SPECIAL SECTION ON MULTISCALE MODELING IN MATERIALS AND LIFE SCIENCES

This special section of *Multiscale Modeling and Simulation: A SIAM Interdisciplinary Journal*, on multiscale modeling in life and materials sciences, is based on a summer program with the same theme, held August 4–30, 2003, at the Università della Svizzera Italiana in Lugano, Switzerland, and organized by the ETH Zurich Computational Laboratory (CoLab). This workshop emphasized that multiscale modeling and simulation can serve as a common scientific language enabling cross-fertilization across disciplines and the definition of new scientific frontiers.

Materials science was one of the first disciplines that emphasized the need for novel multiscaling approaches bridging continuum and atomistic models. In life sciences, the rapid growth of the role played by computational methods has led to the early realization that a multiscaling approach is necessary to tackle inherently complex phenomena involving cells, organisms, and ecosystems. This summer program provided the opportunity to scientists from these different scientific fields to exchange ideas and to pursue research in an interdisciplinary fashion using multiscale computational methods as a common language. These interactions demonstrated that research in multiscaling is a fertile breeding ground for the development of novel powerful computational tools for domains where computing is established as a tool for scientific inquiry and for the dissemination of this know-how to disciplines for which computation is an emerging form of scientific investigation.

This special section of MMS is a representative sample of theoretical and computational approaches to multiscale modeling and simulation in materials and life sciences. The papers discuss multiscale coupling of physical models and time/space multiresolution techniques.

The problem of coupling models across space and time scales is a fundamental issue in multiscale modeling and simulation. Multiscale approaches often require the rigorous integration of diverse physical models, such as the case of blood flow in the circulatory system (Fernández, Milišić, and Quarteroni). The multiscale integration of diverse physical models in nanoscale magnetic systems involves the proper coupling of quantum effects in classical descriptions (Wessel, Trebst, and Troyer). Multiscale simulations of materials with heterogeneous properties are tackled using asymptotic expansions for the case of conducting inclusions embedded in a homogeneous matrix phase (Ben Hassen and Bonnetier). A broad class of multiscale problems involves the description of macroscale systems using only the information available by suitable microscopic models. This technique is demonstrated in simulating the evolution of parabolic homogenization problems with nonlinear reactions, using as a microscopic model a partial differential equation with rapidly oscillating coefficients (Samaey, Roose, and Kevrekidis). A related work extends this concept to problems with a wide separation in time scales. Using as an application a model of bacterial chemotaxis it is shown that projective time integration of coarse variables can be carried out in time scales that are long compared to those of the microscopic dynamics (Setayeshgar, Gear, Othmer, and Kevrekidis). In problems with time-dependent, large space scale variations a new class of multiresolution particle methods enhances their inherent adaptivity and presents an alternative to grid-based methods (Bergdorf, Cottet, and Koumoutsakos).

Future research in multiscale modeling would continue to rely on synergies across disciplines for the development of novel computational methods, the integration of physical models, and the formulation of new challenges. This principle will continue to guide future workshops in multiscale modeling and simulations at the CoLab and, we believe, an ever-increasing number of scientific institutions.

The editors in charge would like to credit, for their hard work and dedication, those editors who helped handle the peer-review process for papers submitted to this special section. Thanks to Emily Carter, Wolfgang Hackbusch, Robert Kohn, Hans Christian Ottinger, Olivier Pironneau, and John Willis. We also wish to thank SIAM Publications Manager Mitch Chernoff for his invaluable advice and help in preparing this section.

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