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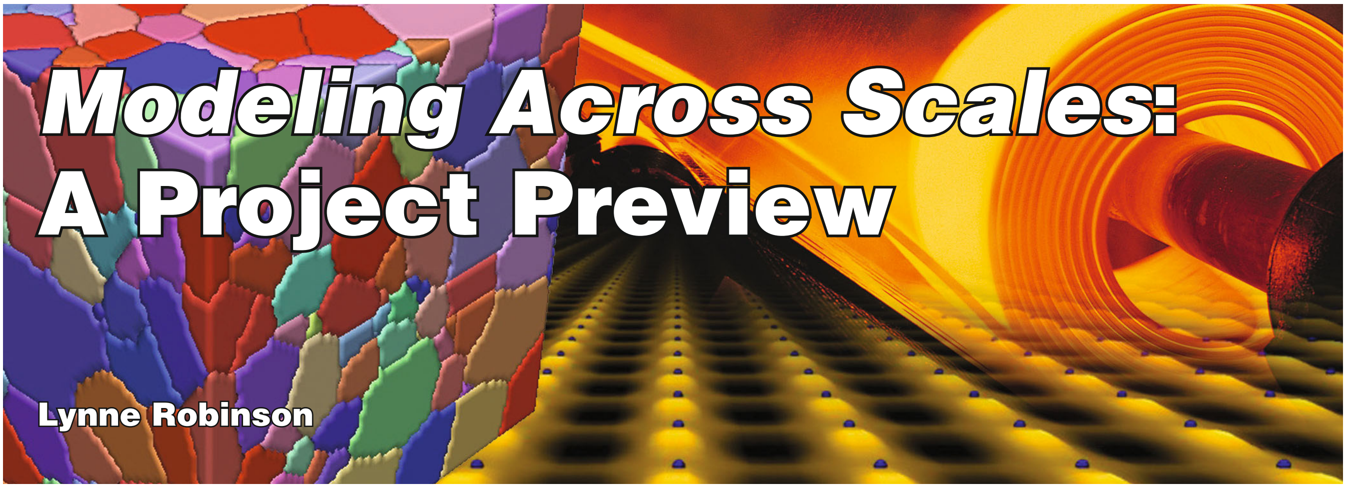


Modeling Across Scales: A Project Preview

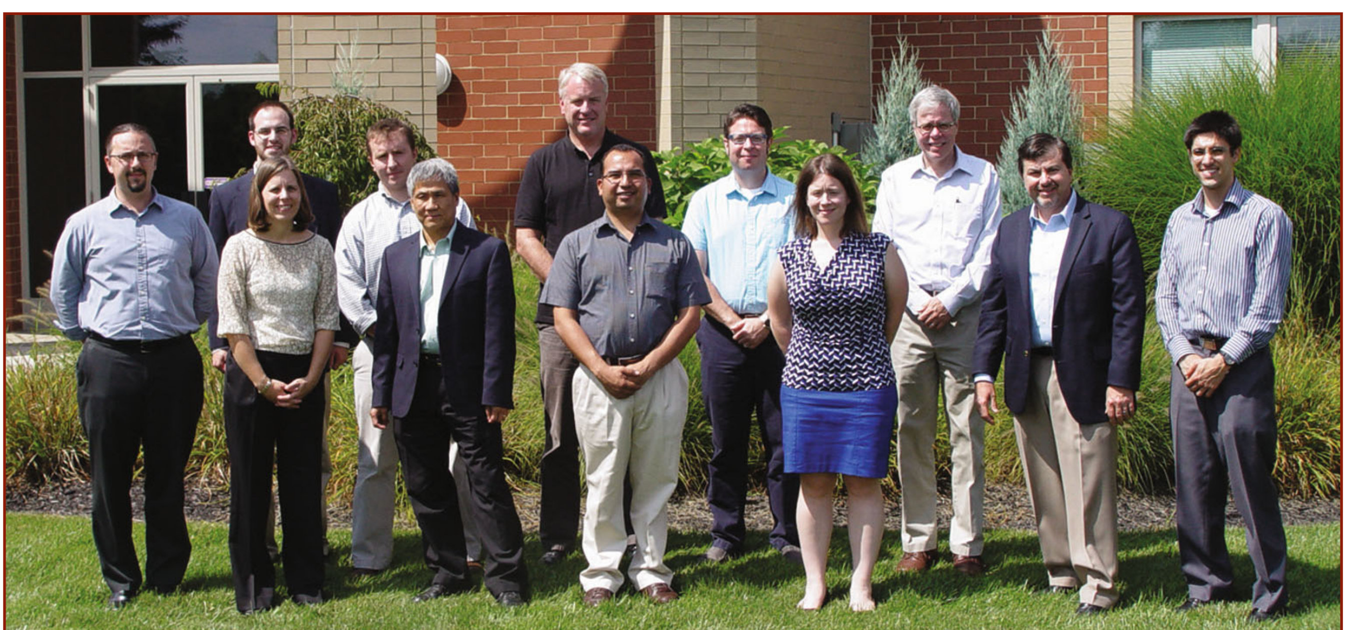
Lynne Robinson

(Image credits, from left: Alexis C. Lewis, U.S. Naval Research Laboratory; National Science Foundation, Kazuhiro Fujita, Cornell University; Office of Science and Technology Policy, *Materials Genome Initiative for Global Competitiveness.*)

Although the official release of *Modeling Across Scales: A Roadmapping Study for Connecting Materials Models and Simulations Across Length and Time Scales* is still a few months away, Peter Voorhees noted that the prevailing theme tying all aspects of the study together emerged fairly early in the development process. "A particularly important thread that runs through the report is the role of collaborations in moving the discipline forward," said Voorhees, Frank C. Engelhart Professor of Materials Science and Engineering, Northwestern University, and chair, TMS *Modeling Across Scales* core team. "These collaborations can be between experimentalists and theorists or among investigators in different fields. This cross-fertilization between disciplines and different approaches to science and engineering is key to success in the future."

Sponsored by the National Institute of Standards and Technology (NIST) Materials Measurement Laboratory and lead by TMS, *Modeling Across Scales* is itself a product of this type of collaboration, starting with the core team of international experts assembled last spring to represent the perspectives of industry, academia, and government. The key deliverable of the team's efforts is a series of concrete recommendations for addressing the gaps and limitations they identified in order to advance the state of the art in model and code linkage.

The core team began its work through series of online preparatory meetings throughout the summer and early fall. They then convened in person for two facilitated meetings



Members of the *Modeling Across Scales* core study team take a break during their work meetings in October 2014. First row, from left: Ross Brindle, facilitator, Nexight; Carelyn E. Campbell, NIST; Wing Kam Liu, Northwestern University; Raymundo Arróyave, Texas A&M University; Alexis C. Lewis, U.S. National Science Foundation; George Spanos, TMS; Jared Kosters, facilitator, Nexight. Second row, from left: David Howe, TMS; James K. Guest, Johns Hopkins University; Mark Asta, University of California, Berkeley; Dallas R. Trinkle, University of Illinois, Urbana-Champaign; Peter W. Voorhees, Northwestern University.

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—Peter Voorhees, Chair, *Modeling Across Scales* Core Team

to develop recommendations for critical steps and pathways needed for linking computational materials models and simulations across various length scales.

Also informing the study report are the results of a working meeting held in conjunction with the 1st International Workshop on Software Solutions for Integrated Computational Materials Engineering (ICME) in June 2014. Conducted by Voorhees, James Warren, NIST Technical Program Director for Materials Genomics, and George Spanos, TMS Technical Director, the session focused primarily on software tools employed in multiscale modeling. In addition, two *Modeling Across Scales* core team members, Mark Asta, Professor and Chair, Materials Science and Engineering, University of California, Berkeley, and David L. McDowell, Regents' Professor and Carter N. Paden Distinguished Chair in Metals Processing, Georgia Institute of Technology, facilitated a meeting coinciding with the 7th International Conference on Multiscale Materials Modeling in October 2014 to gain insights on needs, potential recommendations, and case studies involving multiscale modeling.

"Since the focus of the study is on identifying the gaps present in multiscale modeling approaches, my expectation was that the recommendations would focus on computational methods and hardware," commented Voorhees. "While the study does address these issues, it became clear that certain poorly understood or characterized physical phenomena are major stumbling blocks to progress in the multiscale modeling area. For example, the team identified interfacial properties and phenomena, and the need for publicly accessible, curated, multiscale materials databases as major barriers to progress. It is through an understanding of these issues that the parameters needed for accurate multiscale modeling will become available."

"A particular challenge for the team was defining four or five major length scale regimes, in terms of different models. There are so many gray areas with a great deal of overlap among models," added Spanos. "In the end, they were able to identify four regimes, with two being particularly intertwined. There was also a great deal of fruitful discussion about differentiating fundamental models from tools, and the related concepts of theories, models, and codes. Bridging length and time scales involves addressing all of these entities, as well as their interplay."

Once the core team developed a working draft of its recommendations, an independent review team provided an additional check on the technical aspects of the report in early 2015. While a few details are still being addressed at press time, the final report is on track to encompass the following concepts and resources:

The Modeling Across Scales Review Team

As an additional step to ensuring the quality and relevance of the final *Modeling Across Scales* report, the core study team recruited the following individuals to provide a final technical review of the recommendations:

- Christopher Woodward, Materials Engineer, U.S. Air Force Research Laboratory
- William Curtin, Professor, École Polytechnique Fédérale de Lausanne
- Wei Chen, Director, Integrated Design Automation Laboratory, Northwestern University
- Irene Beyerlein, Scientist, Los Alamos National Laboratory
- Siddiq Qidwai, Mechanical Engineer, U.S. Naval Research Laboratory
- André Phillion, Assistant Professor, University of British Columbia

For a complete listing and biographies of the core study team members, refer to the August 2014 *JOM* feature, "New TMS Study Tackles the Challenge of Integrating Materials Simulations Across Length Scales."

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- **State-of-the art materials models.** The core team will share the results of its work on examining many of the current materials models within different length scale regimes, with consideration of crossing timescales as well. More specifically, existing models at the quantum and atomistics scale, microstructural evolution and materials response (and time) scales, and macroscopic scales are explored. Each of these length scale regimes is considered in terms of the relationships between key overarching model approaches, specific implementation approaches, and model output or property predictions.

- **Current methods and approaches for linking across scales.** The report will present two types of modeling categories. *Hierarchical modeling* involves running calculations independently at different length scales, with optimization methods such as statistical analysis or homogenization. *Concurrent modeling* entails operating multiple scales within the same code and time step within each numerical or calculation step. Brief descriptions of a number of models and existing approaches for bridging length and time scales, as well as some of the software tools available for implementation, provide a valuable overview of the current state of the field.

- **Gaps, limitations, and needs.** The core team has identified more than 30 key gaps and limitations for bridging fundamental models and/or modeling tools across length and time scales, while also rating them in terms of potential impact and probability of success.

- **Recommendations for addressing gaps and limitations.** At the heart of the final report are more than 15 robust recommendations that examine strategies for bridging length and time scales, specific tactics and expertise needed to implement the recommendations, and suggested timeframes for implementation, among other topics. These recommendations are categorized as scientific and technical or programmatic.

The final report and recommendations will be unveiled at the 3rd World Congress on ICME, May 31–June 4, 2015, in Colorado Springs, with every attendee receiving a hard copy. The study will then be made available for free download on the TMS website.

Beyond compiling state-of-the-art approaches to multiscale modeling in one comprehensive document, Spanos believes that the greatest value of the report lies in the detailed recommendations for addressing gaps and needs. "We assembled some of the truly brightest minds in this area—a dream team if you will—who focused tightly on the overall goal of the project. As a result, they developed a number of detailed, actionable recommendations—ranging from highly technical to somewhat programmatic—for moving forward on multi-scale modeling."

Voorhees agreed that extensive engagement of volunteers from across the materials community is the defining factor in the strength and relevance of *Modeling Across Scales*. "The most gratifying experiences for me in this project have been the interactions with the members of the core team and the support of the community," he said. "In addition, I am very grateful for the opportunity to formulate a report that is unique in both its focus and potential to impact the materials field."

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