescales. The disparate length- and timescales associated with biological assemblies are bridged by combining mesoscopic simulation methods with nonequilibrium molecular dynamics (NEMD) at the atomistic level. To demonstrate the multiscale methodology, the authors report on the simulation of Large Unilamellar Vesicles (UUVs) immersed in a solvent.

Properties of molecules confined in carbon nanotubes can be used to design environmental and pharmaceutical applications. Lee and Sinnott report on the comparison of the dynamic transport of methane and oxygen through open single-walled carbon nanotubes using classical nonequilibrium molecular dynamics simulations. The authors report that for nanotubes with diameters below 2 nm, the gas molecules diffuse via normal-mode, single-file, and superdiffusion modes depending on the properties of the nanotubes. They also show that the molecular transport can transition from one diffusion mode to another, and the mass transport system changes from nonequilibrium to near-equilibrium behavior over the course of the simulations.

Wijesinghe and Hadjiconstantinou discuss hybrid atomistic-continuum methods for multiscale hydrodynamic applications. The authors consider both dense fluid and dilute gas formulations and present incompressible and compressible hybrid methods. The incompressible framework is based on the Schwartz alternating method, which provides timescale decoupling. The compressible method is a multispecies, fully adaptive mesh and algorithm refinement approach that introduces the direct simulation Monte Carlo (DSMC) at the finest level of mesh refinement.

Qiao and Aluru present an embedding multiscale approach and its application to the electroosmotic transport in micro and nanochannels. The central idea in the embedding multiscale approach is as follows – to analyze a coarse-scale problem in which atomistic details are important in certain critical regions, atomistic simulations are first performed on a fine-scale system to obtain quantitative information of the system behavior in the critical regions; the quantitative information is then incorporated into the continuum simulation of the coarse scale system. As an application of the technique, the authors show results for electroosmotic flow in a 30 ◎m wide slit channel.

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