

Symposia on Multiscale Material Modeling and Simulation (17-20 June 2003, Cambridge, MA, USA) and Multiscale Modeling and Simulation of Material Behavior (27-31 July 2003, Sandia, NM, USA)

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2004 Modelling Simul. Mater. Sci. Eng. 12

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## EDITORIAL

**Symposia on Multiscale Material Modeling and Simulation (17–20 June 2003, Cambridge, MA, USA) and Multiscale Modeling and Simulation of Material Behavior (27–31 July 2003, Sandia, NM, USA)**

This past year, two distinguished conferences were held that both covered the wide area of computational mechanics. These were the 2nd MIT Conference on Computational Fluid and Solid Mechanics, held on 17–20 June, 2003 in Cambridge, Massachusetts, and the 7th US National Congress on Computational Mechanics, held on 27–31 July, 2003 in Albuquerque, New Mexico and hosted by the US Association for Computational Mechanics. Both conferences consisted of symposia covering a variety of computational mechanics topics, including a set of symposia that featured presentations on multiscale modelling and simulation of materials [MIT2 symposia organizers: Raul Radovitzky (MIT) and Alberto Cuitiño (Rutgers University); USNCCM7 symposia organizers: Alberto Cuitiño, Raul Radovitzky, Michael Ortiz (California Institute of Technology), Jonathan Zimmerman (Sandia National Laboratories)]. This subject has received much attention in recent years and has developed into a field of tremendous interest and activity. A prime example of this attention was seen in the March 2001 issue of the Materials Research Society Bulletin [1], which featured articles centred on the theme ‘Materials research by means of multiscale computer simulation’.

The main objective of modern materials modelling is to enable researchers to assess the mechanical reliability of materials and predict the modes of material failure. These failure modes are characterized by material deformation mechanisms operating at specific length scales, which vary from angstroms to metres. At the symposia in Cambridge and Albuquerque, research was presented that displayed the varying types of modelling and simulation methods capable of accurately modelling phenomena at all of these length scales. Atomistic simulation techniques were shown to model phenomena such as shock propagation in metals, diffusion-wedge and dislocation formation in thin films, grain boundary evolution in nanocrystals, and the atomic-scale origins of both brittle and ductile fracture. Current computational capabilities can be used to treat billion-atom systems, reaching into the sub-micron range for component dimensions. Alternative methodologies have been developed that shatter the micron barrier and were used to analyse systems with dimensions up to hundreds of microns. The ‘fundamental particles’ treated by these methods include material defects and microstructural boundaries. For example, grain boundary deformation and kinematics have been simulated to display how load and temperature affect grain coarsening and refinement. Dislocation dynamics simulations were shown to predict the evolution of dislocation boundaries and the creation of new microstructures in materials. Polycrystalline plasticity models were also used to model the dynamic loading of materials through impact and shock propagation. Still other methods were presented that are continuum-based and capable of modelling systems at the macroscopic scale. These included finite element analysis and phase field simulation, and were used to study deformation of shape memory alloys, solidification of metal–matrix composites, and hysteresis in metal hydrides.

A large number of presentations also discussed strategies for combining multiple simulation methods in order to span the length scales. This coupling was done with methods valid on immediately adjacent length scales, such as quantum calculation and (empirical) atomistic simulation or atomistics and dislocation dynamics, as well as disparate regimes, like quantum calculations done in tandem with finite element analysis. Some combinations of methods were used in a direct coupling sense, while others were used for hierarchical linking, whereby separate calculations done at a fine scale provide parameters or other information used within coarse scale simulation. Among the many questions posed to the symposia participants were: *'Which types of coupling are the most effective?'* and *'Are some of the coupled scales too disparate to enable tools to predict realistic material behaviour?'* Some of the presentations given also showed research that used coupled methods to span not only length scales, but time scales as well. Simulations of dislocation dynamics and grain boundary evolution, which can simulate up to seconds of physical time, used information obtained in the picosecond domain of molecular dynamics. While not many methods exist for directly coupling time scales, a notable exception being the hyperdynamics technique developed by Voter [2], the question was asked: *'How versatile are such methods as compared with hierarchical coupling options?'*

One of the advantages of attending these symposia was the opportunity to discuss some of the concerns that arise when considering the validity and usability of such research. For example, in a field of study which routinely combines methods and concepts from both engineering and physics, one must be concerned with the vocabulary of mechanics. While many researchers have been working fervently to develop ways to couple multiple-scale analysis methods, few have considered the question as to whether such methods have a common enough vocabulary so that information is exchanged easily and has a well-understood meaning. For example, the use of the term 'energy' has many different connotations. Does kinetic energy at the atomic scale translate to kinetic or thermal, or both, at the micron level? What other types of potential energy besides strain energy need to be considered within a continuum simulation when finite temperature or multiple chemical species exist?

Another issue discussed was the significance of dimensionality of a simulation. Many of the presentations given at the symposia verified materials modelling methodologies with two-dimensional problems. While this no doubt benefits the researcher in terms of computational cost and complexity for analysing problems, physical experiments are largely three-dimensional in nature and lower-dimensional physics may not carry over to three dimensions. This point was raised this past year in a fascinating article by Livi and Lepri [3] that discussed the conceptually simple example of heat conduction. This issue is especially relevant for nano-scale devices in which two-dimensional behaviour may be expected and theory and models for two dimensions are more appropriate than those for three dimensions.

A final topic discussed was the maturity of multiscale modelling methods. Most of the presentations given focused on method and model development. These newly developed methods require validation with analytical models and experiments of 'classic' mechanics problems such as simple states deformation, e.g. tension, compression, and shear of standard geometries. One question to consider is: *'When will these methods start tackling complex problems from the engineering community?'* Although this was shown to have already started in some cases, more should be done. Another question posed was: *'Does the engineering community have complex and interesting problems that require these methods?'* This question reveals an underlying uncertainty as to whether multiscale modelling and simulation still lies in the engineering domain of problem-driven research, or if it has become a science, and an art, unto itself.

Although they are not easily answered, the questions posed above display the realization that careful thought and scrutiny must accompany scientific development, especially in the

field of multiscale materials simulation. As you read the articles presented in this special issue (from page S289), I hope that you use these tools to validate the worth of the research presented, and I encourage you to feedback to the modelling community your insights and opinions. Most of all, I would like to thank everyone who participated in the discussions at the aforementioned symposia and welcome suggestions for future conversations, workshops and conferences.

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### References

- [1] Materials Research Society 2001 Materials research by means of multiscale computer simulation *Bulletin* (March)
- [2] Voter A F 1997 Hyperdynamics: accelerated molecular dynamics of infrequent events *Phys. Rev. Let.* **78** 3908–11
- [3] Livi R and Lepri S 2003 Heat in one dimension *Nature* **421** 327