

FROM aeronautical engineers designing passenger aircraft in virtual wind tunnels to molecular biologists designing anticancer drugs in a virtual laboratory, computer simulation is often the research tool of choice. At Lawrence Livermore, home to some of the most powerful supercomputers in existence, computer simulation is a growing part of every research effort. Indeed, the pages of *Science & Technology Review* are increasingly devoted to Laboratory employees' pioneering uses of simulation in fields as diverse as materials science, environmental remediation, and the safe stewardship of nuclear weapons.

But the increasing use of computer simulation has raised fundamental questions. Where is simulation taking science and engineering research? When, if ever, can simulation techniques replace experimental observation? Can scientists really describe "reality" with computer simulations?

Last October, some 60 of the nation's leading simulation experts gathered at Lawrence Livermore to try to answer these questions and explore ways to advance their craft. In discussions that ranged from the philosophy of science to the pitfalls of software, participants passionately cited the accomplishments and limitations of their rapidly evolving field (see boxes below).

The workshop, called "Barriers to Predictive Simulation in Science and Engineering," was held at the University of California at Davis Department of Applied Science, a center of graduate research and training located adjacent to Lawrence Livermore. Laboratory physicist Giulia Galli Gygi, a workshop organizer, said the session was envisioned as a way for experts to explore the entire range of barriers to fully predictive simulations. "Although every discipline has its own simulation challenges, we wanted to bring together the best people in the different fields to look for areas where there were common challenges," she said.

Lawrence Livermore has been one of the leading simulation centers in the world since the 1950s. Laboratory computational biologist and workshop chair Mike Colvin notes, however, that simulation has become such an important tool for every industry and research field that Laboratory researchers have much to learn from other research centers. Consequently, they are seeking to strengthen their collaborations with colleagues nationwide. Colvin, who was a dynamic force behind this workshop, is at the forefront of such efforts.

Simulation Partners with Theory

Lawrence Livermore's Dave Cooper, associate director for Computation, told attendees that simulation has become a full partner with theory and experimentation. He pointed to the significant accomplishments of the Department of Energy's Accelerated Strategic Computing Initiative (ASCI), a vital element of its Stockpile Stewardship Program to assure the safety and reliability of the nation's nuclear weapons. Cooper said ASCI has demonstrated that high-resolution simulations of nuclear detonation can be performed efficiently on supercomputers using thousands of relatively simple microprocessors working in tandem.

He asked participants what would be required to make similarly revolutionary simulation advances in their disciplines. For example, he asked what barriers would need to fall to accurately predict the exact path of a hurricane.

Lawrence Livermore physicist Berni Alder, one of the founders of computer simulation, gave a personal perspective on the growth of the field. "There's too much emphasis on building new machines," said Alder, who did pioneering work in the 1950s using computers that could describe only 100 molecular collisions per hour. Alder's seminal simulations in the early 1960s on Lawrence Livermore's LARC (Livermore Advanced Research Computer, the supercomputer of its day) changed kinetic molecular theory, showing that simulations can significantly affect a scientific field.

Several speakers noted that experiment and theory must evolve together, with each needing the other. However, they described the challenge of comparing even closely related experiments and simulations. "There is not always an obvious relationship between the two—we don't understand all that is involved," said Galli Gygi. She said that setting up a good simulation is similar to setting up a good experiment in that "you have to ask the right questions."

Participants discussed the observation of famed British physicist Paul Dirac, one of the pioneers of quantum mechanics, that even if all of the relevant equations are known, a simulation is often impossible to conduct because it would require far too many supercomputers far too many years to complete. "The fact is," said Colvin, "to simulate a chemical or biological process, you can't simply throw a bunch of atoms together and try to use brute force computational approaches."

Multiscale Modeling

Instead of trying to describe a complex chemical or biological process entirely in terms of the underlying quantum mechanics equations, some simulations are broken into a hierarchy of size and time scales, each involving a different simulation method. Such multiscale modeling was discussed with considerable enthusiasm, although a number of major challenges remain. Under development at Lawrence Livermore (see *S&TR*, December 2000, "[Following Materials over Time and Space](#)") and elsewhere, multiscale modeling was seen as essential because a "single numerical scheme is not feasible in materials and chemistry," according to Princeton University's Roberto Car.

"Multiscale is the only way to go," Car said, but integrating the different length and time scales represents a formidable barrier. As an example, he discussed the challenge of combining a simulation based on quantum mechanics with one

based on classical physics. Lawrence Livermore physicist Tomas Diaz de la Rubia agreed that combining scales is vital for accurate materials models. He also noted that real materials contain impurities and other imperfections that are not addressed in ideal simulations.

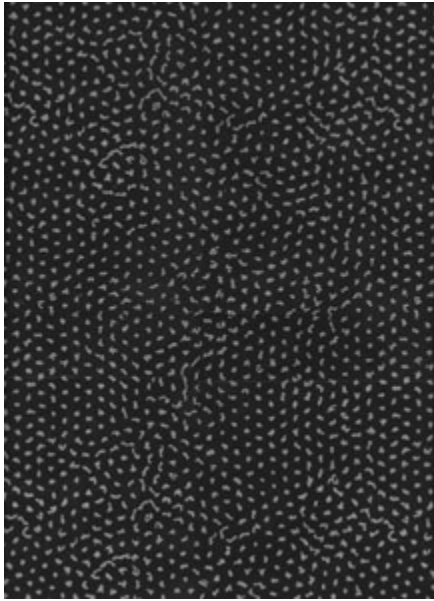
David Ceperley from the University of Illinois said the multiscale approach was mandatory in part because the largest computers can now handle simulations of up to one billion particles, but real-world problems have vastly more particles. "We're never going to be able to do 10^{23} particles [10^{12} is a trillion], so we need to do multiscale," he said.

While it was clear that computer simulation is an important tool for both theorists and experimentalists, Galli Gygi asked if simulations could lead to a major scientific discovery. "Are computational tools an essential part of the discovery path, or will they be?" Most argued that it remained an important open question in most fields, but that with the steady advances in computers and software, the answer would inevitably become "yes." Some, however, questioned whether simulation could ever discover a new field such as, say, superconductivity.

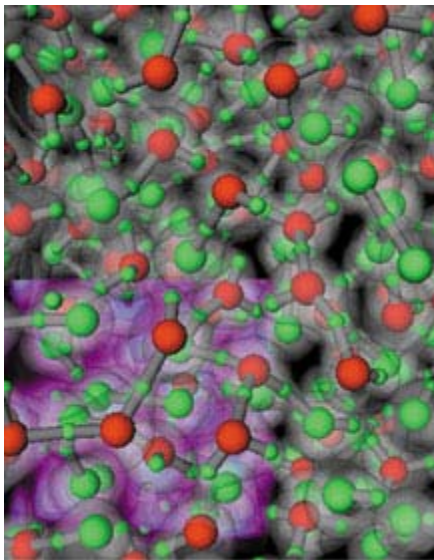
Lawrence Livermore engineer Kim Mish observed a distinction between scientific and engineering simulations when it came to discovery. "Science is concerned about fundamental truth, whereas engineering is an integrative process about systems you know a lot about," he said.

Examples of Barriers to Simulation

- Not knowing the appropriate scientific questions to address with simulations.
- Not knowing the underlying equations to describe the phenomena of interest.
- Intrinsic limitations to computability.
- Inability to meaningfully analyze simulation data.
- Lack of experimental data to initialize or validate simulations.
- Inability to scale algorithms to increased model size and resolution.
- Limitations in the speed and efficiency of computer hardware.



Livermore physicist Berni Alder's pioneering computer simulation work was published in *Physics Review* in 1962. Shown here is an example of Alder's research performed on Lawrence Livermore's LARC supercomputer. This simulation tracked 870 particles over time and contributed to the understanding of matter.



This quantum-level simulation of a mixture of hydrogen fluoride and water molecules at high temperatures and pressures took 15 days on the Accelerated Strategic Computing Initiative machine at Lawrence Livermore. (Image by Francois Gygi, Lawrence Livermore.)

Simulations Still Have Limits

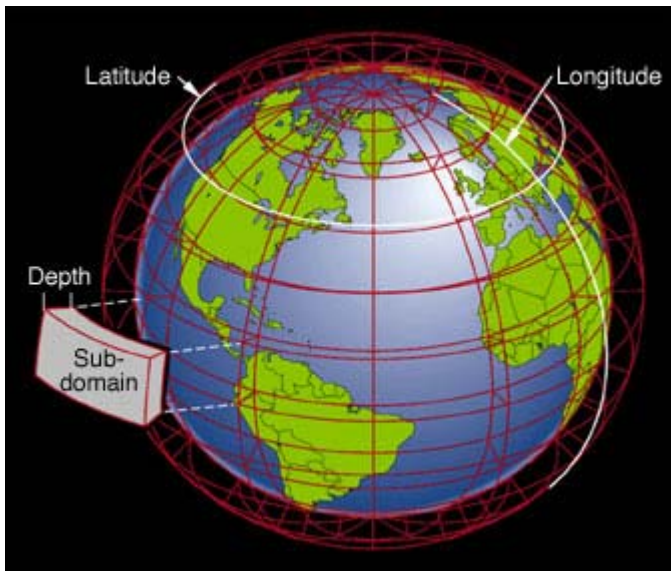
Several speakers discussed the limits of simulation validity, especially in simulations involving many phenomena. Paul Dimotakis, from the California Institute of Technology, noted that many things still cannot be computed, especially those containing heterogeneous materials and phases. Burning a piece of paper involves two phases of matter (soot particles and gases) and more than 2,000 chemical reactions involving more than 100 chemical species. Simulating such a system is probably beyond present capabilities, he said.

Another multiphenomena simulation is global climate modeling, which must take into account atmospheric physics, ocean physics, the effects of Earth's orbit, human activities, and the details of clouds, aerosols, water, and ice. UCLA's James McWilliams said climate modeling has matured as a simulation tool that involves many phenomena continually changing and affecting each other. He cited two grand challenges in the field: turbulence and pattern recognition. Although existing theories don't yet interface well with observed behavior, "We're learning an enormous amount from

simulations," he said.

The University of Michigan's Joyce Penner, a former Lawrence Livermore scientist, traced the increasingly refined model of global warming that has been extended to include scattered radiation, aerosols, biomass burning, soot, and sulfates. How the subsystems combine is impossible to reconcile in full detail, she said. Nevertheless, climate modelers are closing in on the problem of long-term climate prediction.

Lawrence Livermore's Philip Duffy explained the monumental task of simulating climate change that necessitates taking 1 million time steps to calculate grids of areas that are several hundred kilometers per side. Even with such a coarse resolution, it may take up to two months to complete a simulation. "Higher resolution is the holy grail of climate modeling," he said. Improvements will come, he suggested, from better computer designs and better representations of data, as well as better understanding how volcanic eruptions, solar variability, and aerosols affect the climate.



Climate models running on multiprocessor computers are divided into subdomains so that each processor handles a limited range of latitude and longitude and unlimited depth. This approach is typically the most efficient because it minimizes the amount of time spent exchanging information among processors, allowing the computer to perform the maximum number of calculations per second. (Image courtesy of Philip Duffy, Lawrence Livermore.)

Biology: Simulation's New Frontier

Caltech's William Goddard predicted that in the next three years, advanced simulations would reveal the structure and function of many proteins and enzymes. Biologists worldwide, including those at Lawrence Livermore, are studying how proteins--polymers consisting of up to many thousands of atoms--fold in one-thousandth of a second into three-dimensional, functional structures measuring 2 to 3 nanometers in diameter.

Stanford University's Michael Levitt called biology "the ideal system for simulation" and drew similarities between mechanical engineering simulations and protein-folding simulations. Protein-folding studies have been influenced by experiments conducted in the Critical Assessment of Structure Prediction project, which is managed by a team in Livermore's Biology and Biotechnology

Research Program Directorate. In those experiments, the amino acid sequences of proteins are posted on the Internet, and researchers from around the world predict the corresponding three-dimensional structures. The correct structures are concurrently determined experimentally by x-ray crystallography, and the predictions are revealed at a biannual conference. Workshop participants discussed whether this blind process could be valuable in other fields as a means to test different simulation software.

Lawrence Livermore biologist Elbert Branscomb, the first director of the DOE Joint Genome Institute, described a major challenge: simulating the regulatory control of genes. The genome's regulatory logic is "profound and complex," he said, with the locations of regulatory mechanisms seemingly "chaotic and crazy." He compared building a computer model of gene regulation to one describing the functioning of a computer chip. "The real barrier is the complexity barrier," he said.

Models Need Basis in Reality

Christopher Barrett from Los Alamos National Laboratory described novel software that his group has developed to help authorities better respond to emergencies. The software simulates a host of situations such as bioterrorism, earthquakes, or commercial power-grid outages. The software includes models to find how to reduce congestion, thereby allowing faster emergency response. "Computer simulations have become a commonplace, but artful tool for addressing these problems," he said. Lawrence Livermore engineer Dave McCallen discussed what can happen when seismic engineering models are not based on real experiments: "Things can go bad when we don't fully understand the physics of the process." McCallen cited a newly constructed bridge that collapsed in the 1971 San Fernando Earthquake because "we didn't know then how bridges vibrate."

McCallen said engineers now have adequate computer power to model regional seismic activity and the response of structures. He pointed to a collaboration between the Laboratory and the University of California at Berkeley on the seismic response of long-span bridges (see *S&TR*, [May 1999](#), "[The Revelations of Acoustic Waves](#)" and [December 1998](#), "[A Shaker Exercise for the Bay Area](#)"). The major 1999 earthquake in Taiwan provided a wealth of ground-

motion data that validated the occurrence of huge ground displacements that were produced in Lawrence Livermore simulations. The predictions made by these simulations had originally been considered by many seismic experts to be unrealistically large. "Our ability to compute has vastly outstripped our ability to validate," he noted.

Themes Arising from the Workshop

- Limitations in raw computer speed is not the sole barrier to progress in simulation.
- Expectation of outcome varies, ranging from discovering fundamental physical laws to determining the most efficient airfoil shape.
- The observation of Paul Dirac that all of the relevant equations are known but remain difficult to solve.
- Dependence on initial conditions (for example, crack formation, turbulence in some systems may limit results).
- Concept of robustness, in which many emergent behaviors are insensitive to model detail and starting conditions.
- Challenge of comparing even closely related experiments and simulations.
- Need to overcome limits of simulation, especially in multiphenomena simulations.
- Need of computers to do more than just numerics—they need to help set up grids, evaluate outputs, and analyze experimental data.
- Software development and management are major hurdles and perhaps lend themselves to interdisciplinary collaboration.
- The role of blind prediction experiments in protein folding could have valuable applications to other fields.
- Funding for solving problems with existing methods is easier to get than funding for developing better methods.
- Accurate material models are required for realistic computational simulations of macroscopic phenomena.

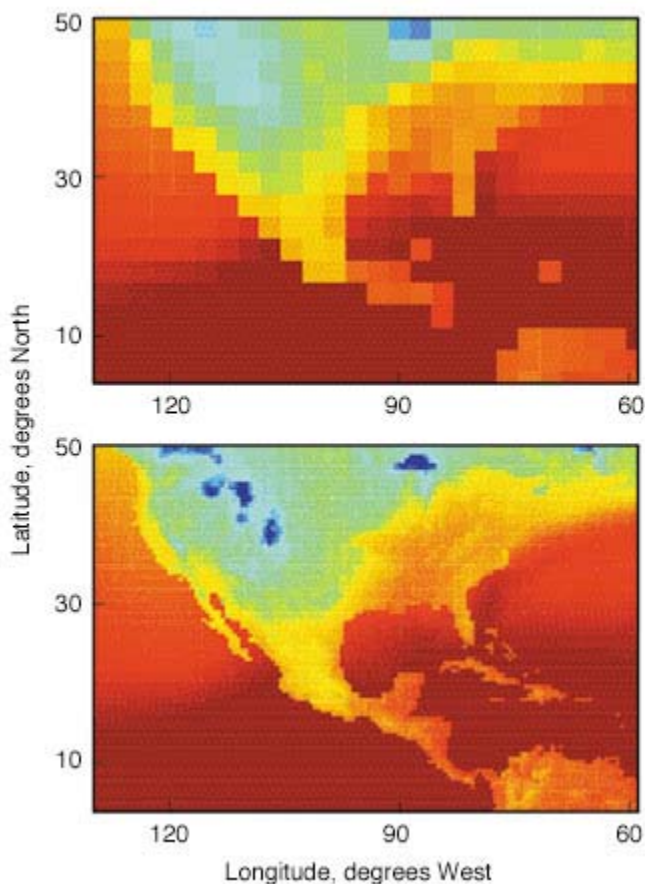
In that respect, participants drew a distinction between verification and validation: verification involves making sure models and equations have been implemented correctly while the process of validation ensures that the simulation represents reality.

K. K. Muraleetharan of the University of Oklahoma said it was difficult to get data on the material properties of soils for use in simulating the seismic response of new structures. Muraleetharan cited two other barriers to civil engineering simulations: a litigation-driven society and the reluctance of people in his field to try new approaches.

Workshop speakers made it clear that in some systems, predictive accuracy may always be limited by dependency on the precise details of initial conditions. For example, the propagation of a crack in a material is affected by what goes on at the crack's very tip. As a result, said Northwestern University professor Ted Belytschko, realistically predicting the formation of cracks is still problematic.

Simulations involving climate change also have a high sensitivity to starting conditions. UCLA's McWilliams noted that numerical weather prediction is 50 years old, but predictions are useful for only about one week in advance. "There is a fundamental limit of predictability because small disturbances become amplified," he said.

Nobel Prize-winning Livermore physicist and Stanford professor Robert Laughlin suggested that some physical properties seem to be protected from sensitivities to starting conditions and model details, and he encouraged the workshop participants to seek out such systems for simulation. One example of such a protected system is a phase transition, such as when water turns to ice.



Higher spatial resolution is needed to accurately forecast both regional and large-scale climate change using global climate models. Typical global models (top image) use grid cells with horizontal sizes of 250 to 300 kilometers, preventing accurate forecasts for specific geographical regions (for example, California). The bottom image shows preliminary results of a simulation at 50-kilometer resolution performed at Lawrence Livermore on computers of the Accelerated Strategic Computing

Initiative. At this resolution, much more accurate forecasts should eventually be possible. (Images by Philip Duffy, Lawrence Livermore.)

Virtual Proving Grounds

Belytschko also described the virtual proving grounds of U.S. car manufacturers that model, for example, a car's suspension system. A virtual car can be run over a pothole, with the resulting stress on the suspension system measured. A realistic simulation must include thousands of welds, some of which inevitably fail, sometimes because of poor workmanship. Predicting which welds will fail, when they will fail, and why is a tough challenge.

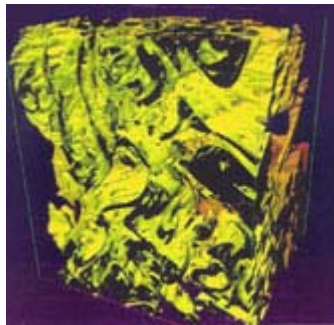
Scientist Jacqueline Chen of the Sandia National Laboratories Combustion Research Facility described efforts to simulate turbulent mixing and combustion found in diesel engines. Turbulent mixing, an irregular process of stirring and mixing, greatly enhances combustion by creating a flame area. Chen noted that in recent experiments by Sandia's John Dec, laser diagnostics of diesel combustion reactions involving 80 to 100 atmospheres of pressure and temperatures of 2,000 kelvins have significantly changed the conceptual understanding of diesel combustion. Further advances in the fundamental understanding of the relevant physics will be aided by first-principles numerical simulations.

Beyond Computer Speed

Although speakers gave credit to the unprecedented power of current computers, raw computer speed was not identified as the sole barrier to progress in simulation. Livermore physicist Bill Nellis challenged the conventional thinking that the key to better simulations was more powerful computers. He said that there are too many "brute force" simulations with not enough thought behind them. "The key to doing good science is using your head," he said. "You need as much intuition to do computation as you need to do experiments."

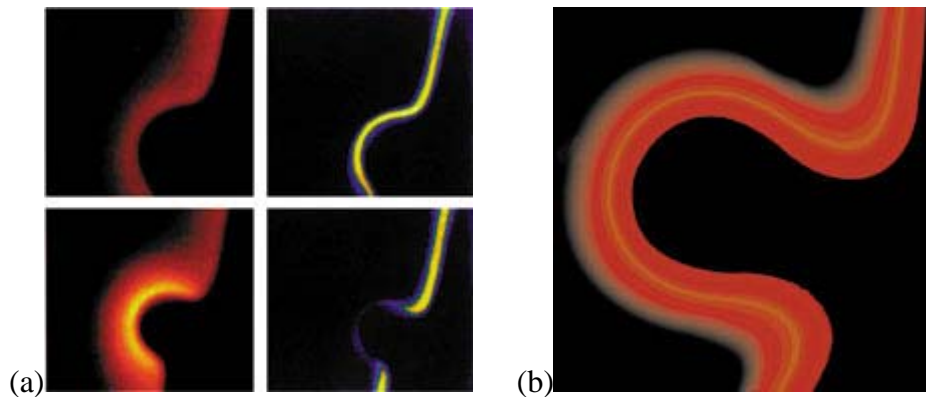
Alder said it made sense to focus more on developing advanced algorithms because the increased speed of computing has been as much due to improvement in algorithms as to new hardware. He also noted that it was easier to develop algorithms on personal computers than on larger machines. Several speakers said there was plenty of room for both greater computational power and better algorithms. They voiced their concerns, however, that policymakers excessively emphasize multiparallel computing designs, such as ASCI machines using thousands of microprocessors. Different kinds of machines with fewer but more powerful processors would work better for some whole-system problems such as climate science, which involves interweaving data from physical, chemical, and biological processes.

Many participants cited the development and management of simulation software as a key barrier. Several regretted that there is no Moore's Law for software. A common request was for robust software with intuitive interfaces that could be used by any engineering student or by a small



Simulating the chaotic nature of turbulence is one of computer simulation's great challenges. This three-dimensional image of laboratory data shows the tremendous complexity of a turbulent jet. (Image courtesy of Paul Dimotakis, California Institute of Technology.)

engineering firm. Lee Taylor, from TeraScale LLC in Albuquerque, New Mexico, raised the issue of accessibility for small firms that may not be able to purchase an advanced computer, yet recognize that simulation "lets you design closer to the limits."

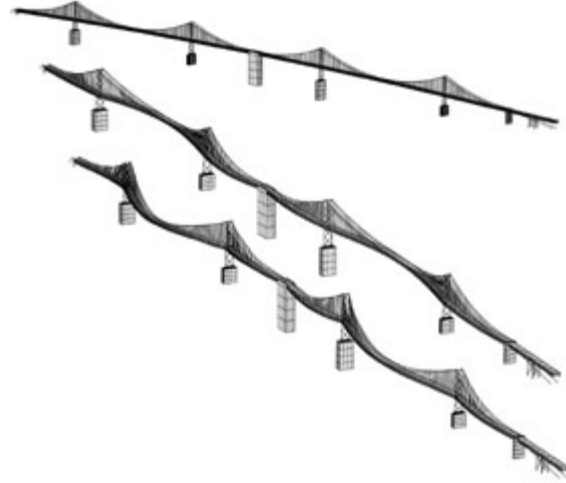


Modeling combustion in an engine demands close links to experiments. (a) Images of OH and CH in an actual flame-vortex interaction and (b) an image of OH from a simulation illustrate the complexity of modeling chemical response to fluid-chemistry interactions. (Image (a) is provided courtesy of The Combustion Institute, and (b) is by Jacqueline Chen, Sandia National Laboratories, Livermore.)

Collaborating on Software

A popular idea was to make software writing more efficient, perhaps by collaboration. UCLA's McWilliams said, "We all do everything for ourselves. We keep reinventing simple solutions that take lots of hours to develop and debug." Several participants urged free exchange of software, but others cautioned that some institutions have cultural barriers against sharing software developed in-house. One suggestion was an interdisciplinary collaboration on common software components. Although such an effort would necessitate going beyond rigidly defined academic disciplines, many felt that the time had come for researchers to have a broader knowledge of science and technology. In that light, Princeton's Car suggested creating new positions such as "software physicist" or "software chemist." Participants also voiced concern that Silicon Valley was drawing off some of the best software minds. Lawrence Livermore's Krzysztof Fidelis commented, "We need better software, but we live in a world where software experts tend to go to industry."

Several participants observed that it is much easier to get funding to solve problems with existing methods than to develop better methods. Many agreed with William Goddard of the California Institute of Technology that funding was needed to explore new directions that offered long-term but sizable payoffs. Unfortunately, funding sponsors want a particular problem solved and are not interested in funding better methods that may not directly solve their problem.



More and more, seismic engineers are using powerful computer models to design seismic retrofits to existing structures. The simulation above shows a severe earthquake in Northern California, and the simulations at right show how the earthquake affects the San Francisco-Oakland Bay Bridge. The topmost one of those simulations is of the bridge before the earthquake, and the bottom two show the aftermath.



Simulations are helping to reveal the three-dimensional structures of proteins. This image shows the structure of a protein determined by computational modeling. (Image by Ceslovas Venclovas, Lawrence Livermore.)

Simulating Extreme Conditions

Two areas of major interest to Lawrence Livermore are nuclear weapons physics and its close relative, astrophysics. Lawrence Livermore physicist David Nowak, ASCI program leader, said, "ASCI has led the U.S. to world leadership in high-performance simulation." The first major barrier to

success, said Nowak, is resources, which include funding, hardware costs, and recruiting and retaining computational experts. The second barrier is technical, for example, validating new software that simulates imperfectly understood processes such as turbulence and materials properties. ASCI simulations, he said, must reflect a host of data that include engineering details, weapon designer comments from 30 years ago, information gathered in nuclear tests, and the results of equation-of-state experiments.

Because astrophysics is not a classical experimental science, simulation plays a strong role in that field. University of California at Berkeley's Christopher McKee said the primary barrier in astrophysics simulations is vast time and distance scales, ranging from atomic nuclear reactions to the formation of entire galaxies, with time scales ranging up to a billion years.

"People are stretching the ability of computers" with these problems, McKee said. He added that computer simulations can perform virtual experiments whose outcomes can be validated with observations. The grand challenge is to follow the simulated gravitational collapse of a molecular cloud to the formation of one or more stars.

Lawrence Livermore physicist Richard Klein said an important barrier to astrophysics simulation is the difficulty in obtaining enough data to validate models. A new testbed for validation is emerging in the University of Rochester's Omega laser and the National Ignition Facility, currently under construction at the Laboratory. Klein has used simulation to predict photon bubble oscillation, a new phenomenon on the surface of neutron stars, with structures the size of New York's World Trade Center.

Lawrence Livermore astrophysicist Dave Dearborn noted that astrophysics simulation incorporates lots of physics, some of it not well known. "We're still human," he said. "We need the brightest people to pose new questions."

Workshop Speakers and Panelists

Simulations History

Berni Alder, Lawrence Livermore National Laboratory

Accelerated Strategic Computing Initiative (ASCI)

David Nowak, Lawrence Livermore National Laboratory

Infrastructure Modeling

Christopher Barrett, Los Alamos National Laboratory

Astrophysics

David Dearborn, Lawrence Livermore National Laboratory

David McCallen, Lawrence Livermore National Laboratory

Richard Klein, Lawrence Livermore National Laboratory

K. K. Muraleetharan, University of Oklahoma

Christopher McKee, University of California at Berkeley

Theofanis Theofanous, University of California at Santa Barbara

Mechanics

Richard Becker, Lawrence Livermore National Laboratory

Biology

Elbert Branscomb, Lawrence Livermore National Laboratory

James Belak, Lawrence Livermore National Laboratory

Krzysztof Fidelis, Lawrence Livermore National Laboratory

Ted Belytschko, Northwestern University

Michael Levitt, Stanford University

Lee Taylor, TeraScale LLC

John Moul, University of Maryland

Physics and Simulation

Robert Laughlin, Lawrence Livermore National Laboratory and Stanford University

Climate and Weather

Philip Duffy, Lawrence Livermore National Laboratory

James McWilliams, University of California at Los Angeles

Quantum Mechanics

Roberto Car, Princeton University
David Ceperley, University of Illinois at
Champaign-Urbana
William Goddard, California Institute of
Technology
Bill Nellis, Lawrence Livermore National
Laboratory

Joyce Penner, University of Michigan

Fluid Dynamics
Jacqueline Chen, Sandia National Laboratories,
Livermore
Paul E. Dimotakis, California Institute of
Technology
Anthony Jameson, Stanford University

Next Steps

Colvin says the workshop was so successful that plans are under way for a number of follow-on meetings. Kalos will be chairing a simulation workshop this summer addressing a number of other simulation fields. Livermore's Materials Research Institute, under director Mike McElfresh, is holding a Computational Materials Science and Chemistry Summer Institute where graduate students can explore cutting-edge computational methods (see <http://www.llnl.gov/mri/> for more information). A workshop on advanced simulation software is being organized by Mish for the summer of 2002. Discussions are also continuing about extended programs involving visiting faculty and graduate students who would research a single topic. More informally, individual researchers are working on ways to build on existing collaborations and newfound friendships formed at the workshop. Fortunately, the barriers to lasting friendship are less formidable than those required for scientific and engineering simulations.

—Arnie Heller



Members of the simulation workshop steering committee, from left, are Malvin Kalos, Mike Colvin (chairman), John Holzrichter, Steve Libby, Paul Miller, Giulia Galli Gygi, and Francois Gygi.

Key Words: Accelerated Strategic Computing Initiative (ASCI), blind prediction experiments, computing speed, Dirac observation, model validation, multiscale modeling, predictive simulations, software.

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About the Scientist



GIULIA GALLI GYGI is a group leader for the Quantum Simulation Group in the Chemistry and Materials Science Directorate. She joined Lawrence Livermore as a staff physicist in 1998, after holding the position of senior scientist at the Swiss Federal Institute of Technology in Lausanne, Switzerland. She received a B.S. in physics from the University of Modena in Italy, and an M.A. and Ph.D. in physics from the International School for Advanced Studies in Trieste, Italy. Thereafter, she was a postdoctoral research associate at the University of Illinois at Champaign-Urbana and then at the IBM Zurich Research Center, Switzerland. Galli Gygi has published over 70 papers in refereed international journals. Her areas of interest are in systems and processes relevant to condensed-matter physics, physical chemistry and materials science, and quantum simulations. Current topics of investigation include modeling of fluids under pressure, DNA in solution, and complex surfaces and nanostructures.