ISCR hosts workshop on multiscale simulations

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The Institute for Scientific Computing Research (ISCR) hosted a workshop on *Multi-algorithm Methods for Multiscale Simulations* in Livermore at the Hilton Garden Inn, January 14-16, 2004. Forty-five attendees, including 26 from U.S. national laboratories with the balance from academia, industry, and abroad, participated in five half-day sessions on various multiscale topics, which were sorted by the organizers into applications in solids, liquids, and gases and crosscutting techniques. Each session concluded with a panel discussion in which the speakers and audience interacted richly and informally. The workshop was sponsored by the ASCI Institute for Terascale Simulation on behalf of the ASCI program, which has numerous multiscale applications.

At a working dinner on the first evening of the meeting, Professor Graeme Bird of the University of Sydney (now emeritus, but still actively writing new codes and papers and consulting in the U.S. as he has throughout his career) provided a historical perspective on the development of Direct Simulation Monte Carlo (DSMC) methods in gas dynamics over the past forty years. Bird noted how scientific progress in DSMC methods has been punctuated by progress in computer architecture and the development of outer atmosphere vehicular dynamics, which provide one of the principal motivations for DSMC, as an alternative to Navier-Stokes.

Co-organizers **Richard Hornung** of the Center for Applied Scientific Computing (CASC) and **Alej Garcia** of the Physics Department at San Jose State University expressed their hope for a "gestalt experience" in which practitioners of multi-algorithm methods from a variety of fields would find common ground and provide cross-fertilization. Materials scientists and gas dynamicists, who are not accustomed to speaking to each other, let alone to the mathematicians and computer scientists also present, found the dialog refreshing. All parties noted challenges in identifying separation of scales and in grafting together representations of the solution from different methods in "handoff" regions in which both are valid, in order to model a global system for which no single method is everywhere valid or efficient. Practitioners also noted the implementation challenges of large-scale discretizations and parallelism. Applied mathematician and chemical engineer Yannis Kevrekidis of Princeton provided one of the most provocative talks of the workshop (which he nick-named "Simulation without Equations") by showing a formalism by which, in some cases, macroscopic variables (e.g., continuum fields) can be solved for without ever writing down macroscopic governing equations, provided that one has a model valid at the microscopic scales. The formalism does not require completely resolving the problem at the microscopic scales, which would be prohibitively expensive.

See the workshop web site for a list of talks and participants.