Multiscale Modeling in Advanced Materials Research: Challenges, Novel Methods, and Emerging Applications

Juan J. de Pablo and William A. Curtin,
Guest Editors

Abstract

The concept of multiscale modeling embodies the idea that a comprehensive description of a material will require an understanding over multiple time and length scales. A multiscale model requires that descriptions at all levels be consistent with each other, which can be particularly demanding for advanced materials and complex fluids. For crystalline materials, emerging modeling approaches have married small- and intermediate-scale descriptions in a highly effective manner, but challenges remain at long time and length scales. For soft materials, such as polymers or liquid crystals, modeling techniques have adopted a more or less systematic coarse-graining approach, in which atomic and molecular details are gradually blurred as one seeks to describe longer length scales. This approach presents its own brand of challenges. And, in spite of rapid advances, entire classes of materials, including amorphous glasses, foams, and gels, have resisted attempts to describe their structure and dynamics over long and relevant length and time scales. This issue of *MRS Bulletin* covers some areas of materials modeling in which enormous advances have been made, but which continue to raise intriguing questions and formidable challenges.

Introduction

Rational design of advanced materials for demanding applications continues to be one of the primary aims of materials research. The concept of "materials by design" has gradually gained acceptance in the materials science and engineering communities, and with that acceptance, the field of materials modeling has tackled increasingly daunting problems. That emboldened attitude has led to a whirlwind of activity in the area of multiscale modeling and to scientific advances that even for the expert have been difficult to digest. For hard materials, available methods have matured to the point where increasingly comprehensive calculations can be performed to address subtle questions about relations between chemistry, structure, and material behavior. But among all the excitement, entire classes of materials have resisted attempts by modelers to reveal their secrets. In the particular case of soft materials (e.g., polymeric glasses and melts, biological macromolecules), widely used modeling approaches require enormous leaps of faith, and well-founded theoretical frameworks for the development of multiscale modeling strategies are only now beginning to emerge.

For this issue of *MRS Bulletin*, we have identified five areas of materials modeling in which enormous advances have been made but which continue to raise intriguing questions and formidable challenges. These five areas are by no means comprehensive, and they represent only a thin slice of the materials modeling community. They do provide, however, a relatively broad overview of current thinking and emerging trends, and they offer a perspective on some of the developments that we might expect over the next decade.

The methodology to be used for a particular problem depends on the length and time scales of interest (Figure 1). The concept of multiscale modeling embodies the idea that a comprehensive description of a material will require an understanding over multiple length and time scales. More subtle is the fact that a comprehensive, multiscale model requires that descriptions at all levels be consistent with each other. That requirement for consistency often demands that models for different processes or pieces of a problem be coupled and solved concurrently, a feat that is often sought but rarely achieved in the study of advanced materials and complex fluids. For some classes of materials, emerging modeling approaches have married small- and intermediate-scale descriptions in a highly effective manner, but challenges remain at long time and length scales. Such challenges are largely due to the computational demands associated with high-resolution calculations over such scales. For some others, modeling techniques have adopted a more or less systematic coarse-graining approach in which atomic and molecular details are gradually blurred as one seeks to describe longer length scales. In the simplest coarse-grained model, a collection of atoms is simply lumped into an individual "super atom," thereby reducing the resolution of the model but alleviating its computational demands. In more sophisticated approaches, a detailed description of a system is mapped onto a handful of carefully chosen variables that are sufficient to describe its overall behavior over long time and length scales.

https://doi.org/10.1557/mrs2007.187 Published online by Cambridge University Press

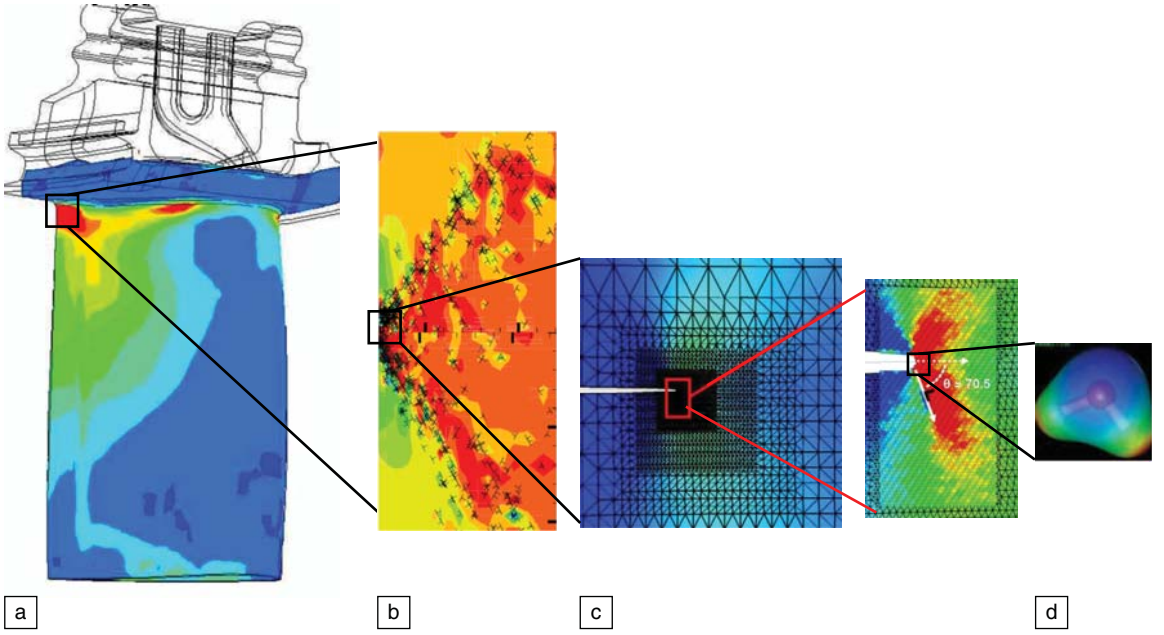


Figure 1. Schematic illustration of multiscale modeling in the mechanics of solids. (a) Component scale, treated via continuum mechanics. (b) Mesoscale, where plasticity is described explicitly in terms of dislocations. (c) Nanoscale, where dislocation plasticity and atomistic models coexist. (d) Quantum scale, for accurate prediction of materials separation or chemical embrittlement.

Figure 2 provides a schematic representation of the coarse-graining concept as applied to multiscale modeling of polymeric materials. At the more detailed level, the object of interest is a small region of a material described at fully atomistic level of detail. At longer length scales, that description can be replaced by a coarser model in which small pieces of the polymeric molecules are described as spherical beads connected by springs. As discussed by Öttinger in this issue, it is now thought that, on even longer time and length scales, the behavior of the material is governed by the existence of entanglements. Individual molecules can be thought of as residing in distinct, tube-like regions, and, when sufficiently long, such tubes can become entangled with each other to constrain the dynamic behavior of the material. The tube, or "primitive path," that each molecule follows can be determined to arrive at a quantitative measure of entanglements, thereby providing the necessary elements and ingredients required by theoretical formalisms developed to describe the behavior of polymers over the long length and time scales that arise in most applications.

A persistent challenge in approaches such as those depicted in Figure 2 remains that of reverse mapping, that is, restoring some of the details after they have been blurred away through an averaging procedure. And, for materials such as glasses and other disordered media, the aim has simply been to gain a fundamental understanding of key structural and dynamic processes, while postponing a multiscale description until the necessary elementary building blocks are discovered. One of the key features to have emerged from recent research on glasses is that of structural and dynamic heterogeneity. That heterogeneity encompasses a wide spectrum of length and time scales and helps explain the challenges associated with a theoretical and computational description.

In This Issue

The first two articles in this issue pertain mainly to crystalline materials, where the emphasis in multiscale modeling has been primarily on predicting mechanical behavior. Mechanical behavior encompasses, however, a wide range of phenomena. Much of the work is on predicting plastic flow phenomena. This is a truly multiscale problem, due to the necessity of capturing dislocation nucleation—an intrinsically atomistic phenomenon—dislocation propagation, dislocation interactions at both short and long range, patterning, and the consequences of all of these parameters on the size-dependent plastic deformation behavior now being observed in many materials systems. Another problem that is intrinsically multiscale is fracture, where crack-tip deformation and the role of chemical impurities in driving embrittlement combine the intrinsic chemistry of bond-breaking and chemical reactions with the larger-scale energy dissipation associated with plastic flow.

To study these and other problems, including, for example, many rate-dependent processes and friction, considerable recent work has focused on appropriate and workable frameworks for finite-temperature multiscale simulations and coupling first-principles quantum mechanical methods to atomistic or continuum models. The overall goal in such development efforts is to create a "seamless" method: a coupled method applied to a problem should produce results that are identical in all important respects to those that would be produced by application of the smallest-scale (i.e., the most computationally intensive) method to the entire problem.

The first article, by Ramasubramaniam and Carter, reviews recent efforts to bring the chemical accuracy of electronic structure/quantum mechanics computations into various materials problems. For bridging length scales, they present a few recent examples of information passing, where carefully selected quantum computations are used to calibrate higher-scale models to describe piezoelectrics and hydrogen embrittlement. The authors also discuss the continued evolution of direct coupling of quantum and atomistic or continuum methods, a subject of prior *MRS Bulletin* articles.[1] This remains a significant challenge both operationally and concep-

https://doi.org/10.1557/mrs2007.187 Published online by Cambridge University Press

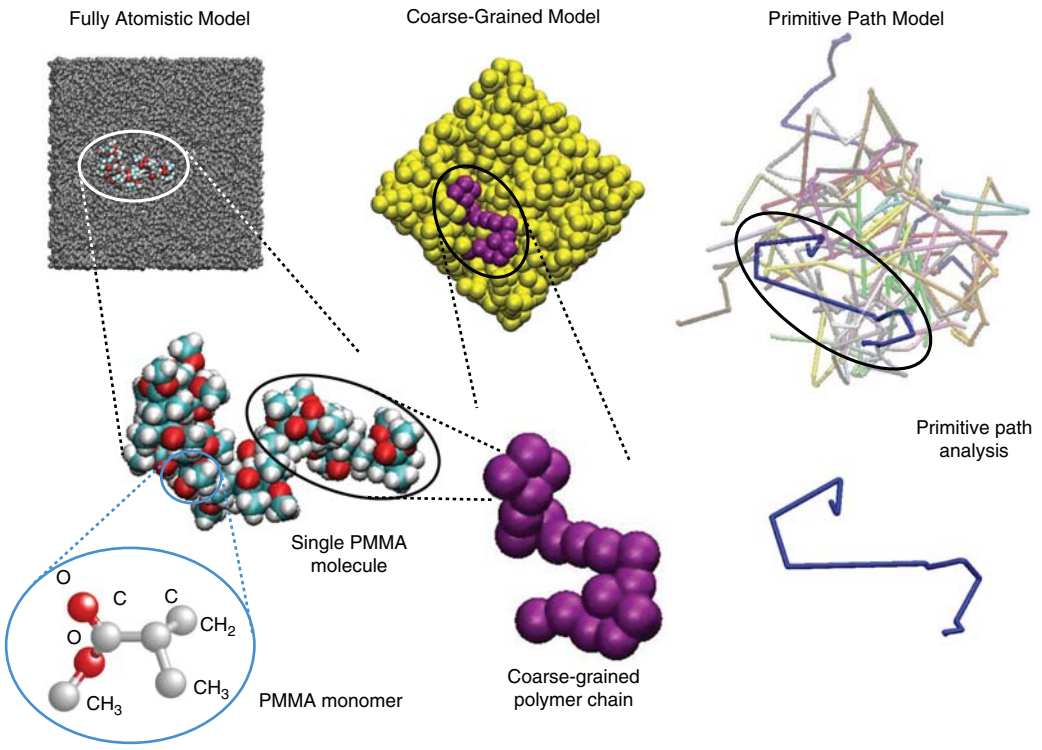


Figure 2. Schematic representation of the coarse-graining concept as applied to multiscale modeling of polymeric materials. The atomistic model on the left includes all atoms. The coarse-grained model in the center uses a spherical bead to represent a collection of polymer segments. The model on the right shows the primitive path that each polymer molecule follows. The entanglements between primitive paths determine the dynamics of the polymeric material over long time scales.

tually, particularly for metallic systems, because of the long-range nature of the electronic interactions. For bridging time scales, the authors review recent progress in imbuing molecular dynamics and kinetic Monte Carlo methods with first-principles information. We note that applications of these multiscale methods extend beyond crystals and mechanical properties to surfaces and chemical reactions, other areas where first-principles input is essential to achieving predictive modeling.

The second article, by Miller and Tadmor, focuses on the methodology for coupling atomistic and continuum descriptions of crystals with defects. The story here begins with the now well-established quasi-continuum model, but shows the evolution of insight into, and understanding of, many subtle details of creating artifact-free coupling methods at zero temperature that has culminated in a range of successful approaches. The authors then report on recent activity in finite-temperature coupling aimed at replacing molecular dynamics. Methods for equilibrium thermodynamic problems, where coarse-graining is performed on the free energy rather than the energy, have emerged. The challenges in handling heat flow across scale-bridging boundaries that arise in nonequilibrium problems are discussed, and some of the recent efforts to handle this issue or circumvent its most deleterious consequences are discussed.

Applications of the methods reviewed in these first two articles, and many other methods such as discrete-dislocation modeling and phase-field modeling, are showing that multiscale simulation methods combined with theoretical models and established metallurgical knowledge are able to push the field forward. The coupled methods enable the study of more complex "unit problems" than previously possible, but results from these unit problems must often still be used within a broader framework of analysis or prediction. The multiscale methods are thus enabling but are not stand-alone. As a result, multiscale modeling has driven multidisciplinarity. Applied mechanicians are now learning quantum and statistical mechanics and dealing with "constitutive laws" in the form of interatomic potentials. Physicists and materials scientists are learning the structure of continuum mechanics that form the basis for exporting physics to larger scales. Experimentalists from all these fields are converging on delicate and beautiful studies at the nanoscale that reveal a richness in phenomena not previously recognized. The field is ripe—computational power abounds, a host of methods exist with their advantages and disadvantages fairly clearly defined, and scientists from different fields are converging. The "big impact" result elucidating new physics/materials behavior or solving a long-standing problem that demonstrates the power of multiscale modeling is still missing. However, steady progress has been made and application successes exist, and the big impacts will emerge in the coming years.

The next three articles in this issue focus on soft materials and complex fluids. Such systems are characterized by a wide spectrum of relaxation processes that occur over an equally wide spectrum of length scales. In a polymeric melt, for example, the relaxation of successive bonds in a chain molecule occurs within nanosecond time scales, whereas the relaxation of the end-to-end distance of the molecules or the recovery of the material after deformation can require milliseconds, seconds, or minutes, depending on the temperature and molecular weight. Such processes are

https://doi.org/10.1557/mrs2007.187 Published online by Cambridge University Press

intimately linked and cannot be uncoupled or treated individually in a straightforward manner; as such, multiscale methods for soft materials have not reached the level of maturity that is encountered in the modeling of crystalline materials.

One strategy that is often pursued is to simply coarse-grain the resolution of a detailed, atomistic-level model by lumping several atoms into an individual "group" having different properties from those of the original model. This decades-old approach has received renewed interest, particularly from researchers dealing with biological systems, and new methods for "systematic" coarse graining are being proposed at a rapid pace. Many questions arise during such coarse graining: Which features of the atomic system is it most important to preserve? Is the resulting coarse-grained model capable of describing the system over reasonable ranges of thermodynamic conditions (e.g., pressure and temperature), or is it only valid at the conditions at which the coarse graining was performed? Is a coarse-grained model derived on the basis of structural information capable of predicting the dynamic behavior of the system? And, once a coarse-grained model has been developed, how can one retrieve the original atomistic model?

A theoretical framework that allows one to address these questions during the process of coarse graining is clearly necessary, and two of our articles address this issue in some detail. The article by Ayton et al. presents a theoretical and computational methodology to develop coarse-grained representations of soft materials including biomolecules, phospholipid bilayer membranes, and gas hydrates. The approach presented by these authors provides a connection between atomistic models of the sort used in traditional molecular dynamics simulations and mesoscopic models that seek to describe systems over scales of hundreds of nanometers. Coarse-graining approaches generally rely on the matching of a structural function, such as a radial distribution function, or a free energy at two distinct levels of description. The centerpiece of the methodology described by Ayton et al. is a variational statistical mechanical algorithm that matches the forces (i.e., the derivatives of the energy with respect to position) determined in atomistic molecular dynamics simulations to those required for a coarse-grained representation, thereby avoiding the calculation of multidimensional potentials of mean force. The question that remains, however, is the extent to which the resulting coarse-grained force field is able to provide predictions at different thermodynamic states, and the degree to which dynamical processes can be captured. To address these questions, the authors discuss three encouraging examples, namely, bilayer membranes, peptides, and carbohydrates.

The article by Öttinger introduces a thermodynamic formalism for systematic coarse graining of material models. Öttinger explains how traditional simulation techniques, such as molecular dynamics or Monte Carlo, can and should be used to derive coarse-grained models for the structure and dynamic relaxation of a specific system. His approach, however, is based on principles from nonequilibrium statistical mechanics, as opposed to strictly at-equilibrium ideas. While he illustrates the application of such a thermodynamic formalism in the context of a polymer, it has the virtue of providing a simultaneous description of structural and dynamic properties, and of being generally applicable to arbitrary systems regardless of their atomic structure, morphology, or overall behavior. Öttinger's contribution is aptly subtitled "Four Lessons and a Caveat." The four lessons are clearly enunciated there for the student to absorb; they provide a step-by-step guide on how to implement a meaningful coarse-graining strategy. The caveat is that any level of coarse graining necessarily introduces irreversibility and additional dissipation. That additional dissipation is often forgotten or ignored, and it limits severely the usefulness and range of applicability of coarse-grained models. Öttinger proposes a general prescription to handle the irreversible nature of coarse graining, and one that remains to be tried on a wide variety of materials.

The final article of this issue, by Barrat and de Pablo, discusses the modeling of glassy, amorphous materials. As noted by these authors, the amorphous, glassy state of materials arguably remains one of the least understood states of matter and represents a true frontier for materials research. Examples of amorphous materials abound in nature and in applications: foams, emulsions, gels, and organic or inorganic glasses are a few examples. Experiments on a wide variety of systems continue to reveal as-yet unexplained phenomena. Beyond explaining such phenomena, one of the goals of amorphous materials research remains that of predicting the relaxation of the system on the basis of knowledge of its structure. Molecular and coarse-grained models of glasses have increased our understanding considerably, but it remains incomplete; we are simply unable to describe essential structural features and dynamical processes occurring over dozens of nanometers and hundreds of milliseconds. In their article, Barrat and de Pablo summarize current models of various mechanical aspects of dynamically arrested systems and their response to deformation and some of the insights they have provided, while also spelling out a few emerging views and the challenges that remain ahead. This is clearly an area of research where much remains to be done, and an area where multiscale modeling is likely to provide much-needed insights in the years or decades to come.

Given the space constraints to which all the authors have been subject, and the limited number of articles that can be included in a journal issue of this nature, the three articles devoted to the study of soft materials only represent a small subsection of the current multiscale modeling activity. We have chosen to emphasize some of the distinct, emerging strategies that are being pursued—for example, coarse graining—and we have unfortunately had to leave out discussions pertaining to the many successes of modeling multiple aspects of the properties and behavior of soft condensed matter. When cleverly used, Monte Carlo and molecular or Brownian dynamics simulations of model systems, for example, have yielded tremendous insights into the structure and relaxation modes of polymeric materials,[2] nanocomposites,[3,4] confined macromolecules,[5,6] liquid crystals,[7] biological membranes,[8] and biological macromolecules.[9] These simulations provide a window into the transport of molecules through porous materials such as zeolites,[10,11] and into the short- and intermediate-time relaxation modes of model glass-formers[12] and colloidal and polymeric gels.[13–15] Multiscale modeling is, without a doubt, a particularly vibrant field of research where the engineering disciplines, the physical sciences, and the life sciences converge. Much of the excitement is being fueled by increasingly sophisticated experiments that are capable of probing matter at the level of individual atoms or molecules. Interpretation of their experimental data requires molecular and multiscale models, and modeling is benefiting from a direct, unambiguous connection to experiment.[4,5,11,12] It is a field where much has been learned, but enormous, exciting challenges remain.

Acknowledgments

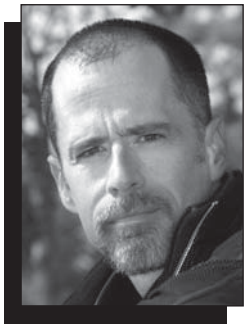
The authors are grateful for financial support from the National Science Foundation's MRSEC program.

References

1. For example, see *MRS Bull*. **25** (5), 11–50 (May 2000); *MRS Bull*. **26** (3), 169–221 (March 2001).
2. C. Tzoumanekas, D.N. Theodorou, *Curr. Opin. Solid State Mater. Sci*. **10** (2), 61 (April 2006).
3. R.B. Thompson, V.V. Ginzburg, M.W. Matsen, A.C. Balazs, *Science* **292**, 2469 (2001).
4. S.W. Sides, B.J. Kim, E.J. Kramer, G.H. Frederickson, *Phys. Rev. Lett*. **96** (25), 250601 (2006).
5. K.C. Daoulas, M. Muller, M.P. Stoykovich, S.-M. Park, Y.J. Papakonstantopoulos, J.J. de Pablo, P.F. Nealey, H.H. Solak, *Phys. Rev. Lett*. **96** (3), 036104 (2006).
6. G.E. Stein, E.W. Cochran, K. Katsov, G.H. Fredrickson, E.J. Kramer, X. Li, J. Wang, *Phys. Rev. Lett*. **98** (15), 158302 (2007).
7. F.R. Hung, O. Guzman, B.T. Gettelfinger, N.L. Abbott, J.J. dePablo, *Phys. Rev. E* **74** (1), 011711 (2006).
8. R. Faller, S.J. Marrink, *Langmuir* **20** (18), 7686 (2004).
9. R.M. Jendrejack, E.T. Dimalanta, D.C. Schwartz, M.D. Graham, J.J. de Pablo, *Phys. Rev. Lett*. **91** (3), 038102 (2003).
10. M.D. Macedonia, E.J. Maginn, *AIChE J*. **46** (12), 2504 (2000).
11. H. Jobic, D.N. Theodorou, *Microporous Mesoporous Mater*. **102** (1–3), 21 (2007).
12. L. Berthier, G. Biroli, J.P. Bouchaud, L. Cipelletti, D. El Masri, D. L'Hote, F. Ladieu, M. Pierno, *Science* **310**, 1797 (2005).
13. J. Largo, F.W. Starr, F. Sciortino, *Langmuir* **23** (11), 5896 (2007).
14. S. Mossa, C. De Michele, F. Sciortino, *J. Chem. Phys*. **126** (1), 014905 (2007).
15. P.I. Hurtado, L. Berthier, W. Kob, *Phys. Rev. Lett*. **98** (13), 135503 (2007). □

Juan J. de Pablo

William A. Curtin



Gary S. Ayton

Jean-Louis Barrat

Emily A. Carter

Juan J. de Pablo, Guest Editor for this issue of *MRS Bulletin*, is director of the Materials Research Science and Engineering Center (MRSEC) on Nanostructured Interfaces at the University of Wisconsin– Madison. He also holds the Howard Curler Chair of Chemical and Biological Engineering at UW–Madison.

His research interests include statistical mechanics, the study of complex fluids and materials, and the development of multiscale modeling methods for the study of such systems. De Pablo has co-authored more than 250 papers in these areas.

A graduate of the National Autonomous University of Mexico (UNAM) in Mexico City, de Pablo obtained his PhD degree in 1990 from the University of California, Berkeley. He has also worked at ETH Zurich.

De Pablo is a fellow of the American Institute of Physics.

De Pablo can be reached at the Department of Chemical and Biological Engineering, University of Wisconsin, 1415 Engineering Dr., Madison, WI 53706, USA; e-mail: depablo@engr.wisc.edu.

William A. Curtin, Guest Editor for this issue of *MRS Bulletin*, is the Elisha Benjamin Andrews Professor in the Division of Engineering at Brown University. Curtin is also director of the Center for Advanced Research Materials and the NSF Materials Research Science and Engineering Center at Brown.

His research is centered on computational materials and mechanics, including atomistic/continuum models of plasticity and fracture, solute hardening in aluminum alloys, and fiber and nanotube composites.

Curtin received a combined ScB/ScM degree in physics from Brown University in 1981 and a PhD degree in theoretical physics from Cornell University in 1986. He worked at the British Petroleum Research Laboratories and Virginia Polytechnic Institute and State University before joining Brown in 1998.

A Guggenheim Fellow in 2005–2006, Curtin has published more than 125 journal papers.

Curtin can be reached at Brown University, Division of Engineering, Providence, RI 02912, USA; e-mail: william_curtin@brown.edu.

Gary S. Ayton is a research associate professor in the Center for Biophysical Modeling and Simulation at the University of Utah.

Ayton is interested in the multiscale simulation of biomolecular systems, with a particular focus on membranes.

He received his PhD degree at the University of British Columbia, Canada, under G.N. Patey and then per-formed his postdoctoral work at the Australian National University, working with Denis Evans on the development of the fluctuation theorem.

Ayton can be reached at the Center for Biophysical Modeling and Simulation, Department of Chemistry, University of Utah, 315 S. 1400 E., Rm. 2020, Salt Lake City, UT 84112-0850, USA; e-mail: gazz@hec.utah.edu.

Jean-Louis Barrat is a professor of physics at the University of Lyon (France) and director of the Condensed-Matter Physics Laboratory (associated with CNRS).

In Lyon, Barrat applies statistical physics and simulation to various problems in soft matter and materials science (glassy systems, confined fluids, polymers).

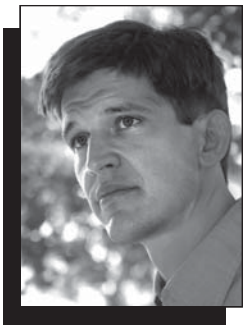
He is a graduate of ENS–Paris and obtained his PhD degree in 1987 from the University of Paris, working on the theory of liquids and crystallization. Barrat has worked in Munich, Santa Barbara, and Lyon. He was a member of Institut Universitaire de France from 1997 to 2002.

Barrat can be reached at Laboratoire PMCN, Bat. Léon Brillouin, Université de Lyon, 43 Boulevard du 11 Novembre, 69622 Villeurbanne Cedex, France; e-mail: barrat@lpmcn.univ-lyon1.fr.

Emily A. Carter is the Arthur W. Marks '19 Professor of Mechanical and Aerospace Engineering and Applied and Computational Mathematics at Princeton University. She is also an affiliated faculty member in chemistry, chemical engineering, the Princeton Institute for Computational Science

https://doi.org/10.1557/mrs2007.187 Published online by Cambridge University Press

Ronald E. Miller



Will G. Noid

Hans Christian Öttinger

A. Ramasubramaniam

Ellad B. Tadmor

and Engineering (PICSciE), and the Princeton Institute for Science and Technology of Materials (PRISM).

Carter's research interests include developing accurate quantum mechanics and multiscale methods for molecules and materials, and understanding materials failure mechanisms in order to design improved materials.

She received her PhD degree from the California Institute of Technology (1987) and was a postdoctoral research associate in physical chemistry at the University of Colorado at Boulder. Before joining Princeton, she served on the faculty of UCLA's Department of Chemistry and Biochemistry.

Carter has authored more than 190 scientific publications and presented over 300 invited lectures. Her work has been recognized by national and international awards and fellowships including, most recently, the 2007 ACS Computational Chemistry Award.

Carter can be reached at the Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ 08544-5263, USA; e-mail: eac@princeton.edu.

Ronald E. Miller is an associate professor in the Department of Mechanical and Aerospace Engineering at Carleton University in Ottawa, Canada.

His research interests focus on understanding the connections between the atomic and continuum scales in the mechanics of materials.

Miller received his PhD degree in mechanical engineering from Brown University (1997) and was a postdoctoral fellow in the Division of Engineering and Applied Sciences at Harvard University (1997–1998).

He has been a visiting professor at Brown University, a Lady Davis Fellow at the Technion–Israel Institute of Technology, and a visiting research fellow with the Institut National Polytechnique de Grenoble and Centre National de la Recherche Scientifique in France. In 2003, Miller received an Ontario Premier's Research Excellence Award (PREA).

Miller can be reached at the Department of Mechanical and Aerospace Engineering, Carleton University, 1126 Colonel By Drive, Ottawa, ON, K1S 5B6, Canada; e-mail: ron_miller@carleton.ca.

Will G. Noid is an assistant professor of chemistry at the Pennsylvania State University.

His current interests include liquid-state theory and developing formal coarse-graining methodologies for complex biomolecular systems.

He attended Cornell University as an Integrative Graduate Education and Research Traineeship (IGERT) fellow in nonlinear dynamics and was awarded an NSF graduate research fellowship in 2002. In 2005, Noid completed his thesis work on classical–quantum correspondence in nonlinear vibrational spectroscopy under Roger F. Loring.

Prior to joining PSU in August 2007, Noid was a National Institutes of Health postdoctoral research fellow at the University of Utah's Center for Biophysical Modeling and Simulation.

Noid can be reached at the Pennsylvania State University, Department of Chemistry, 528 Chemistry Bldg., University Park, PA 16802, USA; e-mail: wgn1@psu.edu.

Hans Christian Öttinger is a professor of polymer physics at ETH Zurich. Öttinger has worked in the Department of Materials at ETH Zurich since 1989; from 2000 to 2002, he was chair of the department.

Öttinger is interested in the flow behavior of polymer melts and solutions based on a molecular understanding of complex fluids and the study of theoretical fundamentals of nonequilibrium systems, the kinetic theory of polymer fluids, continuum mechanics, rheology, applied mathematics, fluid dynamics, and simulations of polymer processing.

He earned his diploma in quantum field theory at the University of Freiburg, Germany, in 1981 and his PhD degree with a dissertation on materials with spatially modulated magnetic structures in 1983. He returned to the University of Freiburg after working as a postdoctoral researcher in the Chemical Engineering Department and the Rheology Research Center at the University of Wisconsin–Madison.

Öttinger can be reached at ETH Zurich, Department of Materials, Polymer Physics, HCI H 543, CH-8093 Zurich, Switzerland; e-mail: hco@mat.ethz.ch.

Ashwin Ramasubramaniam is a research associate in applied and computational mathematics at Princeton University.

Ramasubramaniam's research interests are in self-assembly and morphological instabilities in thin films and, more recently, in multiscale models of crystalline materials.

He received his PhD degree from Brown University.

Ramasubramaniam can be reached at Princeton University, Department of Mechanical and Aerospace Engineering, EQuad D314, Princeton, NJ 08544, USA; e-mail: aramasub@princeton.edu.

Gregory A. Voth

Ellad B. Tadmor is a professor of aerospace engineering and mechanics at the University of Minnesota.

His research focuses on the development of multiscale theories and computational methods for predicting the behavior of materials directly from the interactions of the atoms making up the material.

Tadmor received his BSc and MSc degrees in mechanical engineering from the Technion–Israel

https://doi.org/10.1557/mrs2007.187 Published online by Cambridge University Press

Institute of Technology in 1987 and 1991, respectively. He earned his PhD degree from Brown University in 1996. Prior to joining UM, Tadmor was a postdoctoral research fellow at Harvard University, an associate professor at the Technion, and Erasmus Mundus Scholar at the Ecole Normale Superieure in Lyon, France.

He received the MRS Graduate Student Award for his work on developing the quasi-continuum method as well as numerous awards for excellence in teaching, including the Salomon Simon Mani Award in 2001.

Tadmor can be reached at Aerospace Engineering and Mechanics, University of Minnesota, 107 Akerman Hall, 110 Union St. SE, Minneapolis, MN 55455, USA; e-mail: tadmor@aem.umn.edu.

Gregory A. Voth is a Distinguished Professor of Chemistry and director of the Center for Biophysical Modeling and Simulation at the University of Utah.

His research interests include the theory and simulation of multiscale systems, charge transport, and solvation phenomena in liquid-state, biomolecular, and materials systems.

Voth received his PhD degree in theoretical chemistry at the California Institute of Technology in 1987.

He has authored or coauthored approximately 300 scientific publications and mentored 70 postdoctoral fellows, 30 graduate students, and 10 undergraduates.

Voth can be reached at the Center for Biophysical Modeling and Simulation, Department of Chemistry, University of Utah, 315 S. 1400 E., Rm. 2020, Salt Lake City, UT 84112-0850, USA; e-mail: voth@chem.utah.edu. □

https://doi.org/10.1557/mrs2007.187 Published online by Cambridge University Press