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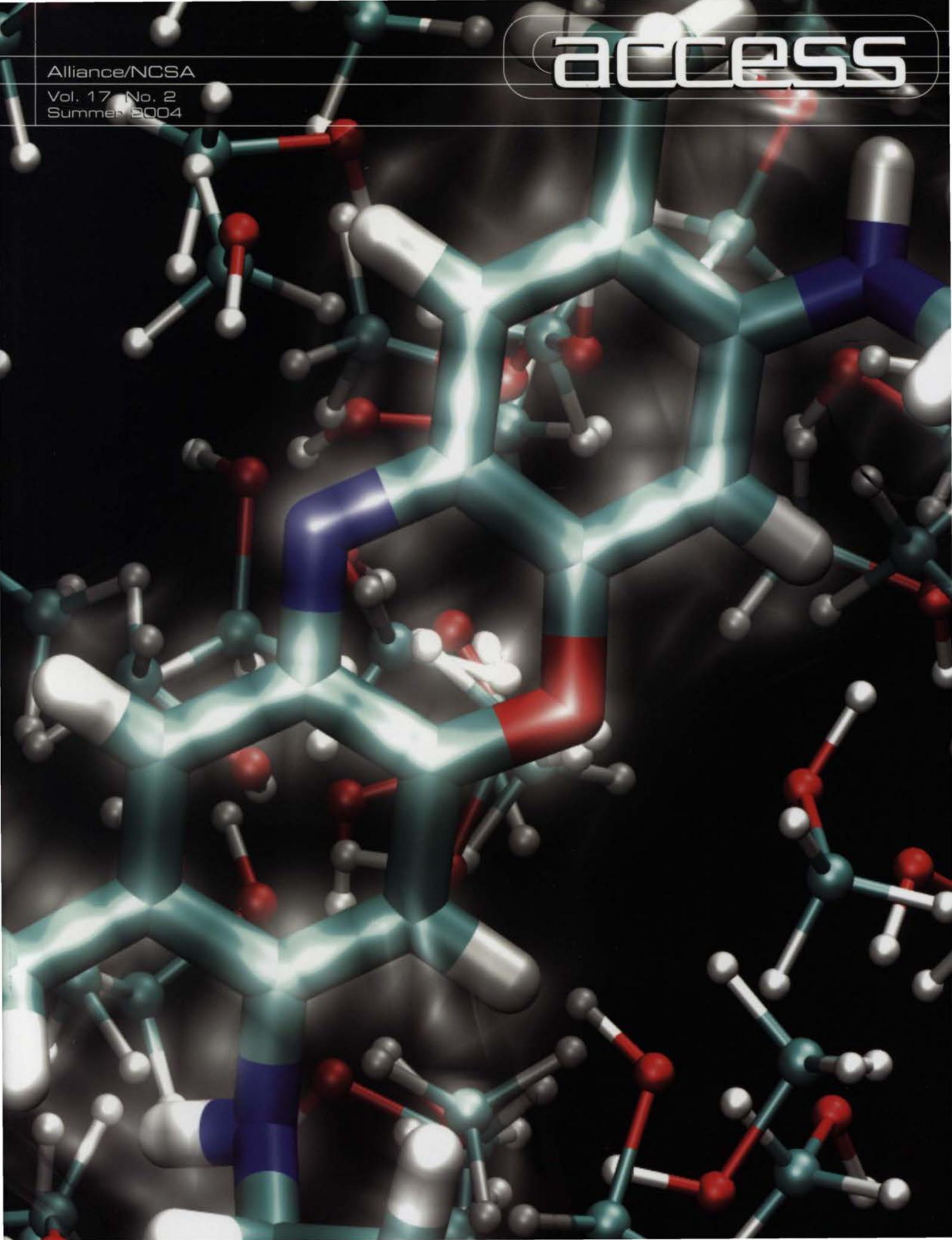

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Who we are

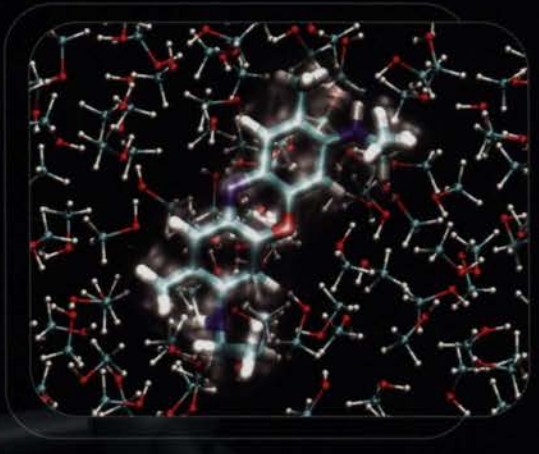
The National Center for Supercomputing Applications (NCSA) opened its doors in January 1986. NCSA earned and maintains an international reputation in high-performance computing and networking and in developing innovative software applications—like NCSA Mosaic, the first readily-available graphical Web browser. Since 1997, NCSA has been the leading-edge site for the National Computational Science Alliance (Alliance), one of two partnerships of the NSF's Partnerships for Advanced Computational Infrastructure program. The Alliance is a partnership among about 50 academic, government, and industrial organizations from across the United States.

In August 2001, NCSA—as part of a four-institution team—was tapped by the National Science Foundation to build one of the world's first computational grids and put it to use. It will be the most comprehensive grid yet deployed for open scientific research, spanning the country and providing the backbone from which tomorrow's global grid can grow. With software developed to make it all work in concert, this TeraGrid will offer the fastest unclassified supercomputers as well as an unparalleled array of visualization tools, sensors and instruments, and mass storage devices. These resources will be linked via a network four times faster than today's fastest.

Major support for NCSA and the Alliance is provided by the National Science Foundation's Partnerships for Advanced Computational Infrastructure program. Additional funding for NCSA comes from the state of Illinois, the University of Illinois, industrial partners, and other federal agencies.

Cover

The laser dye oxazine-4 (solid bonds) dissolved in methanol (ball-and-stick models). The identity and motion of the solvent affect how the dye interacts with light. In simulations of these interactions, the dye is surrounded by 130 angstroms of methanol. Using NCSA's Platinum and Titan Linux clusters, researchers at Hope College are working on perfecting a computational approach that combines molecular dynamics and quantum mechanics to identify and calculate the movements of solvent molecules and their effect on the excitation energy of solute molecules.



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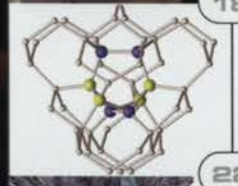
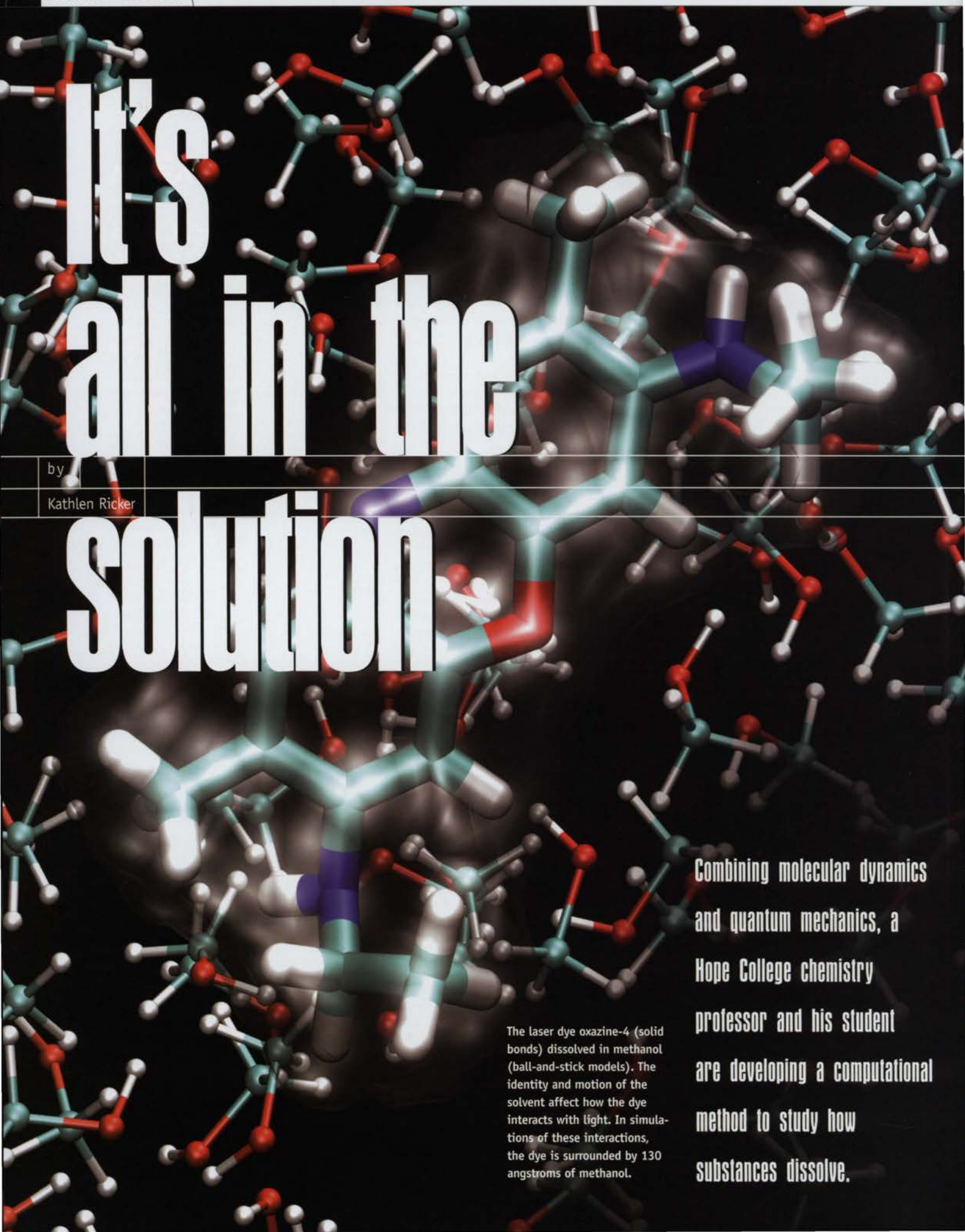


It's all in the solution

by Kathlen Ricker



The laser dye oxazine-4 (solid bonds) dissolved in methanol (ball-and-stick models). The identity and motion of the solvent affect how the dye interacts with light. In simulations of these interactions, the dye is surrounded by 130 angstroms of methanol.

Combining molecular dynamics and quantum mechanics, a Hope College chemistry professor and his student are developing a computational method to study how substances dissolve.

Solvation is an everyday process, one most people don't give much thought. Sugar dissolves in tea, oil-based paints in turpentine, nail polish in acetone. It's also well known that certain substances, like oil, will not dissolve in other substances, like water.

While it seems intuitive that solutes (like salt or sugar) dissolve best in fluid solvents (like water), whether a solute and a solvent are compatible depends on their polarity, that is, how charges are distributed within a molecule. If there is an uneven distribution of positive and negative charges the molecule is polar. Polar solutes will dissolve in polar solvents; hence, sugar will easily dissolve in water, because both substances have some negative and some positive atoms, but because oil is non-polar, consisting of nearly neutral atoms, it will not dissolve sugar.

Solvation is involved in the vast majority of chemical reactions; however, this important process is not entirely understood. "A lot of what's important in chemistry is understanding why a reaction happens in a particular way...or why you mix two things together, A and B, and get C, but not D, when D is a perfectly viable option," says Brent Krueger, an assistant professor of chemistry at Hope College in Holland, MI. "The way solvation happens, and the way solvent affects a chemical reaction, are really the same thing, so if we can understand one of them, we can understand the other in detail."

Solvation on the particle level

Solvation occurs when molecules of a solvent surround and stabilize those of a solute. The solvent molecules are always in random thermal motion—the higher the temperature, the faster they move around. As the solvent molecules move, the solute sees a constantly changing environment—sometimes surrounded by six solvent molecules, sometimes seven, sometimes turned this way, sometimes that. All these different environments yield slightly different solute energies such that the solute energy fluctuates rapidly.

These solvent-driven energy fluctuations have a crucial effect on the outcome of a chemical reaction. The problem, however, is that there are limits to physical methods used to study chemical interactions, such as optical spectroscopy, a technique that uses light to examine molecular interactions. "Spectroscopy can give you a pretty detailed picture of the timescales of motions in the system, but it can't actually tell you what's moving around in the system," explains Matt Zwier, a 2004 Hope College graduate who has been a student of Krueger's. However, says Zwier, simulating the interaction between solvent and solute provides a way to study these movements that spectroscopy doesn't. "A simulation will allow you to see what's actually moving."

Largely using NCSA's Platinum and Titan Linux clusters, Krueger and Zwier are working on perfecting a computational approach that uses a combination of molecular dynamics and quantum mechanics to identify and calculate the movements of solvent molecules and their effect on the excitation energy of solute molecules. Their method is based on an earlier method developed by Ian Mercer, Ian Gould, and David Klug of Imperial College in London. It combines classical mechanics—specifically molecular dynamics (MD)—with quantum mechanics (QM) to calculate the optical properties of a solute-solvent system.

Krueger emphasizes that while there exist a number of both computational and experimental methods for studying solvation, "there's not a strong connection between computational and experimental research. So one of the things we're trying to achieve is to connect our computational method very directly with experimental results." The experimental and computational parts of their work are complementary; each allows them to examine details of the interaction that the other might leave obscure.

Dissolving pictures

The simulation that forms the basis of Krueger and Zwier's work involves a single solute molecule, in this case a dye called oxazine-4. The oxazine-4 molecule is surrounded by about 12,000 methanol molecules, which constitute the solvent. "Basically...we're looking at the fluctuations that occur as the system just sits there at room temperature," says Krueger. "We're not doing anything to the system; it just sits there, with all the oxazine and methanol molecules moving around...all those little fluctuations tell us about how the solute and solvent are interacting."

The molecular dynamics component of the simulation, which is applied classical mechanics, involves sampling all the configurations that take place as the system fluctuates and taking periodic snapshots that show the positions of all the atoms at a given point in time. "The classical mechanics part [of the simulation] is valuable to us because it's a very simple treatment, so that we can afford to have a very large system with 12,000 methanol molecules," Krueger explains. "We can treat it for a fairly long time and get millions of different snapshots that show how all the atoms are arranged."

However, classical mechanics does not work for elementary particles—in this case, electrons. Therefore, a quantum mechanics component, which helps to predict the behavior of electrons, is used to calculate the excitation energy of the solute for each of the millions of snapshots. "The oxazine molecule is bathed in all these tiny charges from the methanol molecules, and in each snapshot the 80,000 charges from the methanol molecules are going to be a little bit different and so, therefore, is the oxazine molecule," Krueger explains. "When we do the quantum mechanics, it registers both the changes in the oxazine structure and the effects of the methanol solvent through all those little charges."

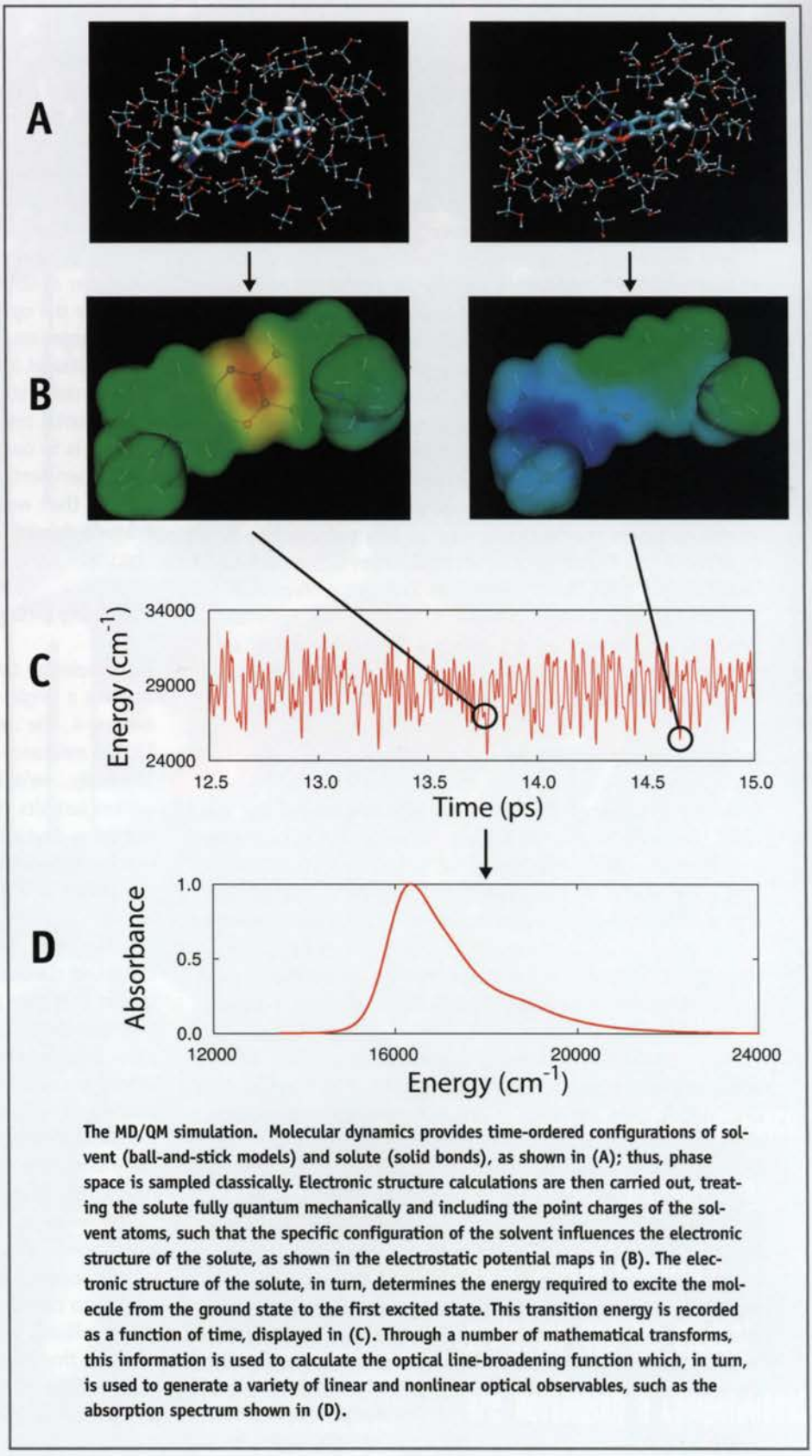
Putting it all together

The system that Krueger and Zwier have put together involves four separate parts. Two are standard applications, including AMBER 7, a molecular dynamics code, and Gaussian 98, which does the quantum mechanics. What's unique about the code is the "glue" that holds the two methods together—dozens of scripts written by Zwier that automate the collection of the molecular dynamics snapshots, convert them into a Gaussian-compatible format, parse out essential information, and send it to an output file for processing later. Performed once or a few times, these are simple procedures. However, Krueger and Zwier need to perform these tasks millions of times—which, as Krueger says, changes everything. "A lot of people write scripts to make their lives easier, but in this case, these scripts are absolutely necessary to doing the calculation."

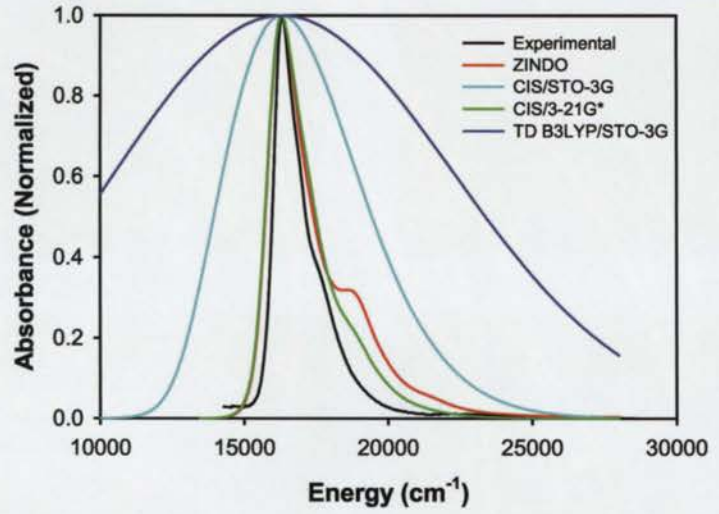
The fourth component of the code has also been developed by Zwier. Deceptively simple, it seems merely to plot the excitation energy of the oxazine molecules over time. However, this information is the key to the whole experiment: It describes the fluctuations in both the oxazine-4 molecules and the methanol molecules. "It turns out that after you've done both the molecular dynamics and the quantum mechanics, that energy versus time is really the only information you need in order to simulate the results from any kind of optical experiment," says Krueger. He anticipates that the code that Zwier has put together, with some modification, will be able to simulate a broad variety of spectroscopic experiments.

Science on a shoestring

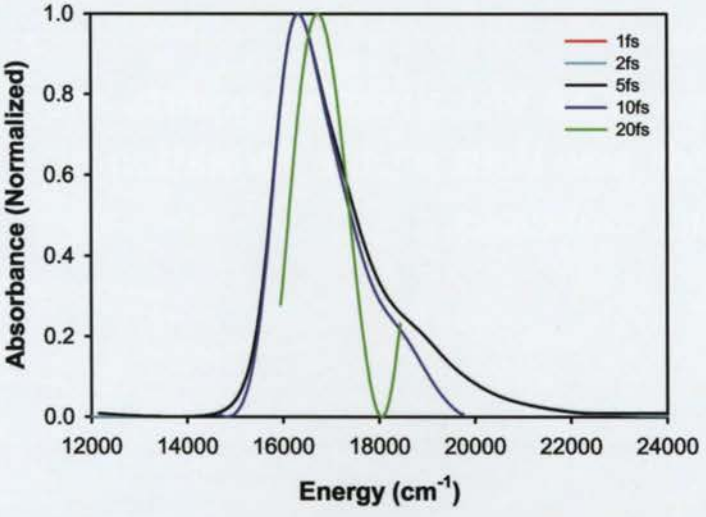
The work of pulling together a complex framework for a scientific application is often done by advanced graduate students as part of a large research group. However, most of the work on this project has been done by Zwier, who doesn't actually begin his graduate work until Fall of 2004, when he will be entering the doctoral program in the Department of Chemistry at the University of Illinois at Urbana-Champaign.



The MD/QM simulation. Molecular dynamics provides time-ordered configurations of solvent (ball-and-stick models) and solute (solid bonds), as shown in (A); thus, phase space is sampled classically. Electronic structure calculations are then carried out, treating the solute fully quantum mechanically and including the point charges of the solvent atoms, such that the specific configuration of the solvent influences the electronic structure of the solute, as shown in the electrostatic potential maps in (B). The electronic structure of the solute, in turn, determines the energy required to excite the molecule from the ground state to the first excited state. This transition energy is recorded as a function of time, displayed in (C). Through a number of mathematical transforms, this information is used to calculate the optical line-broadening function which, in turn, is used to generate a variety of linear and nonlinear optical observables, such as the absorption spectrum shown in (D).



The absorbance lineshape dependence on quantum-mechanical model chemistry. Because quantum mechanical models vary greatly in their computational cost, Krueger and Zwier seek to determine the trade-off between cost and accuracy of simulations. The electronic excitation energy of the simulated system was evaluated every femtosecond over a 20 picosecond period using three quantum mechanical methods and two basis sets. The semi-empirical ZINDO method, shown in red, and the *ab initio* configuration interaction singles (CIS) method over a relatively small basis set (3-21G*), shown in green, produce spectra in reasonable agreement with experiment (black), both in terms of peak width and the presence of asymmetry. CIS over the minimal STO-3G basis set (light blue) and time-dependent B3LYP (dark blue) overestimate system-bath coupling, washing out vibronic structure.



The absorbance lineshape dependence on quantum mechanical sampling rate. Because quantum mechanical calculations are vastly more costly than molecular dynamics calculations, a goal of this research is to determine the minimum sampling frequency for quantum mechanical calculations that still reproduces spectral features with reasonable accuracy. Spectra generated taking configurations every one femtosecond, two femtoseconds, and five femtoseconds (red, light blue, and black, respectively) are essentially indistinguishable in calculated linear spectra. At 10 femtoseconds (dark blue), the bandshape changes significantly, and at 20 femtoseconds (green), peak folding occurs.

"I always was about 70 or 80 percent sure that I wanted to be in research as a career," says Zwier, "but this project has really solidified that. Furthermore, it indicated what I want to do in research—I've got it narrowed down to computational theoretical work or spectroscopy, as opposed to a broader area like physical chemistry or biochemistry."

Krueger says that the development of the code has been a critical component both of his research and of Zwier's undergraduate education. "Many people probably have clusters of 100 CPUs or more, but at a liberal arts college, where our budgets aren't huge, we don't have a lot of local computing resources. NCSA has made it possible for us to do this."

This research is supported by Research Corporation, Hope College, and the National Science Foundation's Research Experiences for Undergraduates program.

Access Online http://access.ncsa.uiuc.edu/CoverStories/mdqm/

For further information:

http://www.chem.hope.edu/~krieg/

Team members

Brent Krueger
Matthew Zwier

Hunt for the

by Trish Barker

A close collaboration between NCSA visualization experts and atomspheric researchers sheds new light on the formation of the most powerful, dangerous tornadoes.

supertwister

In a typical year, 1,200 tornadoes cause 70 fatalities and 1,500 injuries nationwide. Most of the damage, deaths, and injury are due to a very small percentage of these tornadoes, the so-called "supertwisters" whose winds of more than 200 miles per hour put them at the extreme end of the Fujita Scale of Tornado Intensity (the so-called F4 and F5 tornadoes). On average, there are 12 or 13 of these tornadoes in the United States each year.

Ideally, forecasters would be able to provide enough warning that people could protect themselves from these killer storms. While they have successfully identified atmospheric conditions that are favorable for supercell formation, accurately predicting which storms will produce tornadoes and at what time is a feat that continues to challenge forecasters. Researchers from the University of Illinois at Urbana-Champaign collaborated with visualization experts at NCSA in an effort to shed light on how the most violent tornadoes form and to create animations that reveal the inner behavior of tornado producing storms.

Their work was showcased this March in an episode of the PBS TV series NOVA called "Hunt for the Supertwister."

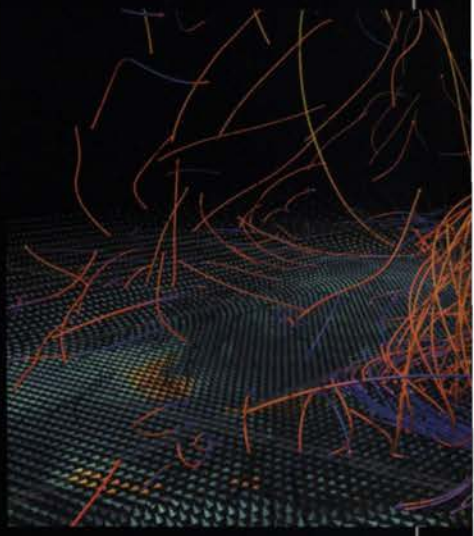
A storm is born

Scientists know that the strongest tornadoes are generated by a particular type of rotating thunderstorm called a supercell. The swirling winds of a supercell can produce tornadoes. But not all supercells lead to tornadoes, and not all tornadoes become supertwisters. In fact, only about 20 percent to 25 percent of supercells produce tornadoes. Why some storms spawn tornadoes while others don't—and why some tornadoes become extraordinarily strong supertwisters—is not yet well understood.

Supercells form in an unstable and adequately deep atmospheric layer that has sufficient moisture and significant change in the horizontal wind speed. An environment that favors the formation of tornadoes also requires high relative surface humidity, considerable low-level horizontal wind, and steep low-level lapse rates (meaning the temperature drops rapidly at greater atmospheric heights).

In an effort to pinpoint what triggers tornadoes, researchers —including NCSA research scientist Robert Wilhelmson—create computer simulations of evolving storms. Just as physicians use X-rays and CAT scans to diagnose disease, these storm researchers use simulations and visualization to analyze tornado formation.

"The big problem in storm science is that with the instrumentation we have we can't sense all the things that we need to know," explains Lou Wicker, a scientist at the National Severe Storms Laboratory who frequently collaborates with Wilhelmson. "From the field, we can't figure out completely what's going on, but we think the computer model is a reasonable approximation of what's going on, and with the model we can capture the entire story."



Images from the animated tornado visualization created by NCSA's experimental technologies group. Orange and blue tubes represent the rising and the falling airflow in and around the tornado, which is shown by spheres that are colored according to pressure.

Wicker developed a model called NCOMMAS (NSSL Collaborative Model for Multiscale Atmospheric Simulation) to computationally simulate thunderstorms and their associated tornadoes. NCOMMAS is based upon an earlier model developed by Wilhelmson.

The simulation begins with data describing the pre-tornado weather conditions—wind speed, atmospheric pressure, humidity, etc.—at discrete points separated by distances ranging from 20 meters to three kilometers. Starting with these initial variables, partial differential equations that describe changes in the atmospheric flow are solved. The numerical solution of these equations proceeds in small time intervals for two to three storm hours as the supercell forms and produces a tornado. A virtual storm is born.

Simulating the supertwister

In the summer of 2003, the 200 mph winds of a supertwister ripped through tiny Manchester, SD. The tornado's path of destruction was caught by the HDTV crew of Tom Lucas, the producer of the "Hunt for the Supertwisters" episode of NOVA. Knowing that weather research combines both daredevil storm chasing and computational simulation, he approached NCSA's Wilhelmson and Donna Cox, leader of NCSA's experimental technologies division, about modeling and visualizing that storm.

Researchers in Wilhelmson's convective modeling group got to work. Starting with the recorded conditions near Manchester, the simulation followed the erupting thunderstorm and resulting powerful tornado as it evolved in a 100 x 100 x 25 kilometer domain. A number of simulations were made using 250 meter and 100 meter horizontal resolution in the active storm region. The result of these simulations was the first ever simulation of a long-track tornado, defined as one that spends 40 to 60 minutes on the ground with a pressure drop of at least 50 millibars.

"The simulation of long-track tornadoes has remained elusive for almost a decade," Wilhelmson says, "and these exciting simulations have paved the way toward understanding the atmospheric conditions that lead to their occurrence."

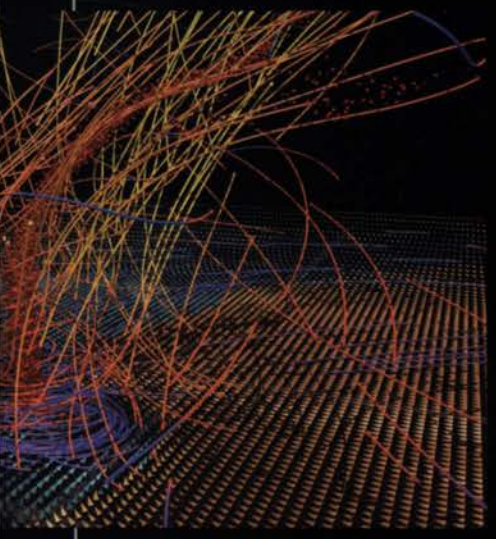
The visualizations included in the NOVA special were made from a simulation performed on NCSA's IBM p690 computing cluster in November 2003. The simulation portrayed the development of a supercell and subsequent tornado—about two and a half hours of "storm time." It was accomplished using 16 processors for approximately eight days.

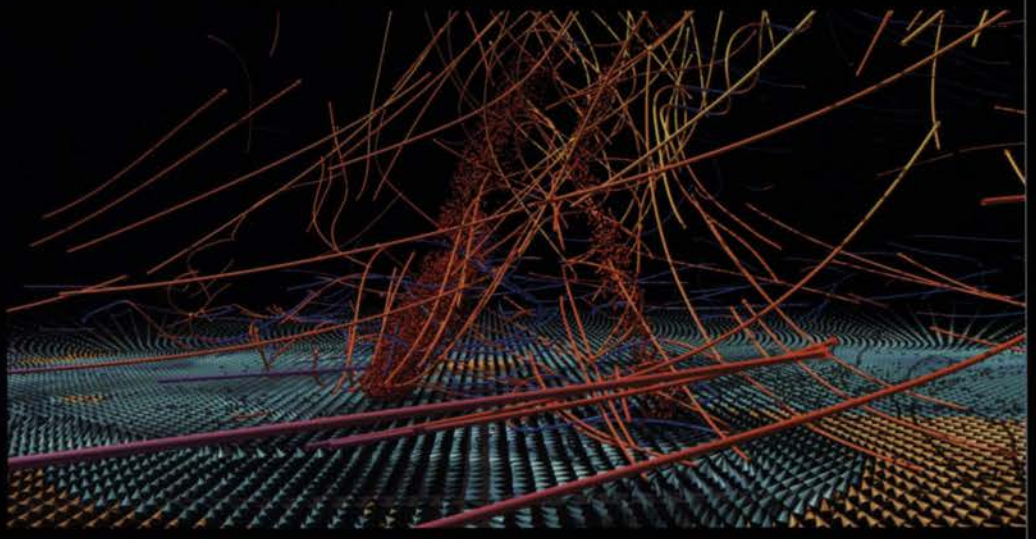
The simulation produced 650 billion bytes of data consisting of snapshots of the evolving storm every second during the tornadic storm phase. These snapshots include wind, temperature, pressure, humidity, turbulence, water, and ice values on a three-dimensional spatial lattice of grid points within the solution domain.

Artfully interpreting data

NCSA's visualization team—Robert Patterson, Stuart Levy, Matt Hall, Alex Betts, Lorne Leonard, and team director Donna Cox—translated the data into a dynamic, high-definition animated visualization of the tornado's birth and growth.

Levy was the first member of the visualization team to work with the raw data from the simulation, computing the trajectories followed by tracer particles to reveal the twister's swirling winds. For the NOVA animations, simple glyphs such as balls and streamtubes were used to represent various aspects of the storm, with variations in color conveying additional information. Cones tilt and sway to show wind speed and direction at ground level, while balls and tubes of varying colors indicate the tornado's pressure and rotation rate.





Hall then worked to develop multiple isosurfaces, the transparent grey-blue clouds that represent the storm cloud, as well as the tilting cones. At each stage, Betts developed Maya plug-ins and scripts to read and control the rendering of the data.

Finally, Patterson tackled the integration and choreography of the visualization, using the Maya software to make rendering choices and to focus on the most significant data and events. Among other daunting tasks, Patterson, in consultation with the storm team, had to edit the thousands of computed trajectories —which together look like a plate of angel hair pasta—down to the few most meaningful trajectories in order to make the data visualization accessible and useful for scientists.

Far from being a unidirectional assembly line, Cox says the visualization process is actually "a very human-intensive, iterative process," in which the members of the visualization team frequently consult with one another and with the storm team. At each stage of the process, human intelligence and collaboration are required to make decisions about what data are most descriptive and how best to draw meaning from the data.

"This has been a very hard-working, collaborative renaissance team," Cox says.

Gaining fresh insights

The visualizations are like "a three-dimensional virtual storm chase," says University of Illinois atmospheric scientist Matthew Gilmore. Using visualizations, events that occur with blinding speed in the field can be slowed to a crawl for close study. The data can be interrogated in many ways, allowing researchers to look at cross-sections, employ different points of view, and zoom in on small-scale effects.

Because of the vast and complex spatial and time datasets involved, the use of interactive visualization tools provides a vital advantage as Wilhelmson's team continues to investigate the mechanisms for tornado formation. In particular, the researchers are examining vortex generation, stretching, and convergence through comparison with theories for tornado formation and through in-depth trajectory analysis.

This project was supported by Intel Corporation, the National Science Foundation, NCSA, and NOAA's National Severe Storms Laboratory.

Access Online http://access.ncsa.uiuc.edu/CoverStories/supertwister/

For further information:

http://www.pbs.org/wgbh/nova/tornado/
http://www.nssl.noaa.gov/
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http://redrock.ncsa.uiuc.edu/AOS/home.html

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Building bridges

by
Kathleen Ricker

As the NEESgrid comes online in September 2004, it brings together widespread earthquake engineering research sites—and two very different research communities.

UIUC's experimental apparatus for the MOST experiment. A partnership between the MUST-SIM team at UIUC, the FHT team at the University of Colorado at Boulder, and the NEESgrid SI team, the MOST experiment provided a preview of the full NEESgrid system, using application software developed by earthquake engineers at UIUC, Colorado, and USC to support domain-specific earthquake engineering simulations.

In the summer of 2003, earthquake engineers and computer scientists around the country created an "earthquake" and studied its effect on the structure of a one-story frame building. One column of the building was at the University of Illinois at Urbana-Champaign; another, at the University of Colorado at Boulder. Meanwhile, the building's central support was simulated on a computer at NCSA. Amazingly, the structure survived an earthquake a thousand miles long.

The experiment was called the Multi-site Online Simulation Testbed, or MOST, and combined physical experiments conducted hundreds of miles apart with numerical simulation. It was the first scientific experiment conducted using the NEESgrid, the cyberinfrastructure for NSF's George E. Brown, Jr. Network for Earthquake Engineering Simulation (NEES), which enables researchers at different institutions to remotely interact with each other, collaborate in research, execute experiments, and publish results.

In September 2004, when the NEESgrid will be fully functional, it will be handed over to the NEES Consortium.

"NEESgrid is NSF's first engineering cyberinfrastructure project," says Bill Spencer, who is the Nathan M. and Anne M. Newmark Endowed Chair of Civil Engineering at the University of Illinois at Urbana-Champaign and principal investigator for NEESgrid.

Spencer says that, by providing common tools that allow individual researchers access to the resources and experiences of a large part of the earthquake engineering community, NEESgrid is making possible research capabilities that have not been available in the past. All of this is accessible through a simple Web interface. "Rather than having to worry about the software," says Spencer, "NEESgrid allows researchers to focus on the earthquake engineering challenges at hand."

Sridhar Gullapalli of the University of Southern California's Information Sciences Institute agrees. "We are building a community of sites to enable sharing of earthquake engineering expertise and resources," says Gullapalli, who leads the effort to prepare equipment sites to participate fully in NEESgrid. "We are well on the way to enabling cooperative, big science, by getting the sites to work together and by developing a standard way to access NEESgrid services across many heterogeneous systems."

As director of both the Mid-America Earthquake (MAE) Center at UIUC and MUST-SIM, UIUC's NEES equipment site, Amr Elnashai says that NEESgrid will help assure that other researchers will be able to access MUST-SIM more easily and use it to its full capacity. "And as a researcher myself," he says, "even if I am not using our own equipment, I am looking to investigate simulation problems that are extremely difficult to resolve either by integrated analysis or integrated experimentation." The tools provided by NEESgrid will facilitate research such as Elnashai's, which combines both physical and computational simulation.

How NEESgrid works

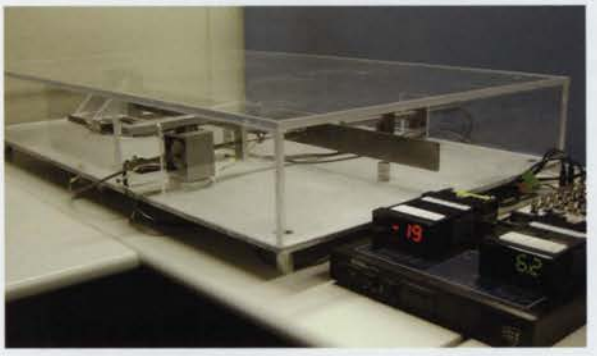
A collaborative NEESgrid experiment typically involves simulating the effects of an earthquake. Data are acquired in a number of different ways, through audio and video feeds, still cameras, and sensors attached to an experimental setup at a NEESgrid node. Through telepresence, data streaming services, and a user-friendly browser interface, researchers at different institutions can observe the experiment in progress or, at a later time, work with the data, which is then stored in a central data and metadata repository currently located at NCSA and accessible through the NEESpop, the collection of NEESgrid services installed at each site.

Making it possible to access data in different ways has been a crucial goal of the project. A recently integrated feature of NEESgrid, Data Turbine, provides multiple users with real-time, networked access to the data from an experiment. Charles Severance of the University of Michigan School of Information, data architect for NEESgrid, describes this new capability as a kind of data TiVo: "While you're watching the data, it's all being recorded, and yet you can play data backwards and forwards in time, you can skip ahead, you can skip backwards, you can actually pull a whole sequence of data out."

Giving data a second life

In addition to the ability to manipulate data, another feature of the NEESgrid that may prove especially useful is the ability to store data easily in a central repository. "All my previous experimental projects have one thing in common: that we use maybe five percent of the data we collect," says Elnashai. He notes that if the data his group has collected and worked with is then stored in an easily accessible form, other researchers will also be able to reuse it for their projects or to use it to verify their analytical models.

The NEESgrid data services, the set of technologies and services with which NEESgrid users store and manage data, were the result of a broad and complex collaboration in which NCSA researchers played a large part. The centerpiece of the NEESgrid data services, the data repository, was designed and implemented by Joe Futrelle, leader of NCSA's Digital Library



Mini-MOST, part of an experimental apparatus small enough to sit on a tabletop. Used during the trans-Pacific experiment with Kajima, Mini-MOST can also be employed to test and verify installed NEESgrid nodes safely and inexpensively before larger experiments are installed.

Technologies Group. The repository stores two kinds of data: the raw data generated during an experiment and metadata, descriptive data that imparts complex, detailed information about the experiment, its design, and the facility in which it is run. The NEESgrid data/metadata team, led by Kincho Law of Stanford University, has developed reference data models for shaking tables and centrifuges.

The challenges of collaboration

NEESgrid has been a breakthrough project in another important way: as a learning experience in conducting a successful large-scale cyberinfrastructure collaboration between two disparate groups of researchers. "NEESgrid has been one of the first serious attempts to coordinate the needs of an engineering community with the development being done by a community of computer scientists," says Doru Marcusiu, who leads NCSA's Grid and Security Technologies Division and the effort to deploy NEESgrid at participating equipment sites around the country.

"In the past," Marcusiu says, "the conventional approach has been that the computer science community develops something, and the engineering community tries to use it, and it either works, it doesn't, or it can be improved." However, NEESgrid's approach has been different in that the SI team tried to identify the earthquake engineering community's requirements and build the NEESgrid infrastructure accordingly, allowing the science to drive every aspect of the collaboration.

What evolved out of intense and frequent discussions between earthquake engineers and SI team members was an iterative process in which the SI team would develop some software and turn it over to an "early adopter" group of earthquake engineers to try it out. With the feedback from the early adopters, the SI team would make adjustments in successive releases that would approach the engineering community's requirements more closely. "The ability to keep an open mind throughout the process has been very important," says Severance. "Each time we released new software we learned new things about it. It required patience on the part of both the developers and the earthquake engineers, but we all learned not to give up just because a particular software release wasn't perfect."

The future of NEESgrid

In March of 2004, the SI team and the UIUC civil engineering department partnered with Kajima Corporation, a leading Japanese civil engineering firm, to conduct the first trans-Pacific experiment using NEESgrid. Like the MOST experiment, the experiment with Kajima involved both computational and physical simulation. Recently, Spencer and other members of the NEESgrid SI team traveled to Kobe, Japan, to discuss how NEESgrid could work with Japan's Earthquake Defense (E-Defense), a project that involved construction of the world's largest earthquake simulator. Similar partnerships are in the works with technological institutions in China and in Europe.

The work of NCSA and the rest of the SI team is almost done, but NEESgrid's work is just beginning.

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Access Online http://access.ncsa.uiuc.edu/CoverStories/NEESgrid04

For further information:
http://www.neesgrid.org

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A collaborative effort

Akira Mita of Keio University, Japan, with members of the SI team, who traveled to Japan to develop collaborative research activities with Japanese earthquake engineering colleagues. One such activity might involve putting E-Defense, the world's largest seismic simulator, on the NEESgrid. From left to right: Mita, Bill Spencer, Carl Kesselman, and Charles Severance.

Members of the NEES System Integration (SI) team, who gathered at the second annual meeting of the NEES consortium in San Diego, CA, in May 2004. Led by NCSA and the Department of Civil Engineering at the University of Illinois at Urbana-Champaign, the SI team was formed in September 2000 and has expanded to include 11 partnering national laboratories, civil engineering departments, computational science centers, and private sector developers. The SI team's purpose has been not only to build the NEESgrid but to help deploy it at a current total of 15 earthquake engineering equipment sites around the country.

The NEESgrid consists of a broad collection of software services. Some of the services have been integrated from existing projects and commercial products; some have been developed specifically for NEESgrid. Their integration into NEESgrid is the result of the intense collaborative efforts of many people at many different institutions.

- Core grid services, such as system, network, and site monitoring, and secure authentication and authorization for users, are provided by the Globus Toolkit (supported by Argonne National Laboratory) and grid technologies developed at NCSA, such as MyProxy. The final NEESgrid installation package was also built at NCSA, using NCSA-developed Grid Packaging Technology.
- The Telepresence Server, developed at Argonne, permits users to remotely view multiple lab spaces and the physical experiment from static and remote telerobotic cameras via ordinary Web browsers. Currently, audio and video from the experiments are streamed through a commercial video server from Broadware, Inc.
- The NEES Teleoperations Control Protocol (NTCP), developed specifically for NEESgrid at the Information Science Institute at the University of Southern California, provides a common protocol that can be used to remotely control physical experiments or computational simulations. By giving users a standard interface to local equipment and simulation capabilities, it provides the transmission standards for the NEESgrid that builds on the TCP/IP protocol, which connects hosts on the Internet.
- The CompreHensive collaborativE Framework (CHEF), developed at the School of Information at the University of Michigan, is a framework for remote collaboratory tools that provides a variety of tools and services for end-users, including virtual workspaces where communication and planning can take place between researchers.
- An electronic "laboratory notebook," called E-NoteBook, developed at Pacific Northwest National Laboratory with support from the Department of Energy, provides researchers with a way to record observations and progress notes that remote team members can easily access.
- A number of simulation tools have been integrated into NEESgrid. OpenSEES, a computational framework for simulating the seismic response of structural and geotechnical systems, was developed at the University of California, Berkeley and has been made available via grid portal by SI team members at Mississippi State University. FEDEASLab, also developed at UC Berkeley, is another simulation tool especially useful for engineering education. ZEUS-NL is the University of Illinois's computational tool for static and dynamic nonlinear frame analysis.
- Data acquired from a NEESgrid experiment are streamed through Data Turbine, a commercial product developed by Creare, Inc. and integrated by SI team members at Argonne and Michigan. Data Turbine allows users to scroll back and forth through data as the experiment is occurring. SI team members at Argonne were instrumental in the initial development of and continue to actively support data acquisition services.
- The data repository services allow users to manage, store, and manipulate data and metadata from past NEES experiments using an XML-based format. The data/metadata effort has been led by NCSA, Michigan, and Stanford.

by

Trish Barker

A snapshot of silica polymorphs formed after several nanoseconds of simulation time in a solution of 38.4 percent silicic acid precursor in water at high temperature. The bonding backbone is shown in ball-and-stick form, with the transparent outer surface showing the "space-filling" molecular structure.

Plotting pores

By studying the porous structure and adsorptive properties of sol-gels, a Washington University researcher might be able to create new materials.

Gels can be found low—nestling amid the packing material for consumer electronics and leather goods to absorb damaging moisture—and high—traveling through space to capture comet dust.

The pebbles of gel in your shoebox and comet-trailing aerogel, the lightest man-made material, share a common origin in the sol-gel process, a versatile technique for making ceramic and glass materials. In general, the method involves the transition of a system from a liquid filled with floating "sol" particles into a solid, but still highly porous, "gel" phase.

Scientists understand how to make a range of materials using this process—from thin film coatings to the aerogel sent on a comet quest by NASA. What scientists lack is a detailed, microscopic portrait of the complex interior structure of a given porous material. That's one of the questions being tackled by Lev Gelb, an assistant professor of chemistry at Washington University in St. Louis. Gelb uses computational resources at NCSA to model the spongelike structure of sol-gel materials. Detailed models of the structure of these materials could be used to explore how gels interact and what tasks different gels can perform. A thorough understanding of gel formation might also make it possible to engineer materials for specific applications.

Creating complex structures

The sol-gel process begins with an aqueous solution of an organosilicon "precursor" compound. The precursor molecules react with each other, connecting to form small particles and then sticking together in larger clumps. This is the "sol" stage, in which solid particles are suspended in the liquid solvent.

What's forming in the solution is "a very complicated branched polymer with many loop structures," Gelb explains. As these polymers continue to interlock and adhere to one another, a liquid that once contained solid pieces becomes a gelatin-like solid riddled with tiny pores.

The structure of the resulting gel "depends pretty sensitively on exactly the solution you start with" and on the temperature, Gelb says, and each gel has a particular "average pore size." The pore size of a material influences the rate at which fluids flow in it, its ability to separate molecules based on their size, and its electrical, optical, and mechanical properties.

The sol-gel process can produce dense silica xerogels that are used in chromatography and studies of gas separations; highly porous aerogels that are used for thermal insulation; and thin films for use in sensors, electronics, and optics.

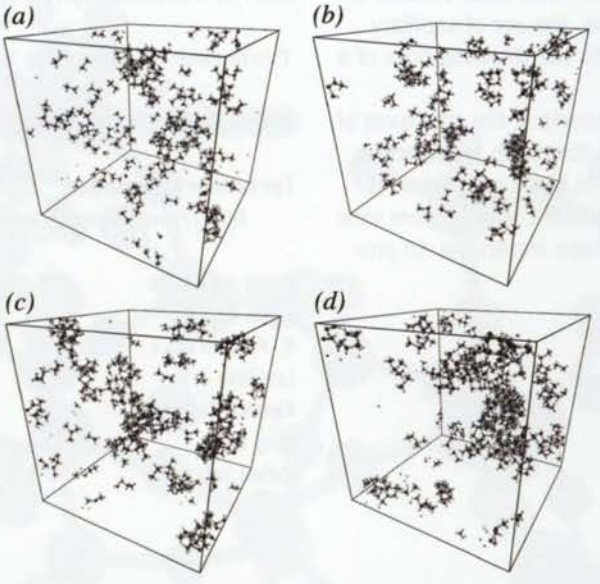
In all of these cases, "the final material is amorphous," Gelb says. "The material does not have a simple periodic crystal structure." In other words, the sizes, shapes, and distribution of the pores vary unpredictably.

Simulating the sol-gel process

To understand the complex structure of these materials, Gelb has turned to computational simulation. His strategy is to simulate each of the steps involved in the experimental preparation of the materials in order to model the resulting structure. Gelb is approaching the problem in two ways. First, his team is developing new models for atomic-level simulations of sol-gel reactions, applying these models, and then comparing the results to structures known from experiment. Secondly, the team is also developing and applying a coarse-grained sol-gel model that is less computationally expensive.

Employing the widely used quantum chemistry codes Gaussian and NWChem on NCSA's IBM p690 cluster, Gelb models the evolution of sol-gel systems using a parallel molecular dynamics code developed by his group.

Gelb has carried out large-scale simulations of the polymerization of silicic acid in aqueous solution, modeling systems with differing water-to-silicon ratios, silicic acid concentrations, and temperatures. Activation energies calculated from the simulations compared favorably with experimental results, encouraging Gelb to attempt to model more complex systems.

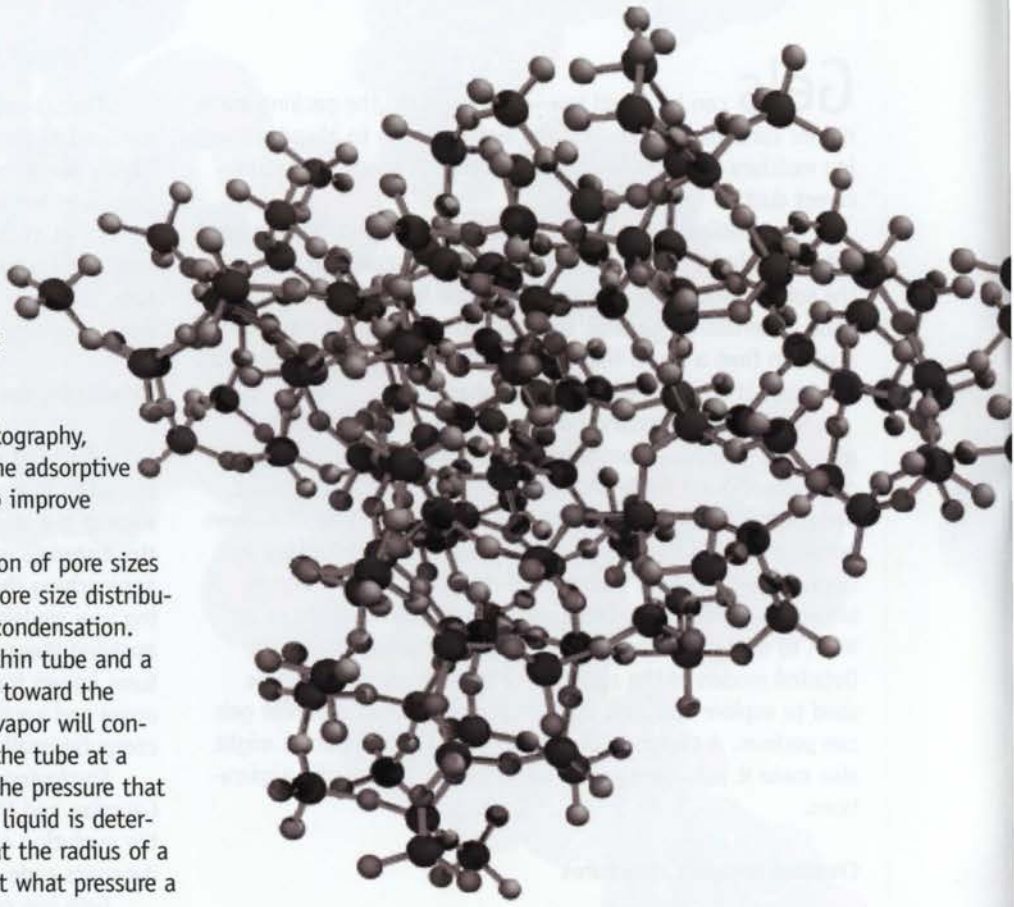


Snapshot of polymerization in a solution of 38.4 percent silicic acid precursor in water at high temperature. Only molecules that contain at least two silicon atoms are shown; these are the early products of the gelation reactions. No water or unreacted precursor is shown, but they fill the remainder of the simulation cell. Also, no hydrogen atoms are pictured. Snapshots are taken from the simulation at (a) 1 nanosecond, (b) 2 ns, (c) 3 ns, and (d) 4.8 ns.

These simulations involve several tens of thousands of individual atoms and millions of femtosecond intervals and require thousands of hours of computation. It can take months to simulate mere nanoseconds.

"The problem is that atoms move very quickly and the forces they exert on each other are very strong," Gelb says. This makes simulating materials at the level of individual atoms very computationally expensive.

Gelb is also developing a coarse-grained model that will track sol particles rather than individual atoms and will represent the solvent with a density field rather than considering each solvent molecule individually. While this method relies on approximations that make it somewhat less detailed than the atom-by-atom approach, it has the benefit of being less computationally intensive.



Capillary condensation

Gelb is also looking at the pores within sol-gel materials from a slightly different perspective, one that considers the relationship between pore structure and adsorptive properties.

Adsorption is employed in many separation and refinement techniques, as well as in chromatography, so understanding how pore structure relates to the adsorptive qualities of a material provides an opportunity to improve applications that use sol-gel materials.

The first step is to understand the distribution of pore sizes in a given material. Scientists typically analyze pore size distribution by leveraging the phenomenon of capillary condensation.

Imagine a closed system containing a very thin tube and a vapor. If the pressure on the system is increased toward the vapor pressure of the liquid (at which point the vapor will condense into a liquid), the vapor will condense in the tube at a lower pressure than it will condense elsewhere. The pressure that is required to convert the vapor in the tube to a liquid is determined by the radius of the tube. This means that the radius of a tube (or pore) can be determined by observing at what pressure a vapor condenses within the tube.

The problem with this technique is that sol-gel materials are much more complex than tiny, isolated tubes. Using this method requires scientists to assume that the pores are regular in size, which they aren't, and that what occurs in one pore has no affect on its neighbors.

"So how descriptive is this measure?" Gelb asks. Instead of really describing the material in question, the use of capillary condensation gives scientists insight into the characteristics of a bunch of hypothetical cylinders.

Gelb's goal is to develop realistic models of the structures of various materials and then to use those structures in molecular dynamics simulations of gas adsorption in these materials. Through simulation, Gelb intends to produce a pore-by-pore view of adsorption; it would be difficult, perhaps impossible, to produce this view experimentally.

Furthermore, by working with computational models, Gelb has the flexibility to make adjustments in structure and observe how these changes affect adsorptive properties. This could lead to identifying and engineering sol-gel materials with properties uniquely suited to a wide range of uses, from earthly concerns such as chromatography and packaging to chasing comets.

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Access Online http://access.ncsa.uiuc.edu/CoverStories/solgel/

For further information:

http://www.chemistry.wustl.edu/~gelb/

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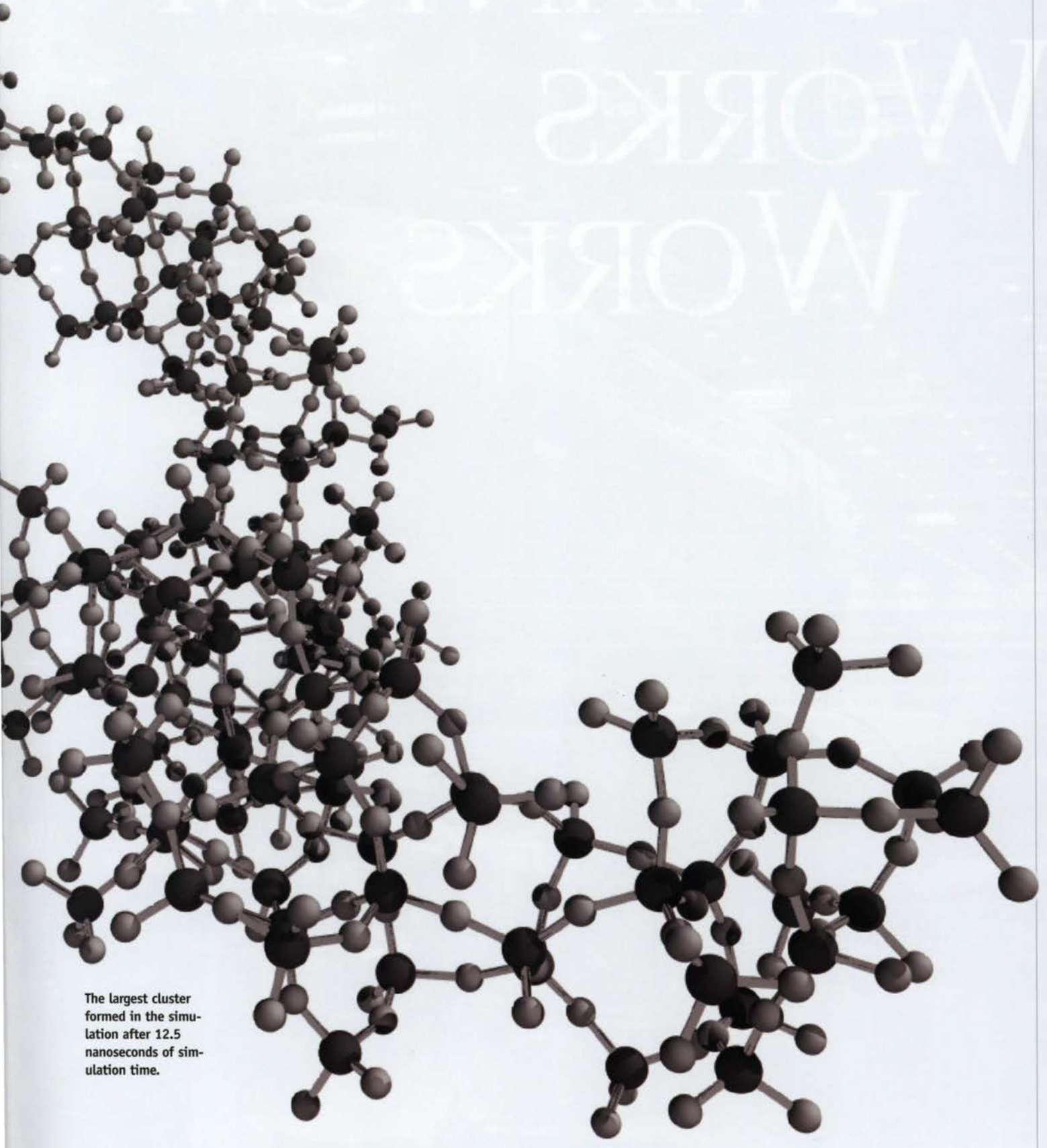
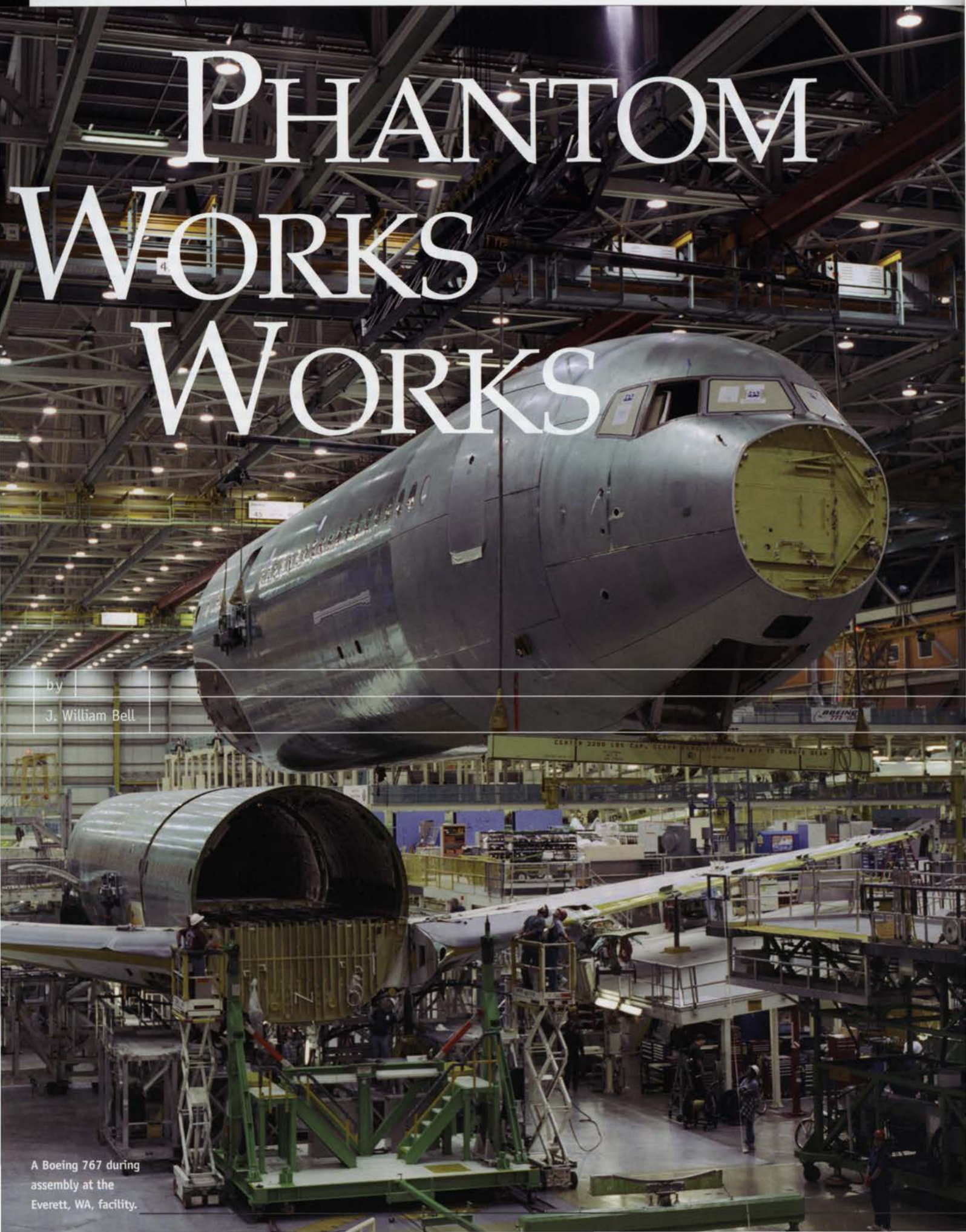


The largest cluster formed in the simulation after 12.5 nanoseconds of simulation time.

Phantom Works Works

by J. William Bell



A Boeing 767 during assembly at the Everett, WA, facility.

The Boeing Company's research and development unit teams with NCSA's Private Sector Program to demonstrate a "distributed task manager" for quality assurance.

The Boeing Company is the world's leading aerospace company and a top U.S. exporter, dedicated to delivering the safest, most reliable, and most technologically advanced airplanes. The 767, for example, has flown more than seven and a half million flights and has carried two billion passengers since it entered service more than 20 years ago. It flies the Atlantic more frequently than all other jetliners combined.

But this sort of performance doesn't come easy.

Like all Boeing airplanes, the 767 contains millions of parts. These parts, and the many complex systems on board the jetliner, must work together seamlessly—and must be checked and rechecked to conform to the highest standards.

"Quality assurance fulfills a very important role at Boeing in that we provide thousands of inspections through the build sequence to ensure that we actually deliver the highest quality and safest airplanes in the world," says Jeff Kleman, quality director of Boeing's 98-acre manufacturing site in Everett, WA. "We take a lot of pride in our activity, and it's a critical aspect of our business."

Meeting a grand challenge

With safety and quality as their goals, Boeing's research and development unit, called "Phantom Works," teamed up with NCSA in 2003. Phantom Works employs 4,000 people dedicated to creating breakthroughs in performance, quality, and cost for the company. Together, over the course of a single year, Boeing and NCSA built a demonstration of a "distributed task manager" that highlights the benefits of network-centric planning and management in airplane inspection. Such software will help Boeing further ensure that their inspectors do the right job at the right place at the right time.

"Short development times are important because our whole business is predicated on time to market," according to Gary Fitzmire, vice president of engineering and information technology for Boeing Phantom Works.

In honor of this vital and rapid effort, NCSA's Private Sector Program presented its 2004 Industrial Grand Challenge Award to Boeing in April. The annual Grand Challenge Award honors breakthrough research completed by private sector partners while working with NCSA.

"NCSA provides a focal point for computer science, computational science, and information technologies. By working with the Private Sector Program partners, we're able to connect real world problems with the necessary infrastructure," says Rob Pennington, NCSA's interim director.

Bob Krieger, president of Boeing Phantom Works, concurs: "The real reason we partnered with NCSA is because they're very experienced in various software systems...Once you partner with somebody that's really expert, you have a lot of confidence and you can get the end objective, which is to have a good product."

Network-centric inspection solutions

Before a Boeing plane leaves the assembly plant, a legion of inspectors make more than 20,000 quality checks on the plane's various subsystems. These systems are tightly interrelated. The wing doesn't pass muster if an aileron is bad, and the instruments are only as good as the miles of electrical wire behind them. And these pieces are assembled over the course of months.

The software that coordinates this long-term focus on very small details is crucial to the quality of the finished product. Every test has to be tracked. Every flaw must be flagged and fixed. Currently, that means opening and closing jobs at a central terminal—in effect filling out paperwork on computers stationed about the assembly plant. Without an automated notification system, subsequent tasks, which can only be started upon the completion of the first, might sit for hours before another inspector knows that they are ready to be taken up.

"One of the keys to the project was job shadowing," explains Scott Lintelman, a project manager for Boeing Phantom Works. "Job shadowing is simply following the inspector around in the factory on his daily job and seeing what he does. It allowed us to gather requirements to ensure that our project was relevant to his needs."

Inspection of a Boeing 767 engine.

The Boeing assembly plant in Everett, WA. It is the largest building in the world by volume, with a capacity of 472 million cubic feet.

Once the Boeing and NCSA team had a clear picture of what the inspectors did and how they did it, they developed a specialized database that tracked inspections and parceled out new jobs automatically. This "distributed task manager" is built on SAMCat, the Secure Active Metadata Catalog created by NCSA's integrated decisions technologies group.

SAMCat is a distributed messaging system based on XML. "We can use any application that can talk XML, which basically any application can. And they can send messages to SAMCat, and other applications that understand XML can take these messages out again," says NCSA's Rob Kooper, who leads SAMCat's development.

An initial test has been conducted, showing the potential of a complete, SAMCat-based, network-centric system. If implemented, inspectors will be able to move about with a hand-held computer or personal digital assistant connected to a central database via a wireless network. The PDA will constantly receive updates on what inspection tasks can be performed. The inspectors, meanwhile, will constantly update their progress on the PDA. The system will then determine which tasks can be performed as a result of that progress. New tasks can be delivered to inspectors in real-time according to their skills, certifications, or roles in the assembly plant. Problems, instead of being trapped in an inspector's notebook until the next time he makes a report, become common knowledge and can be addressed that much faster.

The catalyst for innovation

The benefits of a distributed task manager don't end with efficiency and cost reduction. A network-centric inspection system would give supervisors a look at the state of an airplane that is constantly updated. They'll know where they're at in the inspection process and where the snags are as they occur. Because of SAMCat's flexibility, existing quality assurance software could also be combined into a single system for use in the assembly plant.

"Network-centric solutions are central to the strategy of The Boeing Company, and by that I mean we need to get the right information at the right time to the right decision makers. That has a profound effect on the war fighters in the battle field. It has a profound effect on air traffic management. And it has a profound effect on our customers, because they arrive safely and faster at their destinations," says Fitzmire.

Already, the team is set to work on a proof-of-concept demonstration of a 767 inspection system. Boeing also sees network-centric principles moving into their global enterprise—everywhere from parts manufacturing to purchasing.

What the company learns today will have substantial influence on what they do tomorrow. In 2008, Boeing will roll out its newest airplane, the 7E7. The plane will be the most technologically advanced and efficient commercial jetliner ever built. Most of the plane will be made of composite materials, and it will use 20 percent less fuel than similar planes now on the market.

A visualization of Boeing's upcoming 7E7 "Dreamliner." In April 2004, All Nippon Airways placed an order for the first 50 of these superefficient jets.

Such innovation requires not just technological improvements but also improvements in the ways jobs get done. The relationship between NCSA's Private Sector Program and Boeing brings both.

"Phantom Works is known as the catalyst of innovation for Boeing. What that means is we develop or, through collaborations, find technologies that we can bring into our product line," says Krieger. "The collaboration between Boeing and NCSA worked very well. NCSA brought new emerging technology, we brought the needs for our production floor. We both worked together to interface the two and ended up with a really great product in the end."

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For further information:

http://www.ncsa.uiuc.edu/Projects/PrivateSector/
http://www.ncsa.uiuc.edu/Divisions/PSP/SAMCat/
http://www.boeing.com/

The winning Boeing team with leaders from NCSA and the Private Sector Program. Left to right: Mark Nolan, NCSA; Rob Pennington, NCSA's interim director; Gary Fitzmire, Boeing; Earl Ley, Boeing; Scott Lintelman, Boeing; Danny Powell, NCSA's executive director; and John Stevenson, NCSA.

Salted away silicon

by
J. William Bell

Computer models reveal the process of silicon defect formation—and several previously unknown defect structures.

Ask the stereotypical packrat—just because you replace something doesn't mean you get rid of it. The new television sits on top of the old one, a *TV Guide* mountain abuts the recliner, and someone might use that old bicycle someday. Room for a life amongst the clutter constantly diminishes.

As a silicon wafer is etched to become a microchip, it suffers a similar fate. The silicon is bombarded with boron, and the boron shoves its way into the bulk silicon's crystal structure. This boron, properly implanted, forms transistors and the other minute electronic devices on the chip.

But for every boron atom that is introduced, a silicon atom is knocked loose. These silicon atoms can sit relatively inert in the open spaces of the crystal structure. Unfortunately, loose silicon atoms can also combine with one another and form large "self-interstitial defects."

"Clever reactions take place at low energies in the structure, and the silicons have no reason to leave," explains NCSA material scientist Jeongnim Kim. Instead, the interstitial defects twist the bonds between surrounding silicon atoms. This influence can alter the properties of the structure—leaving you with electronic switches that don't switch or resistors that don't resist. In other words, a microchip that doesn't work as it should.

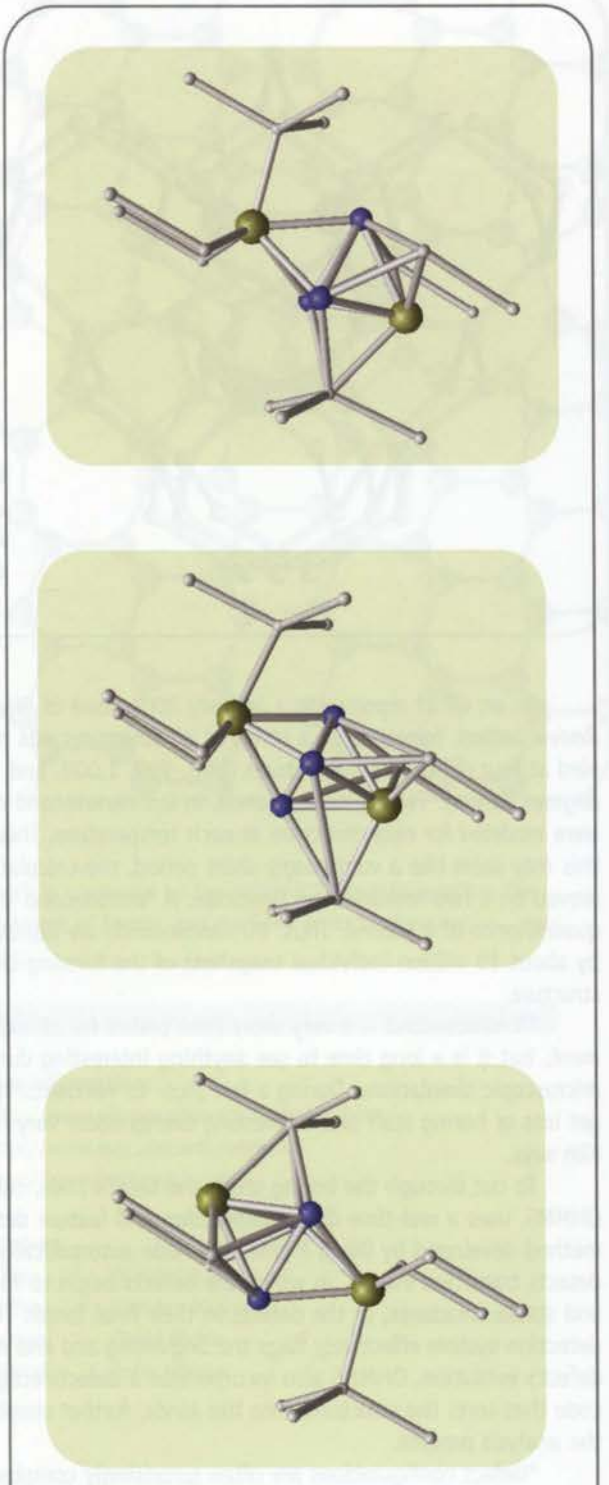
During implantation, the silicon is commonly heated, or annealed, to allow most defects to relax and improve chip performance. However, this process can introduce new complications of its own. As an alternative to implantation, the chip can also be built from the ground up, one atomic strata at a time. The cost of this approach is usually prohibitive.

The fabrication of microchips and other electronic devices goes on, and continues to improve, in the face of these difficulties. But a group of NCSA users isn't satisfied, recognizing that a clearer vision of how defects form will ultimately yield better products. Researchers from the Ohio State University, High Performance Technologies, Inc. in Aberdeen, MD, and NCSA are identifying a series of previously unknown silicon defect structures and modeling the defects' evolution from singleton silicons to large-scale havoc wreakers. The simulations are led by David Richie of HPTi, Richard Hennig and John Wilkins of Ohio State, and NCSA's Kim. They rely on NCSA's Titan Linux cluster and IBM p690 supercomputer.

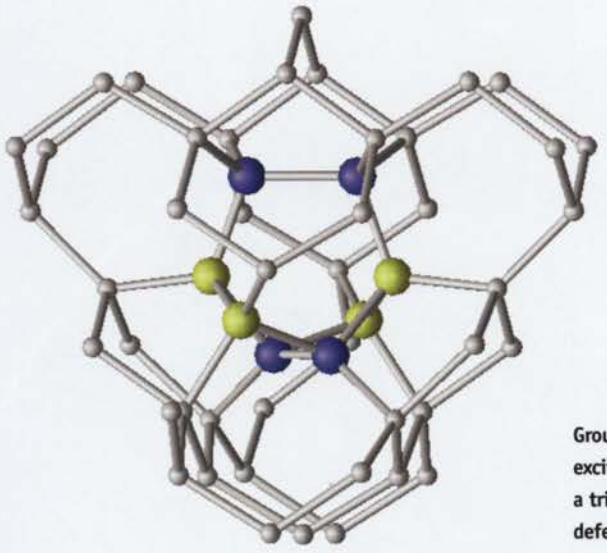
Cheap but reliable

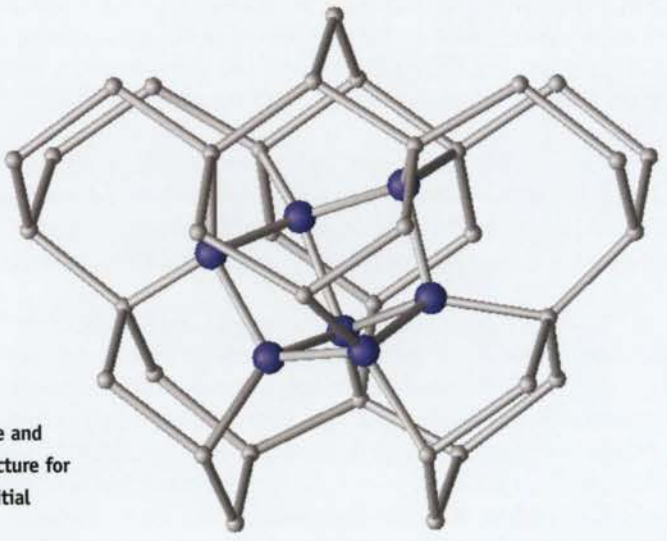
The team's models use a multi-level approach. Accelerated molecular dynamics simulations—which track the interaction of individual pieces of the structures at the atomic level—are completed first. They provide a catalog of possible defect configurations and the energy pathways that the pieces follow as they take on those configurations.

These calculations are the workhorse, representing a computationally "cheap but reliable way to find structures," according to NCSA's Kim. To begin, a relatively small number of silicon and boron structures are established, and the initial conditions for the surrounding environment, such as temperature, are altered slightly in order to produce a variety of defect structures.



Different views of a tri-interstitial defect moving through crystalline silicon.





Ground state and excited structure for a tri-interstitial defect.

In an effort reported in a January 2004 issue of *Physical Review Letters,* for example, a series of 20 structures was modeled at four different temperatures (800, 900, 1,000, and 1,100 degrees Kelvin). Twenty nanoseconds, in 0.5 nanosecond chunks, were modeled for each structure at each temperature. Though this may seem like a vanishingly short period, the calculation moved on a two-femtosecond timescale. A femtosecond is one quadrillionth of a second. Thus, 20 nanoseconds are represented by about 10 million individual snapshots of the forming defect structure.

"A nanosecond is a very short time period for an experiment, but it is a long time to see anything interesting during microscopic simulations. During a few pico- to nanoseconds, you get lots of boring stuff and interesting events occur very rarely," Kim says.

To cut through the boring stuff, the team's code, called OHMMS, uses a real-time data compression and feature detection method developed by David Richie. The code automatically detects transition events, in which the defects begin to form, and stable structures, or the defects in their final forms. This detection system effectively flags the beginning and end of a defect's evolution. OHMMS also incorporates a defect recognition code that sorts the structures into like kinds, further simplifying the analysis process.

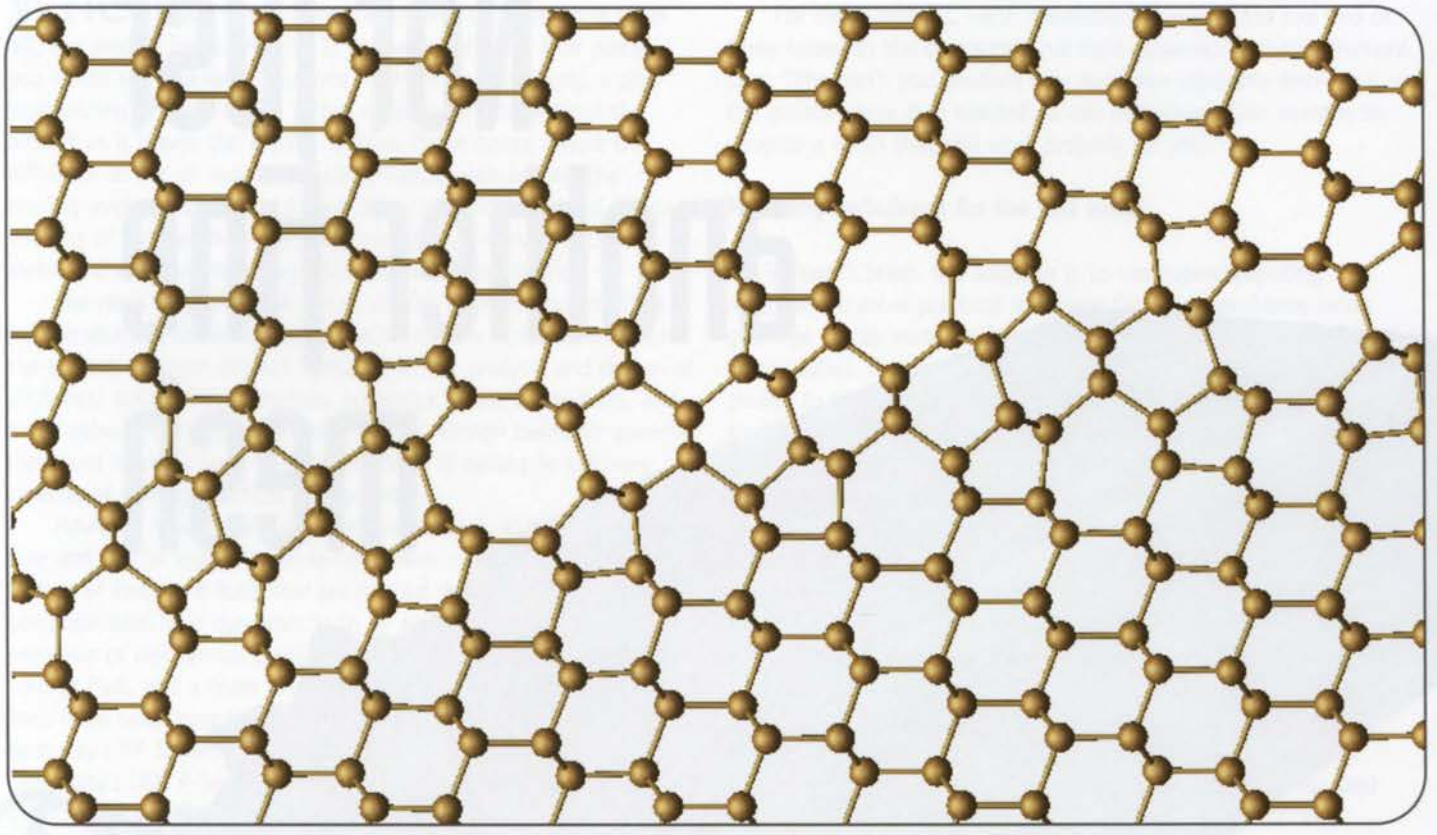
"Defect configurations are often surprisingly complex," the team wrote in a 2003 report, "[and] molecular dynamics simulations performed with OHMMS may lead to thousands of stable configurations. Conventional tools require highly trained individuals to categorize these structures one at a time. [Automated], immediate, and thorough analysis of the massive data amount generated by OHMMS is the key tool for studies of highly complex structures."

OHMMS was originally created by NCSA's Kim in the late 1990s while she was a post-doctoral researcher working for John Wilkins at Ohio State. Development continues in the hands of Richie and the Wilkins research group. In 2003 alone, the team used more than 200,000 hours of computing time at NCSA. They also ran models at the Ohio Supercomputing Center and the U.S. Department of Energy's National Energy Research Scientific Computing Center.

More than molecular dynamics

Once interesting structures are identified, their geometries are confirmed and refined using density functional theory, which is more precise than the molecular dynamics simulations, and a code called VASP. These calculations also determine characteristics of the structures, such as energies and rates at which the structures form. These features are key to chip designers and other applied researchers.

"Device design isn't at the atomistic level where molecular dynamics simulations take place," Kim says.



Planar defect in silicon.

The team's work, especially that discussed in the recent *Physical Review Letters,* reveals not only the higher-order features that researchers need but also some of the flaws in the assumptions that researchers frequently make.

"The complexity revealed in our study is striking compared to the picture uncovered in previous efforts. A good example is the extended chainlike structure of the tri-interstitial ground state, which defies the conventional assumptions of compactness and simple symmetry previously used to investigate these systems," HPTi's Richie says.

In fact, the team has uncovered four structures that were previously unknown. They suspect that these large, complex interstitial structures capture other interstitials at their terminal ends. The daisy-chaining of interstitial silicon atoms that results might explain the observed extended, rod-shaped defects that cause problems for chip designers.

"The practical aim of these and most simulation modeling is to speed the selection of the most likely approaches for detailed experiments that lead to development and manufacture of better chips," says Wilkins, a physics professor at Ohio State. "Of course, we hope improved atomic understanding will also speed up future modeling efforts on new problems."

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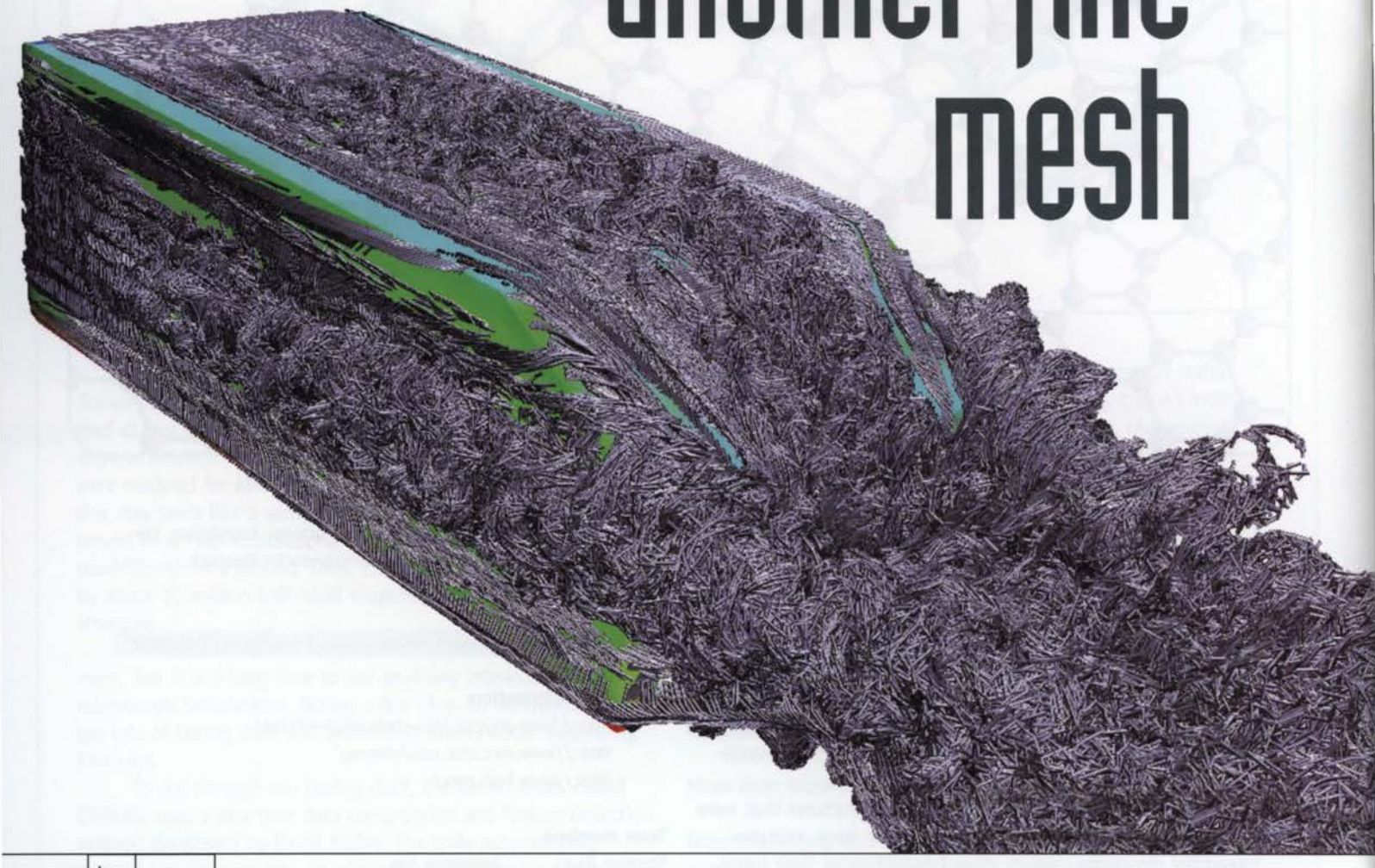
Not just another fine mesh



by Kate Caponi

Researchers create millions of tiny vortices with supercomputers, modeling turbulent fluid flow.

Vortex tubes demonstrate how air flows differently around the sloped window of an Ahmed body.

When you watch from the ground as an airplane takes off, the process looks smooth. If you were riding in that plane, you would see and feel vibrations in the wings and body, a physical inkling of some of the forces working for and against the aircraft as it leaves the earth's surface. These forces reflect the influence of the air making its complicated path around the moving airplane. If you could see the actual airflow, you'd notice millions of little eddies—like tiny tornadoes—skimming the metal and affecting the drag and smoothness of the ride.

The need to predict the forces at play drives turbulent fluid motion studies. Numerical computation of how fluids move around the surface of given objects is crucial to the analysis and design of airplanes, automobiles, engines, computer chips, submarines, and many other technologies. In recent years, design teams in government and industry have invested millions of dollars in software capable of solving practical flow problems.

However, traditional models of turbulent fluid flow are unreliable and can be costly to implement. New capabilities in the prediction of turbulent fluid flow are needed if the full potential of computational fluid dynamics is to be exploited. Peter Bernard, professor of mechanical engineering at the University of Maryland, College Park, and a team of researchers from the company VorCat, Inc., have used more than 60,000 hours on the University of Kentucky's HP Superdome, NCSA's Titan Linux cluster, and Boston University's IBM P-Series supercomputer to develop advanced, grid-free techniques in modeling turbulent flow.

Modeling meshes

According to Bernard, traditional turbulence models are often difficult to apply successfully in new applications with complex physical features. "This reflects the uncertainty in how turbulent flow processes are modeled," he says. "It is also difficult to provide *a priori* numerical meshes that correctly resolve essential flow features. Moreover, special care is needed in solving the highly non-linear partial differential equations appearing in the traditional models."

The availability of supercomputers has spawned the development of a more physically realistic alternative to traditional turbulence modeling, called a large eddy simulation (LES). "In this approach," says Bernard, "turbulent flow is modeled at a small scale and the large scale is computed from the small."

However, despite some significant progress to date, it has proven difficult for researchers to develop small-scale models that reliably produce accurate predictions of complex flows on the large scale. In addition, if LES is to become more useful for real-world applications, the construction of numerical meshes that properly reflect underlying flow conditions near physical boundaries must be automated. Such capabilities are important for reducing the effects of numerical diffusion in which the true solution is distorted due to the lack of enough local mesh points to resolve sharp features of the flow field.

For these reasons, mesh generation is one of the top two or three issues in the computational fluid dynamics industry. Bernard says, "The mesh you produce may not have adequate resolution at the points where it is needed. It can sometimes take months to develop a mesh that will work properly for you."

Modeling turbulence for the real world

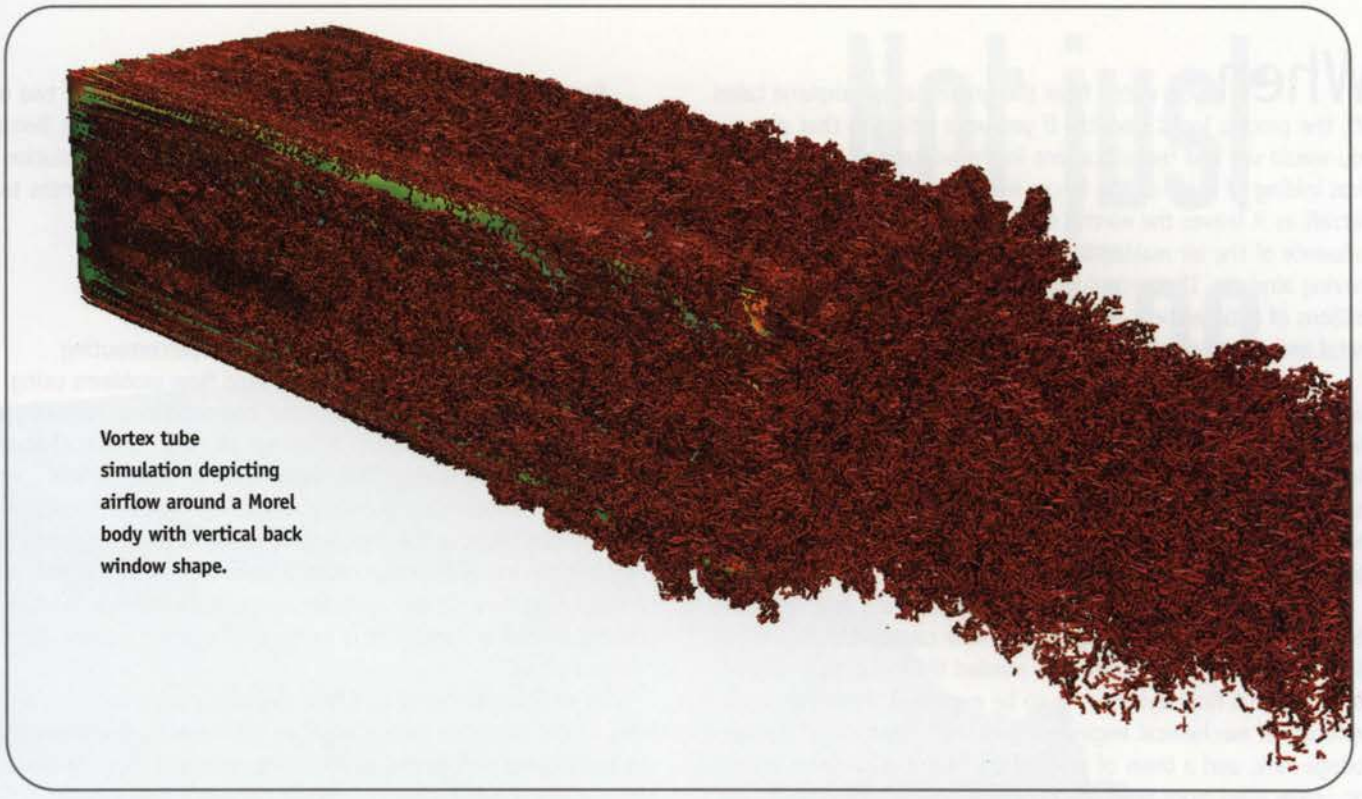
For Bernard's team, the solution is to use supercomputing resources to solve practical turbulent fluid flow problems using grid-free vortex methods in which the computational elements are vortex tubes. He says, "Vortex tubes are physical objects that are similar to little tornadoes. They move around, interact, and stretch. Our models gain accuracy and efficiency over traditional LES methods because the best way to model a physical vortex is with a numerical representation of a vortex. It's a whole new way of simulating turbulence—and because you don't have to worry about developing a mesh, it is easier to use when looking at complicated flows."

In addition to being grid-free and eliminating meshing problems, vortex methods have a number of inherent advantages that are particularly well-suited to modeling turbulent flow. Among these is the self-adaptivity of vortex elements. The vortices actually multiply in the regions where enhanced resolution is needed. Moreover, sharp features of the flow remain sharp, and vortex methods open up a new, more physically appropriate means of modeling small-scale flow phenomena.

One specific turbulent fluid flow problem that Bernard and the VorCat team are working on is a phenomenon called the mixing layer, the region between two fluids of different velocities that are flowing next to each other. The researchers are using the vortex method to look at what happens when you place particles of different sizes in the mixing layer. Bernard says, "Depending on the properties of the particles, they either get sucked in or thrown out of the large-scale mixing layer vortices in a very dramatic fashion."

Another problem that the researchers are looking at is flow past the Ahmed and Morel bodies that serve as prototypes of the kind of flows faced in the automotive industry. These models of simplified car bodies demonstrate how turbulence and drag from airflow are affected when you change the slant of the back window. The vortex method naturally supplies a population of vortices in the regions where the forces at play are most complex, making their model of the car more accurate with less effort than many mesh-based methods.

Such capabilities are important to industry because the answers provided by numerical simulations can form the basis for design. For instance, to see how you might control the flow over wings so as to affect the way a plane flies, you can experiment with surface characteristics that are beneficial. A wing's surface is not flat metal—it is covered with bumps and indentations that cause chaotic airflow. When the plane is taking off, chaotic airflow is desirable because it reduces drag. However, if the plane is flying level, that same chaotic airflow can cause drag. The task of designers is to determine where to put the bumps and dents on the aircraft's wings for maximum fuel efficiency and the ability to climb at a steep angle.



Vortex tube simulation depicting airflow around a Morel body with vertical back window shape.

Arvin Shmilovich, associate technical fellow at The Boeing Company, says, "The promise in grid-free methods such as the one being pursued by VorCat lies in the opportunity they provide in achieving substantial economic gains in the form of improved vehicle designs, reduced design cycle times, and lower vehicle costs. Not only do the methods simplify or eliminate the laborious grid generation process but also provide turbulence modeling that performs reliably under a wide range of flow conditions and without user intervention."

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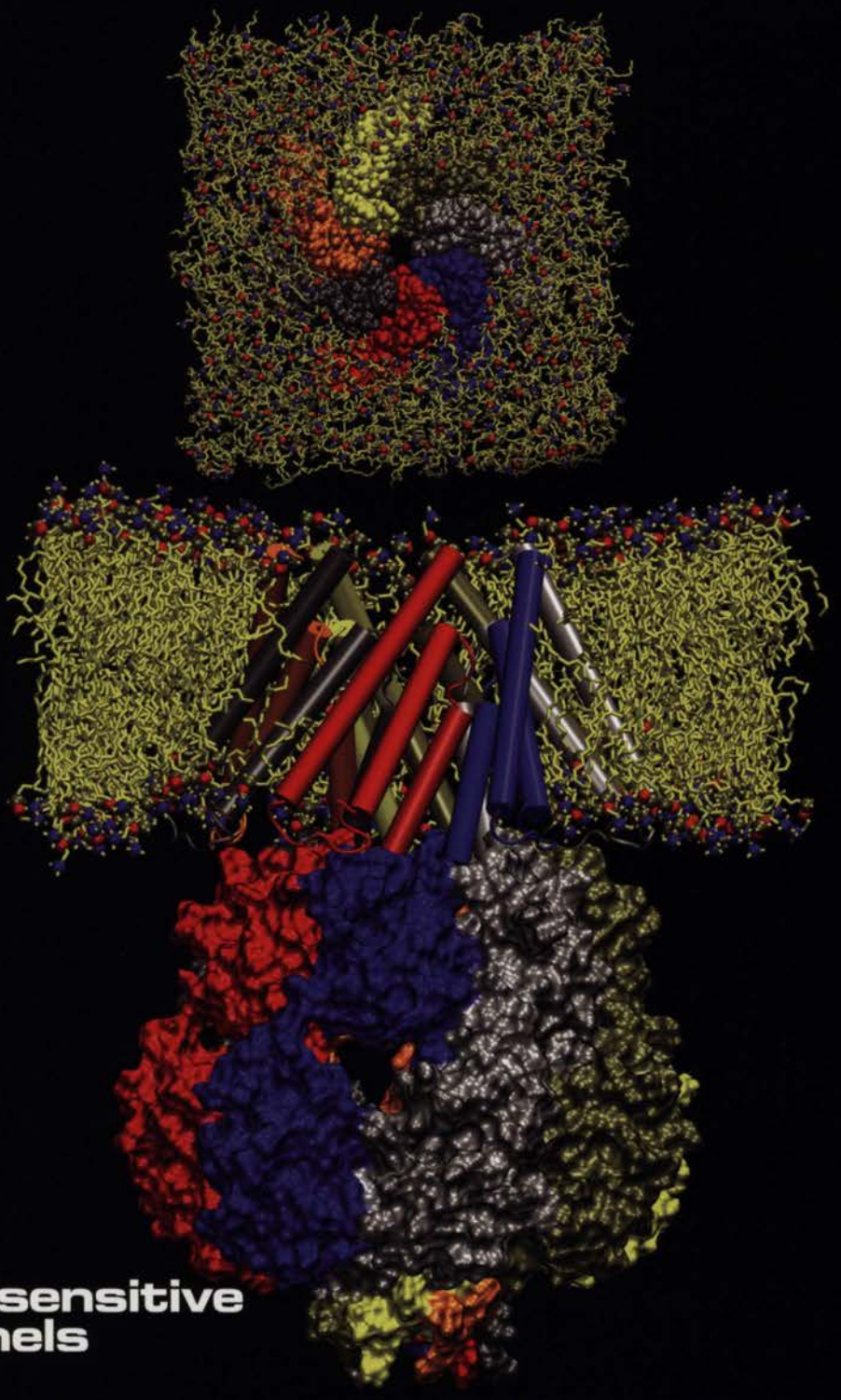

Mechanosensitive ion channels

The ability to perceive and react to different stimuli from the surrounding environment is essential for all living organisms. Mechanical forces produced by sound, gravity, or osmotic stress, among other stimuli, are sensed by organisms through various mechanisms that all involve mechanosensitive ion channels. These membrane proteins open in response to mechanical stimuli, generating an ionic current that eventually triggers an electrical signal. Mechanosensitive channels also play an essential protective role in lower organisms through regulation of cell volume under osmotic stress conditions.

These top and side views of a mechanosensitive channel called MscS embedded in the membrane of a cell were created by Marcos Sotomayor and Klaus Schulten of the University of Illinois at Urbana-Champaign's Theoretical and Computational Biophysics Group. They were simulated using with their NAMD software and visualized with their VMD software. The models include the channel, a large patch of membrane composed of POPC lipids, and sufficient water on both sides of the membrane to fully solvate the system. The combined system includes more than 220,000 atoms. The simulations were performed on NCSA's Linux clusters, with additional calculations on systems at the Pittsburgh Supercomputing Center.

These simulations are the first to examine the free dynamics of the protein in a membrane. They revealed expected and unexpected characteristics that are likely essential to the channel's function. Through an extensive series of multi-nanosecond simulations, the team observed, among other things: the intermittent permeation of water molecules through the channel, the channel's strong tendency to close under constant pressure conditions, and an increase in the size of the channel when surface tension is applied to the embedding membrane. Meanwhile, the large balloon-shaped cytoplasmic domain of MscS spontaneously diffused ions through its side openings rather than its bottom central opening.

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