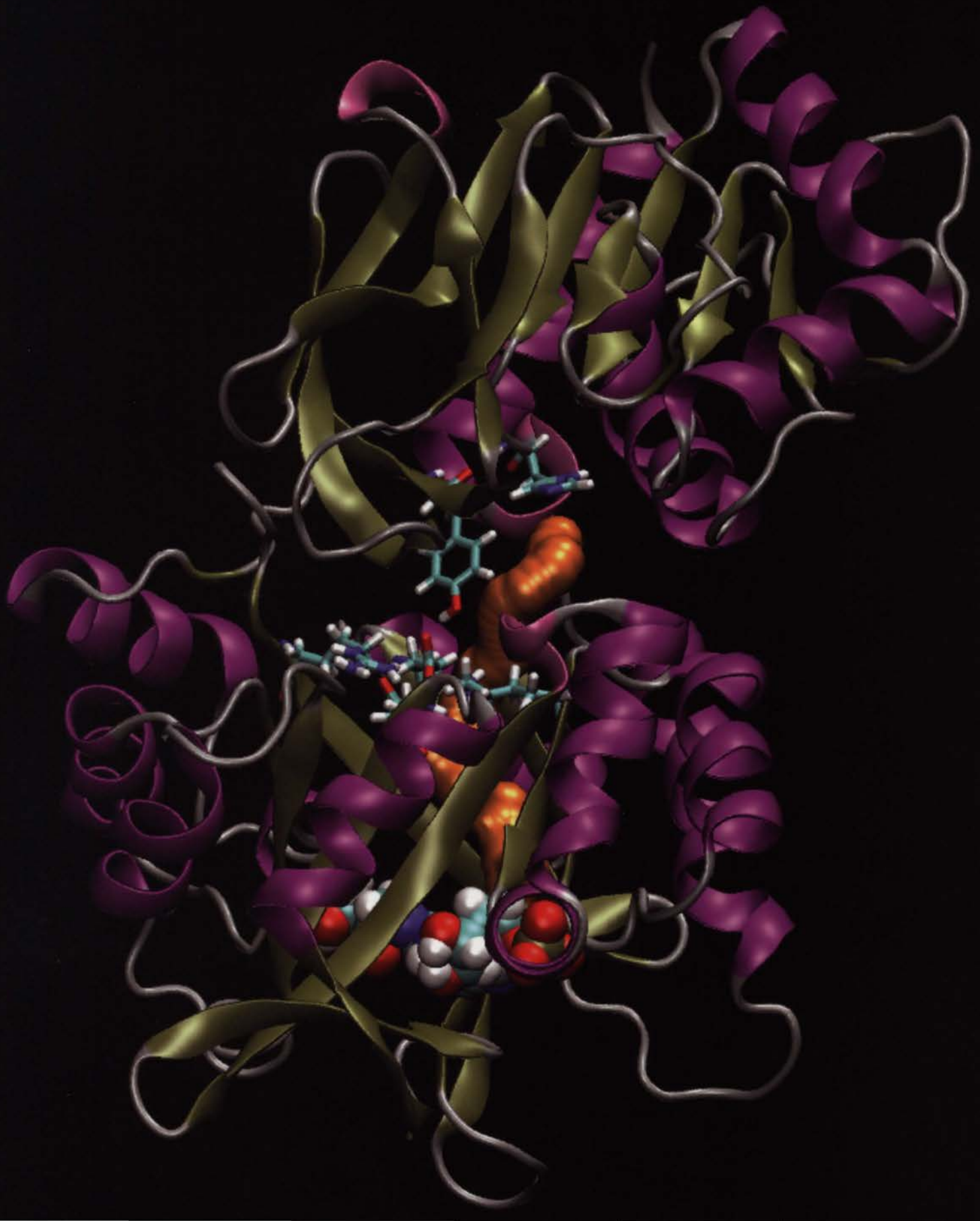
access

NCSA | Vol. 18, No. 3 | Fall 2005



access
Vol. 18, No. 3 Fall 2005

Executive Editor
Karen Green
kareng@ncsa.uiuc.edu

Managing Editor
J. William Bell
jbell@ncsa.uiuc.edu

Art Director
Carlton Bruett
cbruett@ncsa.uiuc.edu

Illustrator
Blake Harvey
bharvey@ncsa.uiuc.edu

Copyeditors
Trish Barker
Kathleen Ricker

On the Web
http://access.ncsa.uiuc.edu
Access is published on the Web every two weeks, covering the latest developments from NCSA and its partners.

National Center for Supercomputing Applications
University of Illinois at Urbana-Champaign
1205 West Clark Street
Urbana, IL 61801
217-244-0072

Who we are

The National Center for Supercomputing Applications opened its doors in January 1986. NCSA earned and maintains an international reputation in high-performance computing, networking, storage, and data mining. It is the recognized leader in developing innovative systems and software for science and engineering.

NCSA's overriding mission is to partner with diverse research communities to create the cyberinfrastructure that makes possible new scientific discoveries. Its specialty is shaping the most cutting-edge computers into working systems complete with software applications and tools for visualization, data mining and analysis, and collaboration. These innovative systems are the heart of an emerging cyberinfrastructure that links disparate systems into a single, seamless resource.

NCSA is a key partner in the National Science Foundation's TeraGrid project, a $100-million effort to offer researchers remote access to some of fastest unclassified supercomputers as well as an unparalleled array of visualization tools, application software, sensors and instruments, and mass storage devices. NCSA also leads the effort to develop a secure national cyberinfrastructure through the National Center for Advanced Secure Systems Research, a project funded by the Office of Naval Research.

The center leaves its mark through the development of networking, visualization, storage, data management, data mining, and collaboration software as well. The prime example of this influence is NCSA Mosaic, which was the first graphical Web browser widely available to the general public. NCSA visualizations, meanwhile, have been a part of productions by the likes of PBS's *NOVA* and the Discovery Channel.

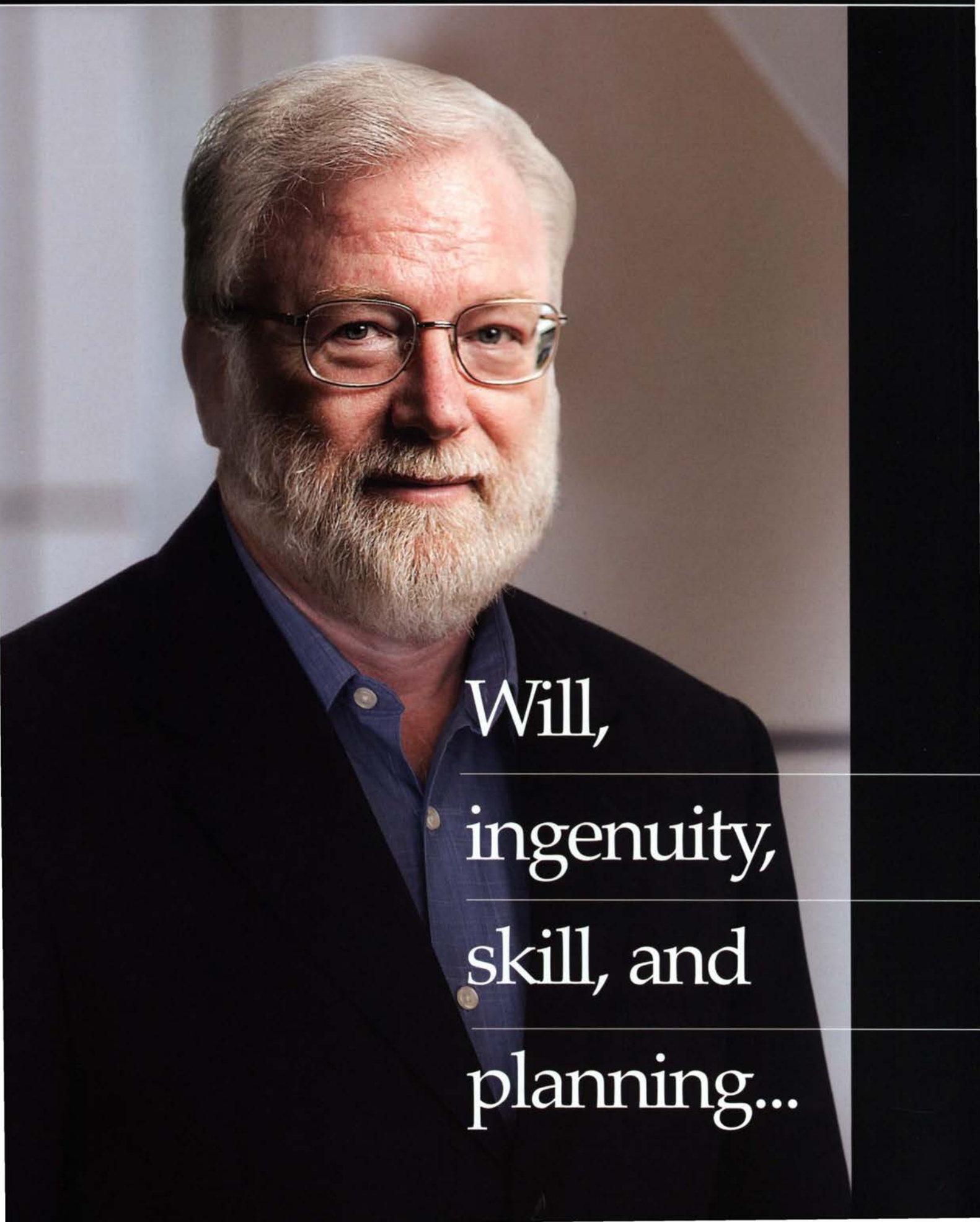
Major support for NCSA is provided by the National Science Foundation. Additional funding comes from the state of Illinois, industrial partners, and other federal agencies.

Cover

Zaida Luthey-Schulten and Rommie Amaro trace the path that ammonia takes between the enzyme IGP synthase's two parts. Their work was recently featured in *Biophysical Journal*. The computations behind it were completed on NCSA's Tungsten cluster.

NCSA

contents



Will, ingenuity, skill, and planning...

The Director's View

Spaceflight in the heady days of the Apollo moon missions represented an enormous amount of ingenuity, to be sure. Solutions to seemingly intractable problems were born apace. Some were triumphs of technical skill; others were triumphs of common sense in the face of knotty issues. All sorts of genius were required to achieve the goal.

But two other things were crucial. The first was will. The U.S. made major investments in Apollo. In 1966, 420,000 NASA employees and contractors were at work on the project. Second, there was careful planning. It's not necessarily something a scientist enjoys, but it's the only way to land a man on the moon when the president has given you a deadline of "before this decade is out" and you only have 16 minutes of manned spaceflight experience under your belt.

Missions steadily increased in scope, a carefully plotted stairstep toward success. Suborbital missions gave way to orbital missions, rendezvous in space gave way to spacecraft docking, orbiting the moon gave way to landing on it. NASA's leadership set out a "regimentation," classes of missions "from the very beginning...with a great amount of discussion and work. We had certain goals and objectives...We were able to build on our experience and learned from each one of those things," Chris Kraft, flight director of many early American flights and eventual director of the Johnson Space Center in Houston, once explained.

With such a model in mind, NCSA recently completed a strategic planning effort to guide us through the next five years. The central conclusion was that to serve the future needs of the nation's scientific and engineering communities, NCSA must undertake a major new effort to create cyberenvironments for science and engineering. We must make the cyberinfrastructure as easy to use as Mosaic made the Internet to use.

The national cyberinfrastructure will consist of a vast array of distributed resources—computers, data stores, and data sources like telescopes and sensors. Using such a powerful collection of resources will be daunting. To realize the full potential of the cyberinfrastructure, scientists and engineers must be able to access and marshal those resources to solve the cutting-edge problems that confront them. Cyberenvironments will provide scientific and engineering communities with the integrated set of tools and services needed to coordinate the end-to-end use of these resources to analyze, visualize, and model the natural or engineered systems of interest.

This will be our mandate in the coming years, and its implications are clear. Cyberenvironments will enable scientists and engineers to draw on the full power of the cyberinfrastructure to advance scientific discovery and the state-of-the-art in engineering. Raw computing power is still very important, but cyberenvironments will allow the scientist or engineer to fashion her own course, knowing that all of the capabilities in the cyberinfrastructure are reliably behind her.

The tools and services in the cyberenvironments will include scientific and engineering applications and Web services, graphical user interfaces and portals for easy interaction with the applications, and workflow and collaboration software to support complex, collaborative projects. A major component of this effort will be an integrated data analysis and visualization capability, which is needed by an increasing number of scientific and engineering communities.

Cyberenvironments will not be born full blown. Like the moon missions, they will be created in stages. Each stage will provide an increased set of capabilities and, at the same time, will lead to a better understanding of the issues and to the creation of the next version of the cyberenvironment.

To realize the full potential of the advanced tools and services in the cyberenvironments, NCSA will provide access to these tools and services on leading-edge computing and data storage resources. To ensure that these resources continue to meet the rapidly increasing computational needs of the scientific and engineering communities, NCSA will establish a new effort in innovative systems for science and engineering. This effort will first focus on new computing technologies, as these technologies are now undergoing a major change, but over time its scope will broaden to encompass the entire system needed to solve cutting-edge problems in science and engineering.

Development of plans for implementing this vision is underway. The course becomes clearer each day. But each endeavor that we laid out in our strategic plan represents only the broadest of strokes. I hope that it helps give everyone at NCSA and all of our partners the will and enthusiasm to imagine the finer points and to begin to define them and integrate them into a complete picture. The whole—whether we're talking about our center and its collaborators or about cyberenvironments—can truly be greater than the sum of its parts.

Thom Dunning
NCSA Director

'That's why it's called research'

In July 2005, Duncan Buell keynoted the Reconfigurable Systems Summer Institute at NCSA. Buell directed the Splash 2 reconfigurable computing project in the 1990s and now leads a university research team supported by the Department of Defense. NCSA's J. William Bell interviewed Buell as he moved into new digs as interim dean of the University of South Carolina's College of Engineering and Information Technology.

Q: Many people are just starting to get interested in reconfigurable computing. Could you give a definition of the field?

A: The field started almost as soon as these FPGAs [field-programmable gate arrays] started to exist in the '80s....[Y]ou have a chip that can take on different hardware characteristics or different gate characteristics depending on what it is configured to do...The idea is that if you have a computation that is not supported successfully by the traditional instruction set that Intel or whoever hands you, then you can essentially design your own arithmetical logic unit to handle exactly the computation you need.

Q: Why should this be on the radar screen of the discipline scientist—the chemist or the astronomer who's doing simulation or data analysis?

A: In the last couple of years, the chips have gotten big enough and fast enough that you could think about laying out the circuitry for floating point [operations]...And that's something that the scientific computing people are taking note of...

[Y]ou can create a number of processing units and have them all functioning in parallel. If they're all on the same chip, all the data stays on the chip. You don't have to go back to memory, not even back to cache...Now, of course, you have to realize that the floating point FPGA is going to be slower than an Intel processor, so the speedup's not necessarily a factor of 100. But you've eliminated the overhead, so maybe you only get a factor of 50. You need to have at least a factor of 50 before people take notice. Anything less than that, and they just ride the technology curve. They just buy another dozen clusters or something.

Q: How do you see this shift expanding out to more discipline scientists?

A: Part of my assumption in all of this has been that if you demonstrate success, people will notice. As long as you're talking about the performance advantages you might be able to get, people will smile nicely, be polite, and do whatever they're doing...The big deal in all of this is that having the hardware is only part of the game. The really important part is the programming environment, so that ordinary programming types are able to make use of the machine.

Q: What are the key features of that software environment?

A: I would maintain that they are going to be willing to look at the hardware as something that will require a special version of something like C or C++...They're not going to be willing to learn a real hardware language...

The other big problem always has been that debugging has to be something that looks like debugging...There has to be something like a software simulator that you can run a debugger on because the first 90 percent of the programming environment is just getting the right answers out and has nothing to do with the hardware and not a whole lot to do with performance.

Q: And what can someone in your position or NCSA's position do to ensure these sort of things actually happen?

A: If you had a few people at the edge, and you had someone willing to undertake an implementation, one message is: "I did the implementation and it was successful, but it would have been more successful and I would have gotten done a lot faster if in fact the programming environment had been the sort of thing it should have been." I think it's going to take a few evangelists to demonstrate they're willing to put in the effort and then point out that they really shouldn't have to put in that much effort...

It's a shakedown cruise. You're going to go see what works, what doesn't work, what could be better...[T]he more applications, the more you expose the features that need to be included that for some reason weren't.

Q: In your keynote, you talked about the "must haves" for reconfigurable computing. The big speedups, the software environment. But you also discussed it being something people choose to do again.

A: When I ran Splash 2, I figured we'd start with a dozen applications that might have potential. Given that we had a fixed set of hardware constraints, probably half of the dozen we would look at briefly, and they wouldn't match the architecture we had. That would leave us with six that we might actually implement. Of those, three might work, have a performance improvement, but say the improvement is 10 or 15 times. Then you sit back, and you say that was a nice experiment.

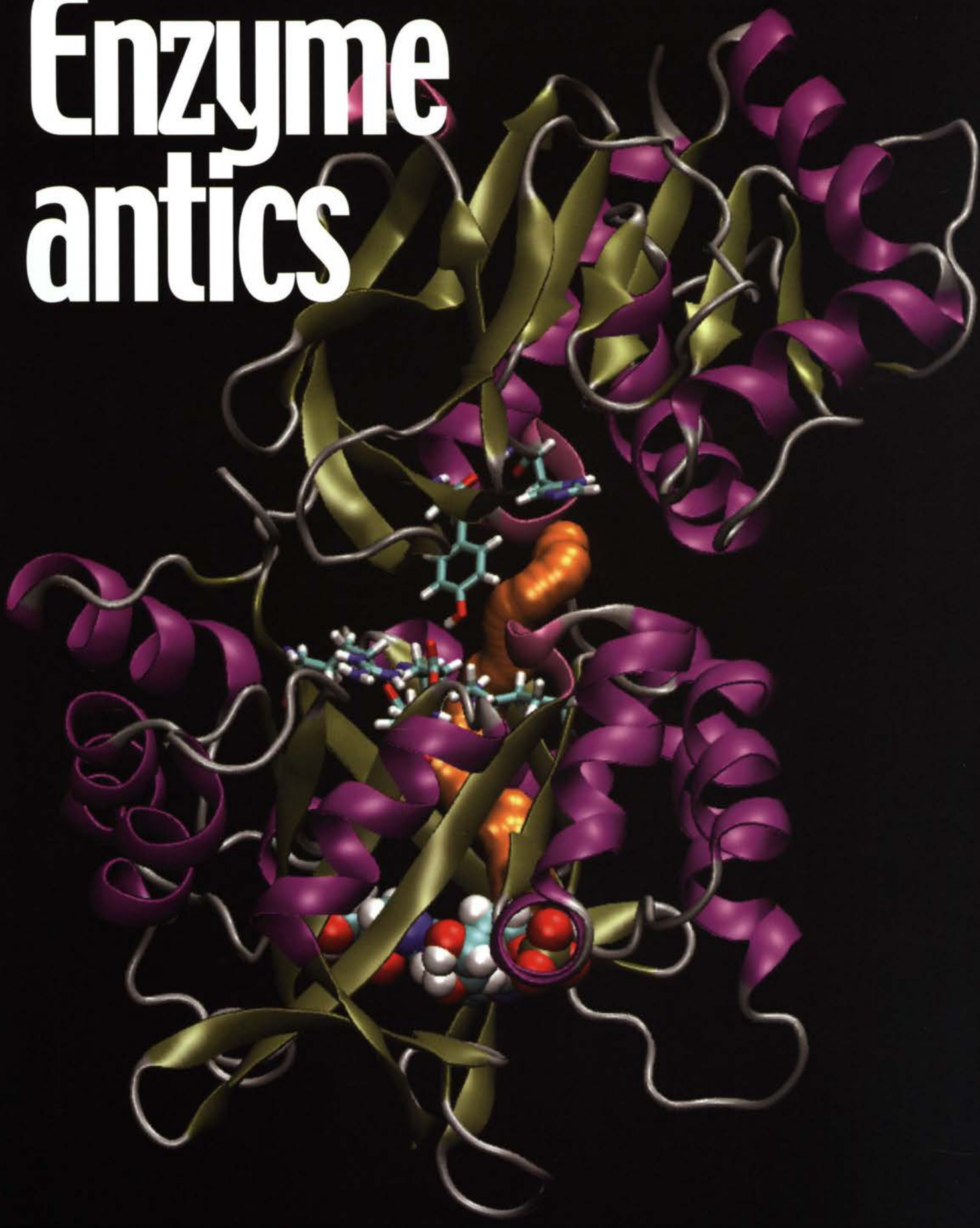
Q: So there's hardware overhead and then there's human overhead?

A: If it's going to be a serious application, it's going to be six months or nine months worth of programming effort. In six months or nine months, machines get better. So really it's the people cost. Is it worth doing it in a somewhat unconventional way compared to doing it in a much more conventional way and just not getting as good performance? From the point of view of a middle management person, is it really a good use of all the resources?

Q: It's interesting to hear you talk about it like that. Rob Pennington [NCSA's Chief Technology Officer] and the people in our Innovative Systems Lab have acknowledged that aspect of it and are looking at a number of different—as many as a dozen, as you just described—applications. They make a full admission up front that some of this is just exploring the space.

A: That's why it's called research. If there isn't a significant possibility of failure it's not research, it's just work. That's not where the "Ah-ha! Gotcha!" big breakthrough comes.

Enzyme antics



by Kathleen M. Wong

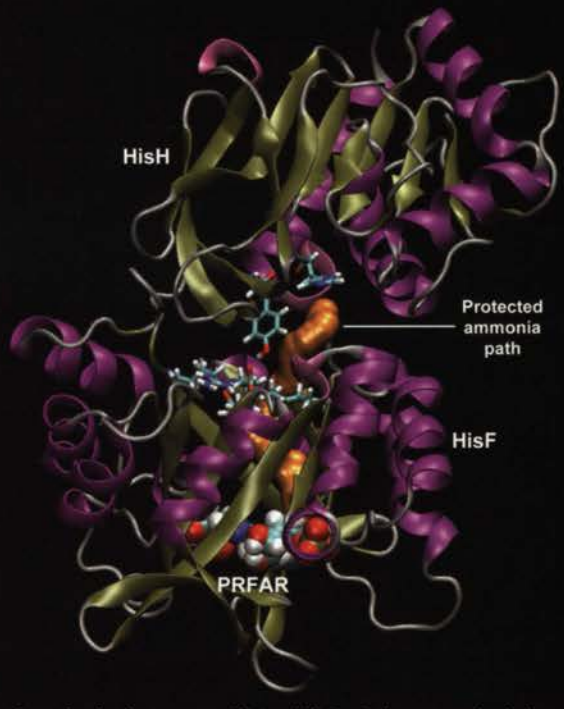
Computer models of enzyme function are revealing how nature's biochemical gadgets operate.

The world's smallest Rube Goldberg devices are manufactured by Mother Nature. Known as enzymes, these fiendishly complex proteins perform life's most basic tasks—transforming air and food into tissues and metabolic energy. Like Rube's ridiculous contraptions, they have parts that grip and bend, swing and rotate. But in place of ball bearings, dominoes, and springs, enzymes use amino acids to accomplish their feats.

How enzymes operate, however, has proven daunting to decipher. For one thing, they're too tiny to be observed by the most powerful microscopes. For another, they're constantly in motion, flexing and drifting in the soupy innards of a cell.

Scientists have long relied on static snapshots (x-ray crystallography) and protein sequences to gain insights into enzyme structure and function. But using this information is like reconstructing a car engine from a parts list and a glance below the hood; it's impossible to understand how it works until you see it running.

Now scientists are doing the next best thing: animating enzymes with models run on supercomputers. Using molecular dynamics modeling, scientists can track the behavior of each of the tens of thousands of atoms that make up enzymes, solvents, and substrates—and watch nature's microdevices in action.



IGP synthase showing its two parts, hisH and hisF, and the protected path that ammonia takes between the two.

A tough nut to crack

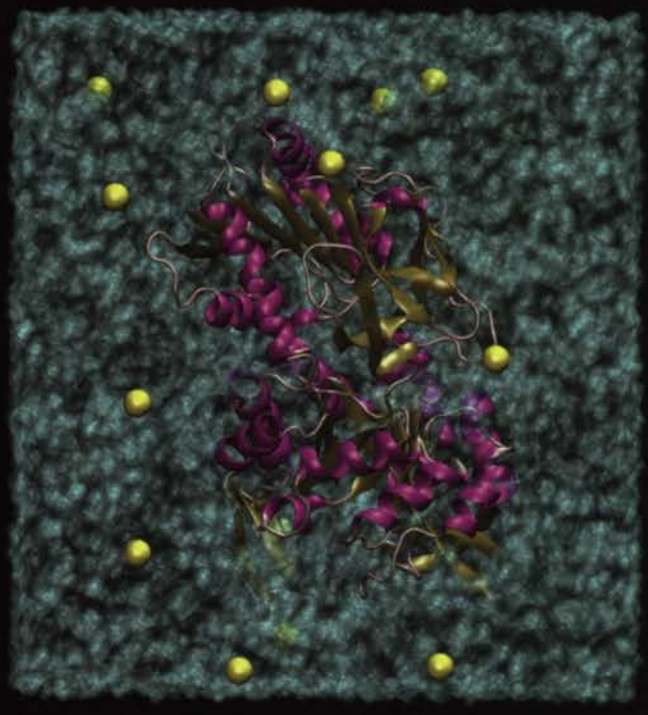
Among those taking this tack are Zaida Luthey-Schulten, professor of chemistry at the University of Illinois at Urbana-Champaign, and Rommie Amaro. Amaro recently completed her PhD with Luthey-Schulten and is starting a post-doc at the University of California at San Diego. They are using NCSA supercomputers to model the workings of an enzyme that helps manufacture the amino acid histidine. Together with the experimental group of V. Jo Davisson, professor of medicinal chemistry at Purdue University and his student, Rebecca Myers, Amaro and Luthey-Schulten have recently nailed down a key step in the production of amino acids and the building blocks of DNA. Their work made the cover of the July 2005 issue of *Biophysical Journal*.

"One of the really fabulous things about molecular dynamics simulations is they allow you to see things on an atomistic level. There is no other way to see these types of behaviors right now. And when it's consistent with the experimental results, you can have really profound insights into these systems," Amaro says.

The enzyme in their sights has a name as complex as its function: imidazole glycerol phosphate (IGP) synthase. The enzyme "is really the epitome of complexity in enzyme catalysis," Amaro says. Its job is to make both IGP and AICAR, an ingredient necessary to make DNA and RNA.

Previous research had shown that IGP synthase consists of two parts, hisH and hisF. Each subunit performs half of the enzyme's duties: hisH transforms the abundant amino acid glutamine into ammonia and glutamate, while hisF uses the ammonia to produce IGP and AICAR.

Though the two subunits might appear to act independently, they always remain docked together when the enzyme is active. The reason behind their close association appears to be ammonia. If released from the enzyme and into the cell, ammonia would instantly react with water and other solvent molecules. Its escape would leave hisF bereft of a substrate. Instead, the scientists realized, ammonia must follow a protected path within the enzyme to travel from hisH to hisF.



IGP synthase surrounded by water and ions, as in the simulations.

Ammonia's mysterious path

Initial studies suggested the handoff occurred at something resembling a molecular gate. Four strategically placed amino acids appeared to block the entrance from hisH and into the tubelike interior of hisF. Two of the amino acids were positively charged, and two were negatively charged; their strong electrostatic interactions appeared to seal off the mouth of the hisF barrel completely. "Everybody thought that in order for ammonia to make it from one active site to the other, these would have to move aside," Amaro says.

Previous sequencing studies had indicated that all four of these gate residues were conserved; that is, the same amino acids occupied these positions in both the bacterial and yeast versions of the enzyme. (In biology, conserved structures tend to be critical for an organism to function. They remain unchanged because without them, creatures don't survive to pass along the defect.)

To determine the role of each gate residue, the scientists replaced them one by one with a generic amino acid and observed what went awry. Checking the experimental and computational results against one another, they reasoned, would narrow down what was actually going on.

One of their substitutions poked a big hole in the gate by substituting a smaller, uncharged amino acid for a bulky, charged one. This nearly derailed the reaction in the laboratory. Normally, the enzyme uses one molecule of glutamine to make one molecule of IGP, an efficient 1:1 substrate/product ratio. The mutation changed the ratio to an abysmal 122:1. "On the computational side, we introduced that same mutation but could really watch the system on an atomistic level. We saw that the water molecules from the solvent rushed into the hole and filled the protected ammonia chamber; it basically flushed the ammonia out," Amaro says.

A molecular trapdoor

Even more interesting, however, was how the normal, or wild-type, enzyme behaved in the simulation. When the ammonia moved near one of the four gate residues, a lysine, "the lysine actually bent, and ammonia slipped through this newly discovered side opening," Amaro says.

Once the ammonia had passed inside, the simulation revealed, the lysine swung shut behind it. Once inside, ammonia was forced to remain in the barrel, and water could not chase it out.

Swapping the lysine for a smaller molecule essentially propped this side door ajar. In the laboratory, the reaction's efficiency slipped from 1:1 to 3:1. The computer simulation showed that while the mutation allowed ammonia to slip into the barrel more easily, it could also diffuse right back out.

"We actually saw the side opening at the beginning and didn't quite believe it," Luthey-Schulten says. In earlier simulations, they had pulled a virtual molecule of ammonia through the enzyme using a technique known as steered molecular dynamics (SMD). SMD allows the scientists to recreate events that would take too long—and use up too much computer time—to simulate

otherwise. In this case, the researchers used SMD to measure the strength of the chemical bonds ammonia makes with enzyme amino acids at each step of its journey. "By knocking on that gate long enough, we saw a heck of a high barrier, and knew ammonia was not going through that very easily," Luthey-Schulten says. "A subtle change, and it just went through the side door. We though nah, we must've done something wrong."

In fact, they had discovered the hidden entrance to the kingdom.

SMD also gave the scientists insight into the role of water in the reaction. Water competes with ammonia to bond with amino acids in the barrel's lining, they found. So having a couple of water molecules in the hisF barrel prevents ammonia from getting stuck. In other words, water helps lubricate the chamber.

A dedicated computing team

The researchers used the NCSA Tungsten cluster to run their 50,000-atom simulations. "NCSA has always been a valuable resource for us; it's my location of choice. Their system is stable, the programs run very well on it, and the people are just fabulous," Amaro says. She singles out John Towns, senior associate director of NCSA's persistent infrastructure directorate, for particular praise. "He's so responsive to our needs as scientists. If we need dedicated time, he can usually help us out. It's also really nice to have people you can talk to; those human relationships make a big difference."

In fact, Amaro and Luthey-Schulten liked working at NCSA so much that they transfered all of their time at another supercomputing center to NCSA.

Thanks to the data-crunching power of supercomputers, Luthey-Schulten says, "this whole field is really coming into its own. We can seamlessly go from bioinformatics to molecular dynamics simulations and energy landscape studies, and learn enough to apply it to other systems very easily."

She, Amaro, and colleagues have already applied their findings to an even more intriguing mystery about IGP synthase—how molecules bound at opposite ends of the enzyme somehow work together to turn the device on. Their discoveries promise to help biochemists everywhere decipher how organisms build such elaborate enzymatic mousetraps.

This research is supported by the National Science Foundation and the National Institutes of Health.

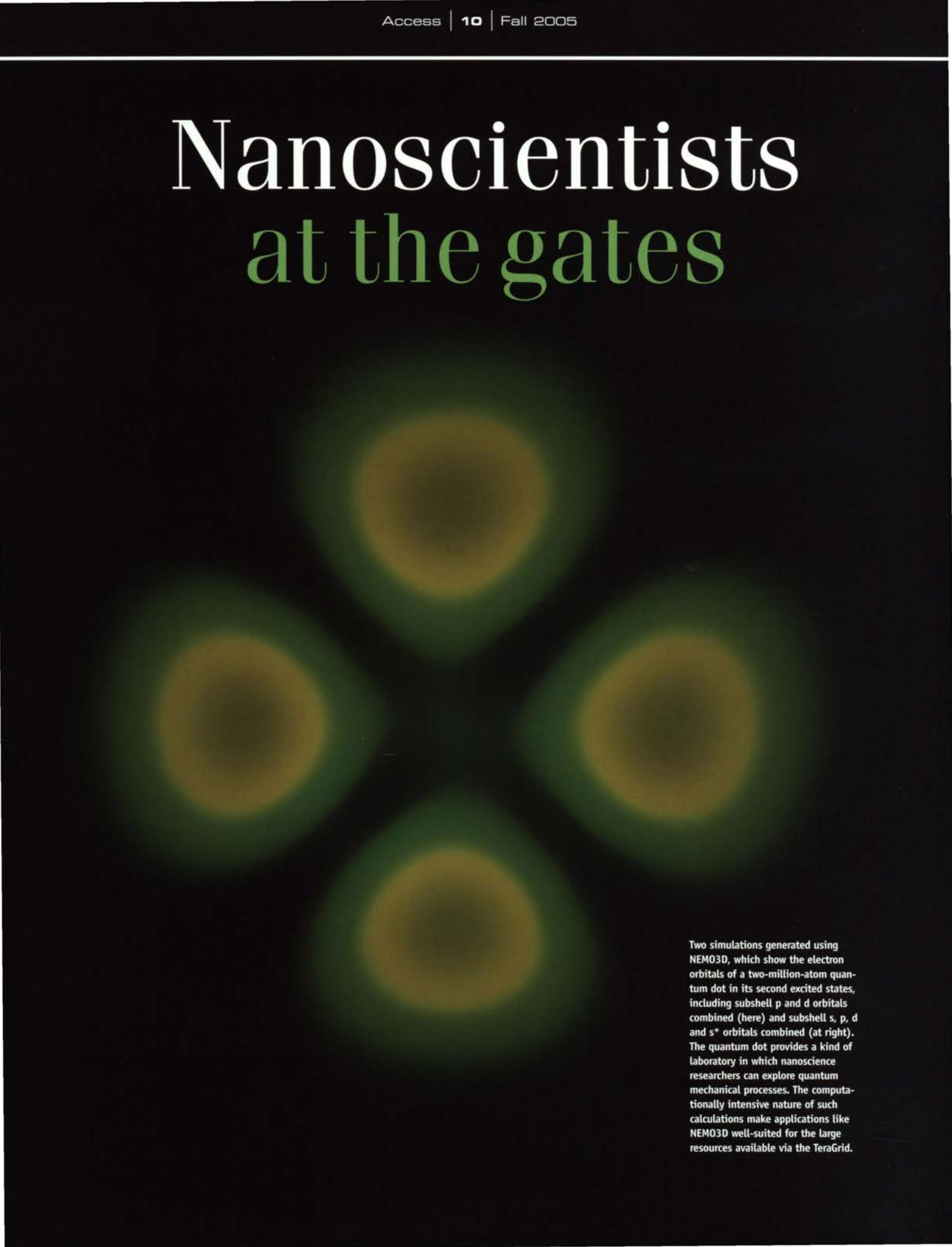
Access Online: http://access.ncsa.uiuc.edu/CoverStories/IGP/
For further information: http://www.scs.uiuc.edu/~schulten/
http://vidar.scs.uiuc.edu/~rommie/

Team members

Rommie Amaro
V. Jo Davisson
Zaida Luthey-Schulten
Rebecca Myers

V. Jo Davisson, Rommie Amaro, and Zaida Luthey-Schulten.

Nanoscientists at the gates



Two simulations generated using NEMO3D, which show the electron orbitals of a two-million-atom quantum dot in its second excited states, including subshell p and d orbitals combined (here) and subshell s, p, d and s* orbitals combined (at right). The quantum dot provides a kind of laboratory in which nanoscience researchers can explore quantum mechanical processes. The computationally intensive nature of such calculations make applications like NEMO3D well-suited for the large resources available via the TeraGrid.

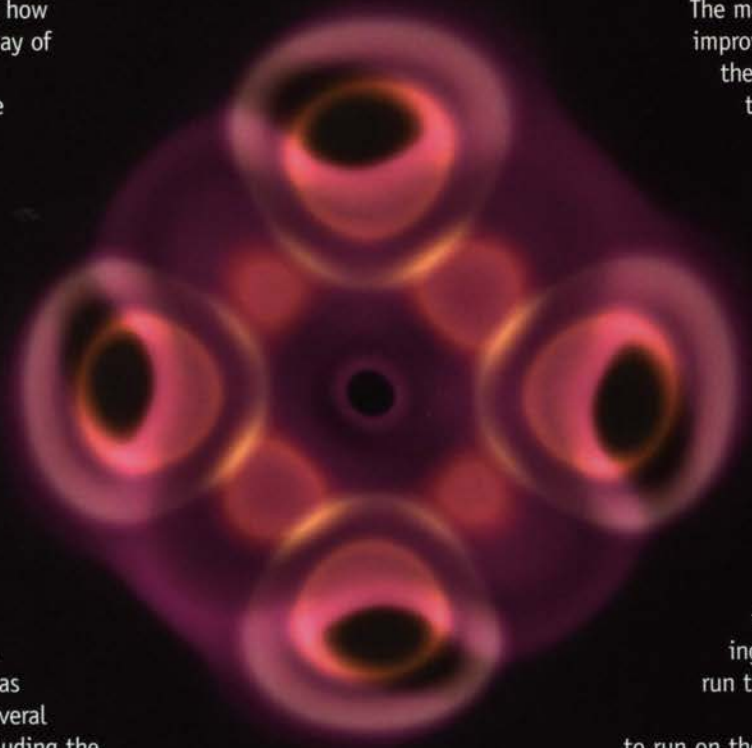
by Kathleen Ricker

Soon to become the nanoscience gateway to the TeraGrid, the nanoHUB is pioneering ways to make the Grid accessible to any user.

As research communities make the leap to scientific computing, at some point they all face the hurdle of user-friendliness. The engineering community is no exception, according to Gerhard Klimeck, technical director of the NCN (National Science Foundation Network for Computational Nanotechnology) and professor of electrical and computer engineering at Purdue University. "I'm an engineer—I want to get results done, and I have plenty of examples of how supercomputing can get in the way of getting results," says Klimeck.

Back in the early days of the Web, the lack of application portability got in the way of results. "The theorists were writing Unix-based applications for semiconductor device modeling," Klimeck explains. "But the experimentalists who wanted to use these tools didn't have Unix systems—they deal with PCs."

Thus, in the mid-1990s came the development of PUNCH (Purdue University Network Computing Hub), middleware that allowed non-Unix-users to run Unix-based applications. Since that time, PUNCH has supplied the infrastructure for several research networks or "hubs," including the nanoHUB, a network that since 2000 has provided a Web interface that makes tools and instructional materials available to experimentalists, theorists, and students in a number of areas of nanoscience, a set of disciplines that examines the physics, biology, and chemistry of extremely small objects. "In a practical sense it solves a lot of problems," says Klimeck, "especially for educators at many universities who don't have the IT staff to install all these different applications on local computers. Instead, they can just manage them from their browsers."

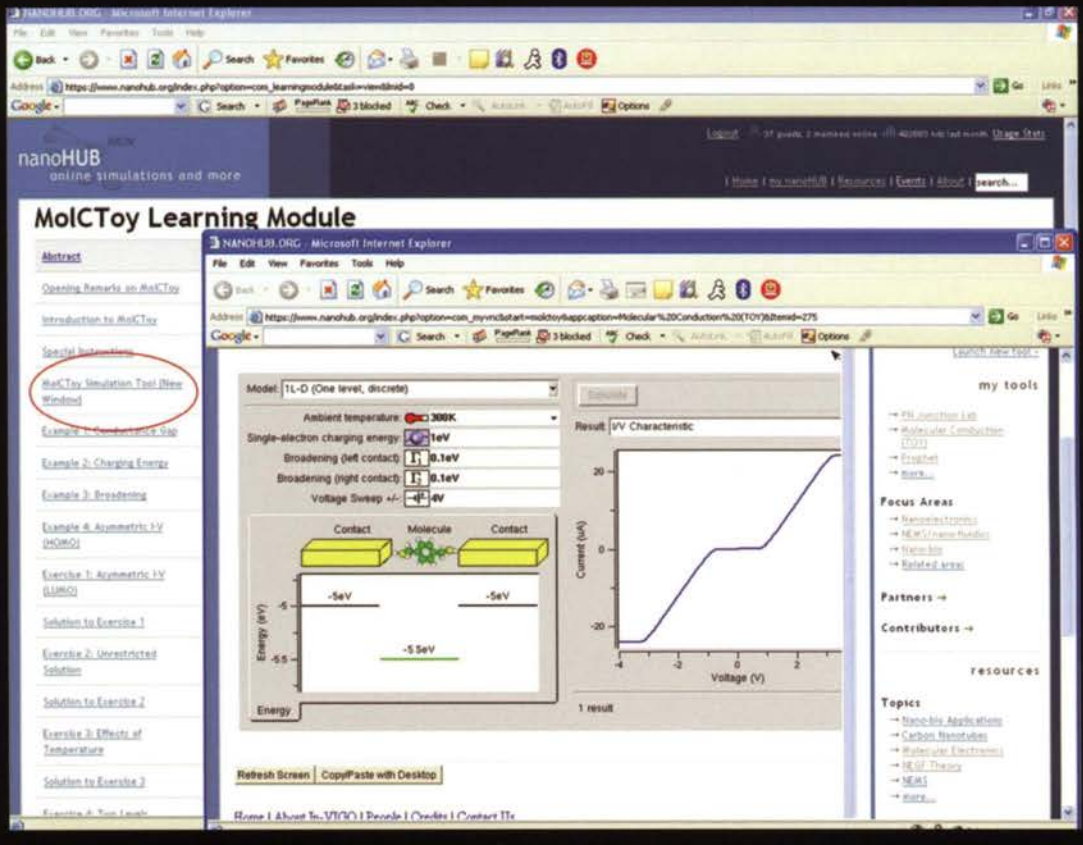


Upgrading to the TeraGrid

Now, the nanoHUB's architecture is being redesigned. By late 2005 or early 2006, the original PUNCH middleware will be replaced entirely by middleware based on In-VIGO, a distributed environment that provides users with their own, individual, secure virtual environments in which to run applications—all coexisting on the same physical resource.

The most elegant aspect of the new and improved nanoHUB, however, is that these features are utterly invisible to the end-user. This is especially important as the nanoHUB takes on its new role as one of the science gateways being created to enable access for various research communities to the TeraGrid's computing power. The integration of In-VIGO with Condor, and particularly with Condor-G, a task manager capable of managing thousands of jobs on a distributed grid, means that researchers running applications on the nanoHUB will be able to submit these jobs to the TeraGrid, drastically reducing the amount of time it takes to run them.

"We want our users to be able to run on the TeraGrid without having to be geeks, writing allocation proposals and installing certificates and having multiple logins," says Klimeck. "They may not even realize they're running on the TeraGrid...they may say, 'What's the TeraGrid? I don't care.' This is our definite end-goal: for people to see as little of what's under the hood as possible and still be able to run their stuff."



One of the tools available on the nanoHUB, Molecular Conduction (Toy), in action. MolCToy computes the conduction properties of a molecule sandwiched between two metallic contacts. Here, MolCToy is used as part of an interactive learning module, also available via the nanoHUB, which introduces students to the basics of molecular conduction.

Is it real, or is it In-VIGO?

Formerly, says Jose Fortes, professor of computer science at the University of Florida and principal developer of In-VIGO, "applications would never be able to run in a physical machine if they expected a different environment, and users who might have conflicting requirements would not be able to share that machine. Now we have software that makes the physical machine appear as multiple virtual machines."

Although two users share the same machine, one user—a theoretical researcher, for example—might be running his or her applications on a Unix platform, tailored to that user's specific requirements, while the other—an experimentalist—might be running on Windows XP. However, they would never be aware of each other's activities, because the physical machine would appear, simultaneously and separately, as multiple virtual machines. In-VIGO creates a virtual address space that assigns each virtual machine its own IP address independent of the IP address of the actual physical machine. The virtual addresses are each mapped to the physical address and translation mechanisms are established between the physical and each of the virtual addresses that rout messages to the appropriate users. "It's like renaming the address of your house for just a few friends and then having the postman know how you did the renaming," explains Fortes.

The capability for multiple, separate virtual environments also has important implications for user security. "You can think of the virtual machines as two separate machines located in the same room—it would be impossible for what happens to one machine to affect what happens to the other," says Fortes. Thus, the damage caused by any serious but unintended errors a user makes is limited only to that user's virtual machine. Likewise, in an era of devastating viral attacks that can bring down entire large machines or networks, any malicious code inserted by a rogue user is limited only to that user's environment and does not affect other users or applications.

Expanding the Grid user community

The nanoHUB's success has been overwhelming. In the past year alone, it has provided the interface for more than 65,000 job submissions launched by more than 1,000 users—70 percent of whom are students using it for university coursework. And another 6,000 members of the nanoscience community have used the nanoHUB to access online workshops and seminars.

"The NCN is defining a new model to serve the computational community and the public at large," says Sebastian Goasguen, a research scientist at ITaP (IT at Purdue) who leads the deployment effort of the nanoHUB funded through the NSF Middleware Initiative (NMI). "Each application is packaged with all the materials researchers or students need to learn and do research on specific subjects." This packaging takes the form of portable, XML-based "learning modules" that can be downloaded via Web browser and accessed in any user environment.

Ultimately, the hope is that the nanoHUB's function as a TeraGrid science gateway will provide other science and engineering communities with an idea of what's possible—that what works for one area of science can be transferred into other areas as well. Says Tim Cockerill, project manager for the TeraGrid, "TeraGrid's relationship with nanoHUB is a prime example of how our science gateway partners utilize some of the National Science Foundation's most powerful high-performance computing resources. Through science gateways we are able to reach out to communities of engineers, scientists, and educators who most likely would not have this opportunity otherwise."

This research is funded by the National Science Foundation, Indiana 21st Century Fund, and ARO.

Access Online: http://access.ncsa.uiuc.edu/CoverStories/NCN/
For further information: http://www.nanohub.org

Team members
Renato Figuireido
Jose Fortes
Sebastian Goasguen
Gerhard Klimeck

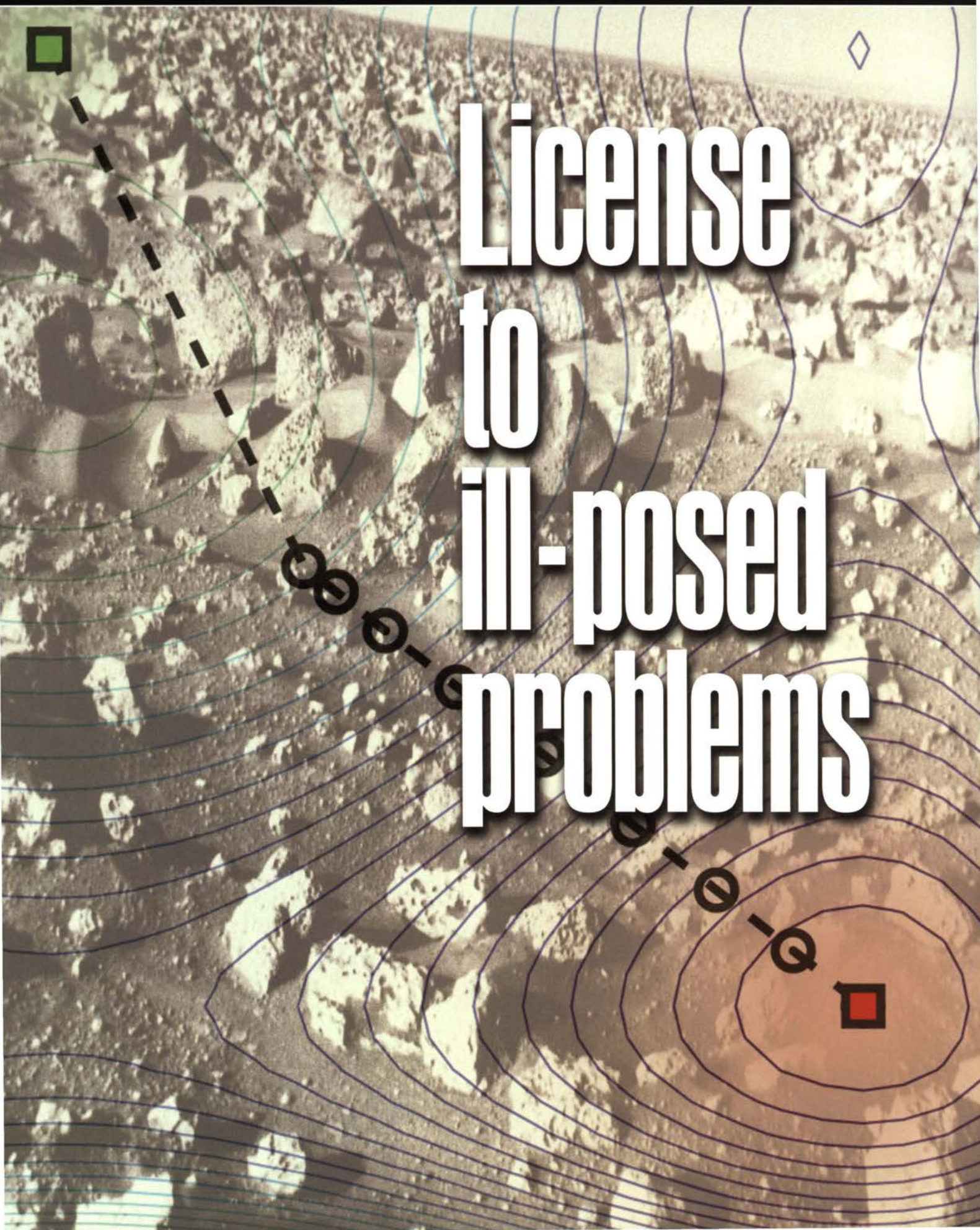
Getting science done

The research tools that the nanoHUB will be making available in the near future focus on three areas of nanoscience: nanoelectronics, nanomechanics, and bionanointerface (which examines the ways in which electrons interface to biological systems). Deployment of these applications, geared toward researchers experienced in computational science, is anticipated within the next six months.

As an engineer, Klimeck himself is hoping to make applications available via the nanoHUB that enable users to do cool nanoscience on the TeraGrid. Klimeck is one of the principal developers of NEMO3D, an application that performs nanoelectric modeling of quantum dots—nanostructures that, while consisting of large numbers of atoms, behave like artificial atoms in their ability to confine a number of electrons to a small space. The size of a typical quantum dot is around 10 nanometers, or 100 times the size of an atom. Klimeck describes a quantum dot as a kind of "little laboratory where you can study a quantum mechanical system, but large enough to extract information out of that system."

By using NEMO3D to calculate the eigenvalues and eigenvectors in the quantum dot's closed system, Klimeck is able to compute the orbits of individual electrons within the dot. Recently, using NEMO3D on NCSA's TeraGrid Itanium cluster, Mercury, Klimeck and his group modeled the largest quantum dot simulation ever, consisting of 21 million atoms. Because NEMO3D is computationally intensive—requiring 200,000 service units or more to model even a small quantum dot—Klimeck sees it as precisely the kind of application that could best exploit the enormous computing resources the TeraGrid makes available.

Another such prospective application for the nanoHUB is BioMOCA, developed by the computational electronics group of Umberto Ravaioli, an engineering professor at the University of Illinois at Urbana-Champaign and member of NCN. BioMOCA, a Monte Carlo solver for biological nanodevices, is currently being used to simulate electrolyte conduction in ionic channels in three dimensions. "BioMOCA has been developed by adapting our framework utilized for semiconductor devices," Ravaioli says, "and it is intended to complement the accurate but time consuming molecular dynamics simulations used in computational biophysics." In contrast to the vast number of atoms represented in a quantum dot, these Monte Carlo ion channel simulations typically involve only a small number of particles (ions) since water molecules are introduced implicitly as a continuum. However, applications need to run for very long times to resolve biological current flow phenomena, which are much slower than in electronics devices, resulting in just as compute-intensive simulations. Ravaioli hopes that this work will facilitate interdisciplinary collaboration between engineers and biologists by providing a tool that delivers a system description of device-like biological functions. Like NEMO3D, BioMOCA is currently being developed with NCSA support, in this case, as part of NCSA's Strategic Applications Program, which provides Ravaioli with large-scale computational resources and crucial assistance from NCSA staff.



License to ill-posed problems

by J. William Bell

An Oak Ridge National Lab computer scientist explores ways to solve ill-posed problems in scientific computing.

It's only fair that a puzzle have only one solution, right? That's the great thing about a crossword or one of those Sudoku number games that the lifestyle pages can't stop talking about right now. There's only one way to fill in the boxes and get a complete answer.

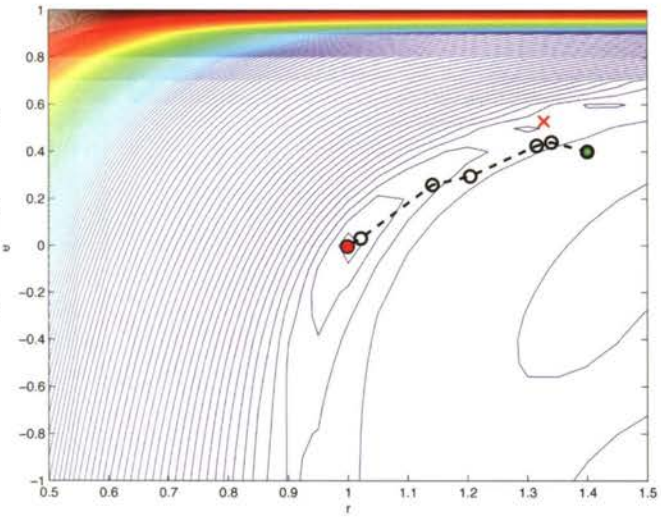
Well, nobody said science was always fair. In what are known as ill-posed problems, there is no unique solution. A slight change in the data fed into the system of functions that rule a given ill-posed problem can produce a large, unpredictable change in the results.

"In the late 1800s, a scientist named Hadamard proposed that ill-posed problems didn't exist [or those that did weren't scientifically significant]. He was totally wrong. They're everywhere," says Rebecca Hartman-Baker, who recently completed her PhD in computer science at the University of Illinois at Urbana-Champaign.

They're found, for example, in medical imaging, financial modeling, environmental modeling, and astronomy. Though Hartman-Baker's PhD thesis focused on an ill-posed problem found in the field of geoprospecting, the approach applies to any of those fields.

"Any ill-posed problem for which you have an educated guess of where to start could use this," says Hartman-Baker, now a post-doc at Oak Ridge National Laboratory. "As a scientific computing type, the thing that brings me the most joy is to contribute to real-world scientific problems through my little thing. I want to get people who didn't know they needed to be involved in computer science to be in it."

Making hundreds of runs on NCSA's Platinum and Tungsten clusters, she developed a selection method for choosing the parameters that go into the problem and an optimization method for finding the ideal result among a sea of solutions.



The way that the diffusion equation method homes in on the global minimum of the geoprospecting problem. The green circle represents the starting point. Using a local optimization method to discern the minimum results in the point at the red X. Using the diffusion equation method traces the path of the dotted line until it finds the true minimum represented by the red circle.

Not just approximate, but quasi

Geoprospecting typically involves placing transmitters and receivers deep in the earth. The transmitter projects electromagnetic energy, or in some cases sound, that is picked up by the receiver miles away. The electromagnetic energy is altered in transit, based on the conductivity of the rock, water, oil, or other materials in the ground. From the data collected by the receiver, researchers can deduce what lies between it and the transmitter.

The challenge is—and this is where the ill-posed problem comes in—that different sizes, shapes, and orientations of underground deposits can produce the same data profile.

"Basically, you're trying to find the size and shape of an ellipse [that represents the deposit that a geoprospector might be targeting, such as oil]. Where the center is at. The rotation or orientation. How you do that is really indirect—kinda backhanded," Hartman-Baker says.

The traditional method of solving this sort of ill-posed problem, known as Tikhonov regularization, gives a blurry picture of this ellipse. It stabilizes the problem around a single solution by adding things like smoothness constraints to the functions. But in situations like this, researchers tend to prefer distinct boundaries. To get these boundaries, Hartman-Baker proposed another class of stabilizing, known as selection methods. With selection methods, the solution is limited to some reasonable set of possible solutions, and the parameters fed into the problem are reduced to a manageable number (about 10 in the case of Hartman-Baker's work). These decisions limit the computational expense of solving the problem and provide a distinct ellipse.

"We're bringing selection methods back into the world. People have forgotten about them," she says. In her numerous runs on NCSA's systems, she tested the viability of the approximate quasisolution method.

Going global

The selection method reduces the number of parameters and shrinks the size of the solution space, but the optimal solution still has to be found. To do so, researchers make an educated guess of the input that will produce the optimal solution, run a simulation using that input, and compare the output to real-world data. They repeat the process until they find the input that most closely resembles the real-world output. In the example used by Hartman-Baker, that reveals the shape of the ellipse that produces the output.

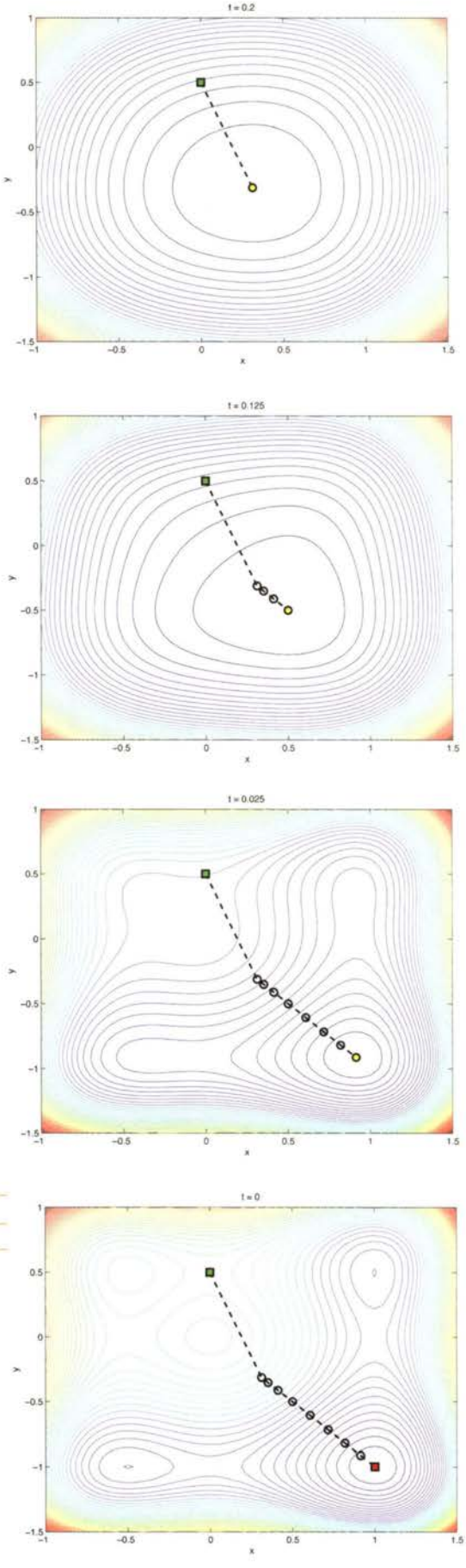
To find the output that most closely resembled the real world, Hartman-Baker's example required finding the global minimum for a system of mathematical functions. After again trying several different methods, she settled on the diffusion equation method (DEM), which finds local minima and then traces back through a series of those local minima to the global minimum. Hartman-Baker compares this process to finding the lowest point in Kentucky. It's easy to find the lowest point in a region; you just head downhill until you are forced to start uphill again. But there are a lot of regional low points spread about, so ensuring that you've found the lowest of the low is no small task. DEM blurs the function "so that at first you just see overall trends, but not all the details. Then as it progresses, you unblur the function more and more until the full features [of the global minimum that you homed in on] are visible," she explains.

As part of her thesis work and again using time at NCSA, Hartman-Baker discretized this involved method so that it can be parallelized and can use multiple processors at the same time. Currently, the evaluation of a function can be run on eight processors and takes about a minute. This has to be done several thousand times to solve a single optimization problem in geoprospecting.

This research was supported by the National Computational Science Alliance and, more recently, the UIUC computer science department's Fulton Watson Copp Endowed Chair held by Professor Michael Heath.

Access Online: http://access.ncsa.uiuc.edu/CoverStories/ill-posed/
For further information: http://www.cse.uiuc.edu/~rjhartma/

Team members
Rebecca Hartman-Baker
Michael Heath



The diffusion equation method at work on a quartic test function of two variables. The first image shows the objective function smoothed until only a single minimum remains. The green dot represents the starting guess for the minimum, and the dotted line traces the path to the global minimum found in that step. The second image shows the path of minima being traced as the function is unsmoothed, and the next image shows the minimum converging to the global minimum as local features reappear. The final image shows the completely unsmoothed function, and the path tracing to the global minimum.

Learning and teaching

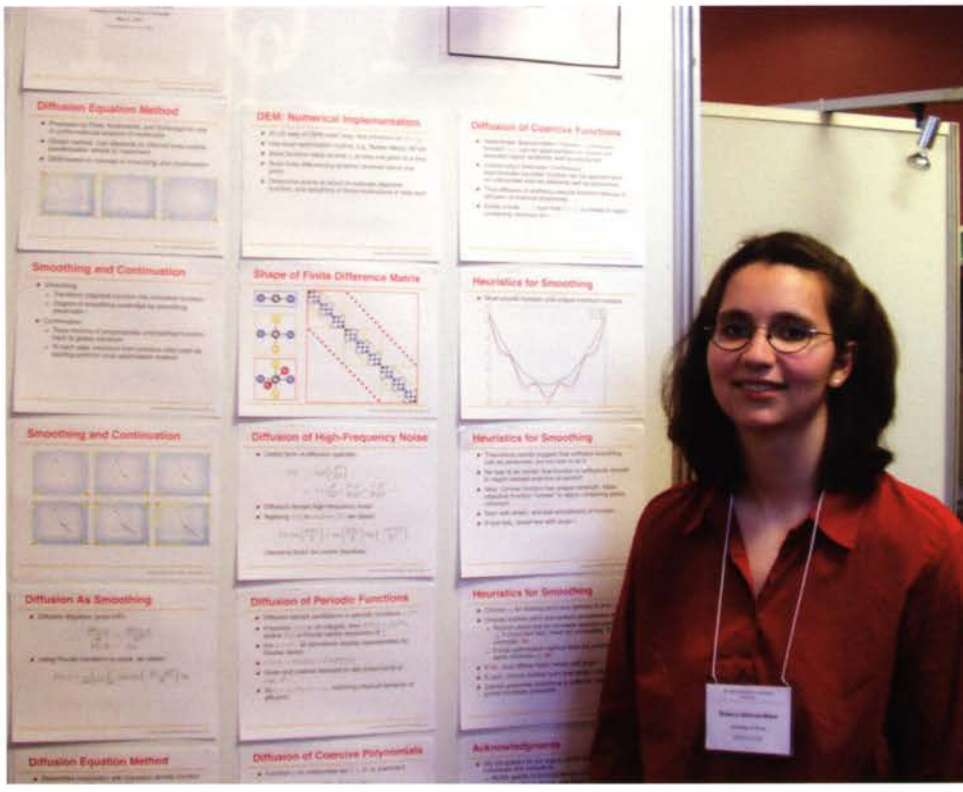
Hartman-Baker finding her way to NCSA was almost as indirect as methods of solving ill-posed problems. Her husband, who worked for the local cable company, hit it off with a customer and NCSA employee and began talking about his grad-student wife's search for a research assistantship. The employee pointed him to NCSA and particularly Sudhakar Pamidighantam, a research scientist with the center's consulting group. She ended up spending a year in the position developing GridChem, a portal for those using computational chemistry codes on resources like the TeraGrid.

"That was the best job I ever had," she says. "I studied physics [as an undergrad] and didn't know anything about CS. It forced me to learn things I was afraid of, like MPI [a method of programming for parallel computing systems]. It made me a lot more comfortable with the sorts of things I was going to be doing."

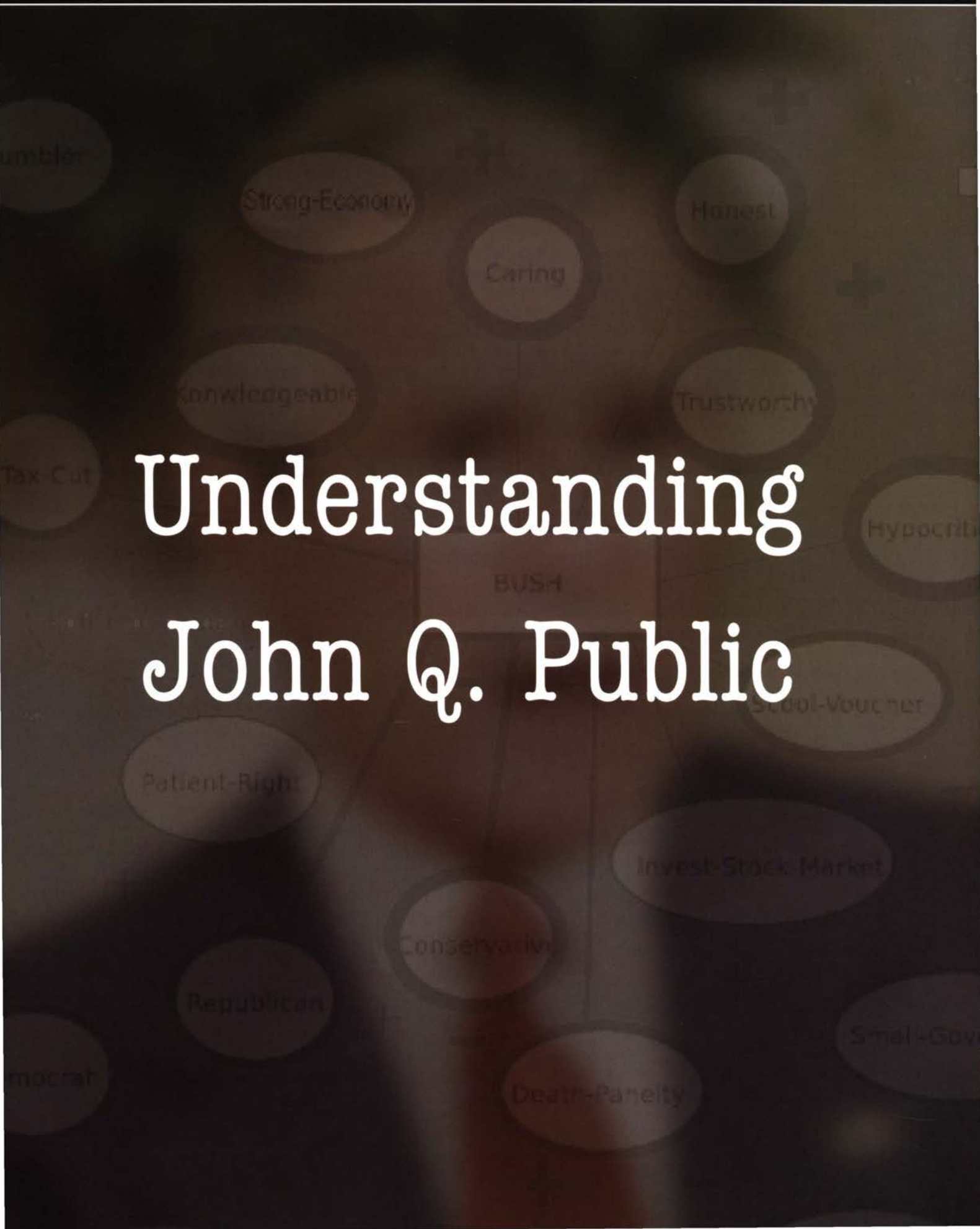
Soon after, she received—with her advisor Professor Michael Heath, a longtime NCSA user from UIUC—the first of two allocations on NCSA systems that made her thesis work possible. Having those in hand, however, didn't slow her interactions with the center.

In 2003 and 2004, she received a GK-12 fellowship through NCSA. This program teamed her with a high-school physics teacher in Hinsdale, Illinois. Working together, they devised a supercomputing project for the Hinsdale students in which they completed the structural analysis of a truss to be used in a hypothetical roller coaster. The analyses were conducted on a Linux cluster at the Office of Naval Research's Technology Research, Education, and Commercialization Center, which is administered by NCSA. More recently, she also taught a brief summer course on computing for minority students at NCSA's ACCESS Center in suburban Washington, D.C.

"Rebecca had the right background when she joined but grew into a more mature scientist through the period she spent in our group...I believe such opportunities to learn technical and other skills is what is significant at a graduate level. [They create] responsible and successful scientists in future," Pamidighantam says. "I hope this great tradition of supporting graduate students from internal resources continues for interesting projects like GridChem that benefit both the graduate students and scientific communities at large."



Rebecca Hartman-Baker.



Understanding John Q. Public

by Trish Barker

A computational model of political information processing maps fluctuations in voters' opinions during the 2000 presidential race.

In 1948, a *Chicago Tribune* front-page headline trumpeted "DEWEY DEFEATS TRUMAN," the bold capital letters incorrectly announcing the defeated challenger as the presidential victor. Many newspapers and broadcasters committed the same gaffe in 2000, when a tight race between George W. Bush and Al Gore see-sawed throughout the night of November 7.

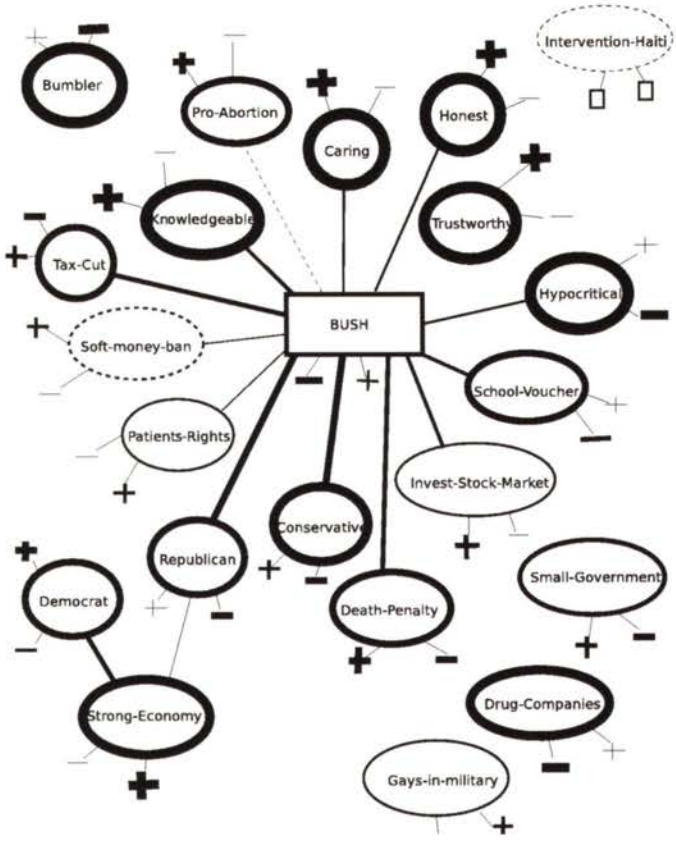
These two incidents show the pitfalls of political prognostication. Anticipating which box voters will check on Election Day and understanding how their attitudes and preferences have been shaped are complex challenges. Political scientists Sung-youn Kim, a visiting assistant professor at the University of Iowa, and Milton Lodge and Charles Taber, professors at Stony Brook University in New York, have developed a novel approach to these questions, creating a computational model that simulates the vicissitudes of political opinion. Recent calculations using TeraGrid resources at NCSA and the San Diego Supercomputer Center (SDSC) demonstrated that their model returns results that accord well with actual polling data. Their research was presented at both the 2004 Midwest Political Science Association Conference and the 2004 American Political Science Association Conference.

Integrating theories

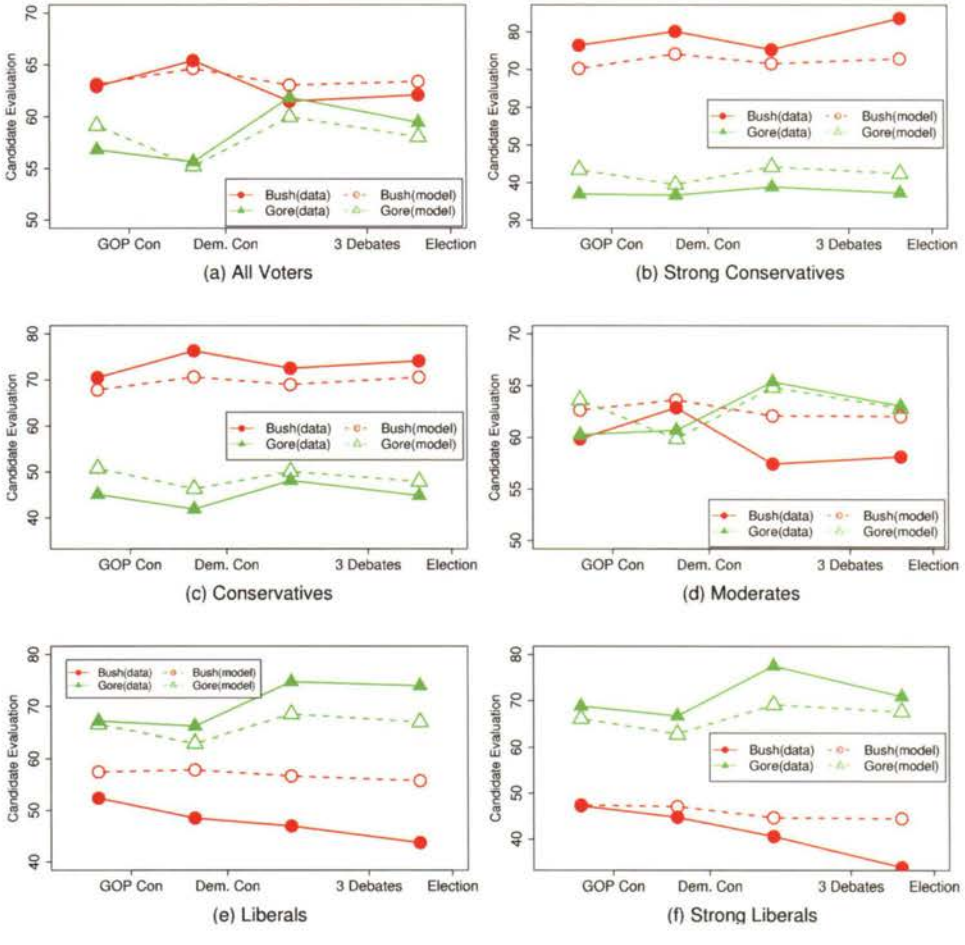
How do people assess candidates? How do campaign events and new information change their views? While there are various theories that address these questions, Kim (then a doctoral student at Stony Brook), Lodge, and Taber saw gaps between existing models and empirical findings. Several theories seemed to partially explain actual political behavior and judgment, but none seemed complete on its own.

"There are two classes of empirical evidence and theories that our model is built upon: the classic cognitive paradigm and the theories of political information processing, including the on-line processing and memory-based processing models," Kim explains. "The model is built by integrating and incorporating what these theories postulate."

Both the on-line and memory-based processing theories—theories regarding how people evaluate political objects, including candidates—were integrated into the model as its judgment mechanism. The on-line processing theory asserts that the affective summary evaluation (or valence) linked to every object in memory is updated continuously whenever an individual is exposed to new information; the individual



George W. Bush knowledge structure for an average liberal. Each oval or rectangle represents a concept node, with the thickness of its boundary representing its base-level accessibility (familiarity). The plus and minus signs attached to each node are its affective summary judgment (evaluative tag), with the size of each sign representing its strength. Each line between nodes represents a semantic association between them, with its thickness reflecting the strength of association.



Fever charts showing how the modeled candidate evaluations (dashed lines) compare to actual polling data (solid lines).

maintains a running evaluative tally for each object. Although the original information that entered into the judgment process may be forgotten, the evaluative tallies are immediately accessible. In other words, on seeing or hearing the name "George W. Bush" a person will immediately know how she feels about the candidate, even though she might not be able to say why she feels as she does.

The memory-based processing theory holds that different, often conflicting, considerations and feelings that come to mind at a particular moment influence the evaluation of an object. The accessibility of these concepts in memory determines what comes to mind and thereby influences how those concepts influence evaluation of the object. When a person is asked for his evaluation of Al Gore, for example, his answer will depend in part on which of the many facts about Gore held in his long-term memory are uppermost in his mind at the time.

Kim, Lodge, and Taber developed six algorithms to represent their amalgam of theories in a computational model. They cleverly dubbed this integrated computational model John Q. Public.

Creating virtual voters

To put the model to the test, they needed to construct virtual voters, or agents, each with a unique initial mindset that could react to campaign information according to the theories integrated into the model.

The agents were provided with the information about general concepts (honesty, determination, right, wrong, etc.) from a standard data set and with information about political objects (parties, candidates, issues, etc.) gathered from the pre-election survey of the 2000 National Annenberg Election Survey (NAES), which was conducted from November 1999 to January 2001 and was at the time the largest-ever survey of the American electorate.

The tens of thousands of NAES respondents were asked to place themselves in one of five ideological categories: strong conservative (7 percent), conservative (29 percent), moderate (41 percent), liberal (19 percent), or strong liberal (4 percent). Kim examined the responses given by members of each self-identified group before the pivotal Republican National Convention, calculating the mean and standard deviation for each group's attitudes toward the candidates, parties, issues, and their perceptions of the candidates' traits and stances on the issues. From these group profiles, Kim then generated 100 knowledge structures with random variations, each one representing the knowledge and attitudes held in long-term memory by a simulated survey respondent.

These weblike *associative semantic networks* use nodes to represent concepts or objects (such as a candidate, an issue, etc.), with the links between nodes standing in for the associative strengths (implicational beliefs) between them. Attitudes are represented by positive or negative valences attached to each node.

Processing campaign messages

The population of agents was now ready for the simulated 2000 presidential campaign to unfold. Real-world voters, of course, are inundated with political messages from newspapers, television news broadcasts, billboards, radio and TV ads, talk radio, televised debates, and personal conversations. The researchers needed to limit the information processed by the agents, however, so all campaign information was obtained from two New York newspapers, *Newsday* and *The New York Times*. News reports on five key campaign events were boiled down to simple sentences ("Bush said Gore is dishonest" and "Bush said Bush is anti-abortion," for example).

The computational model parses each sentence, retrieves relevant concepts from the long-term memory of each agent, and updates each agent's knowledge and attitudes accordingly. For example, an ideologically conservative agent begins with a positive evaluation of George W. Bush and of tax cuts. A news report on the GOP convention indicating that "Bush said Bush supports tax cut" would be "read" by the agent, which would pull its knowledge and evaluation of the object "George W. Bush" and the concept "tax cut" from its long-term memory. The positive evaluation of the tax-cut concept influences the agent's evaluation of Bush. The agent's knowledge map is updated with this new evaluation of Bush, guiding the agent's response to subsequent survey questions.

For the simulation, the 100 agents first responded to the NAES 2000 survey questions, providing a baseline akin to the responses recorded before the GOP convention. Campaign information was gleaned from newspaper reports after the GOP and Democratic conventions and after the three presidential debates. Model surveys were conducted after each event to gauge the agents' reactions. This simulation was repeated 100 times due to the model's stochastic components, which create randomized variations in how readily each agent accesses information, how strong associations are between objects in long-term memory, and how each agent interprets information.

Because the simulation employed multiple independent agents, with each one representing a single voter, each agent had to be loaded in a separate thread. Because of this complexity and the sheer computational intensity of the simulation, the researchers relied on the computational power of the TeraGrid, employing systems at both NCSA and SDSC. Using 10 processors, the simulation took about five hours and produced 10 gigabytes of output.

Comparing simulation to survey

The researchers averaged the results of the 100 simulations they conducted of the changing candidate evaluations of the 100 virtual voters. They compared these results to the fluctuations recorded by the 2000 NAES, finding a strong correlation of about .80. They also compared the simulated and actual evaluations across the five ideological groups to determine how well the simulation matched the actual distribution of candidate evaluations across the five groups, finding a correlation of .98.

There were some discrepancies between the simulation and reality, however. The simulated changes tended to be less pronounced than the fluctuations in the survey data, and in some cases the direction of change was different. For example, while actual moderate voters had a more positive evaluation of Gore after the GOP convention, the simulation showed that moderates had a more negative opinion of Gore at that time. Kim believes that incorporating additional information-processing theories will refine the model and improve the correlation between simulation and survey results.

Now that the simulation's accuracy has been demonstrated, it can be used as a platform to develop and test hypotheses. By incorporating new parameters, researchers can see how these changes affect candidate evaluations. As the model is refined further, it could even be used by political strategists to predict how the electorate will respond to information and how framing an issue or candidate can sway public opinion.

This research is supported by the National Science Foundation.

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

For further information: http://www.ic.sunysb.edu/stu/sungyoki/download/jqp-voting-manuscript-031505.pdf

Team members
Sung-youn Kim
Milton Lodge
Charles Taber

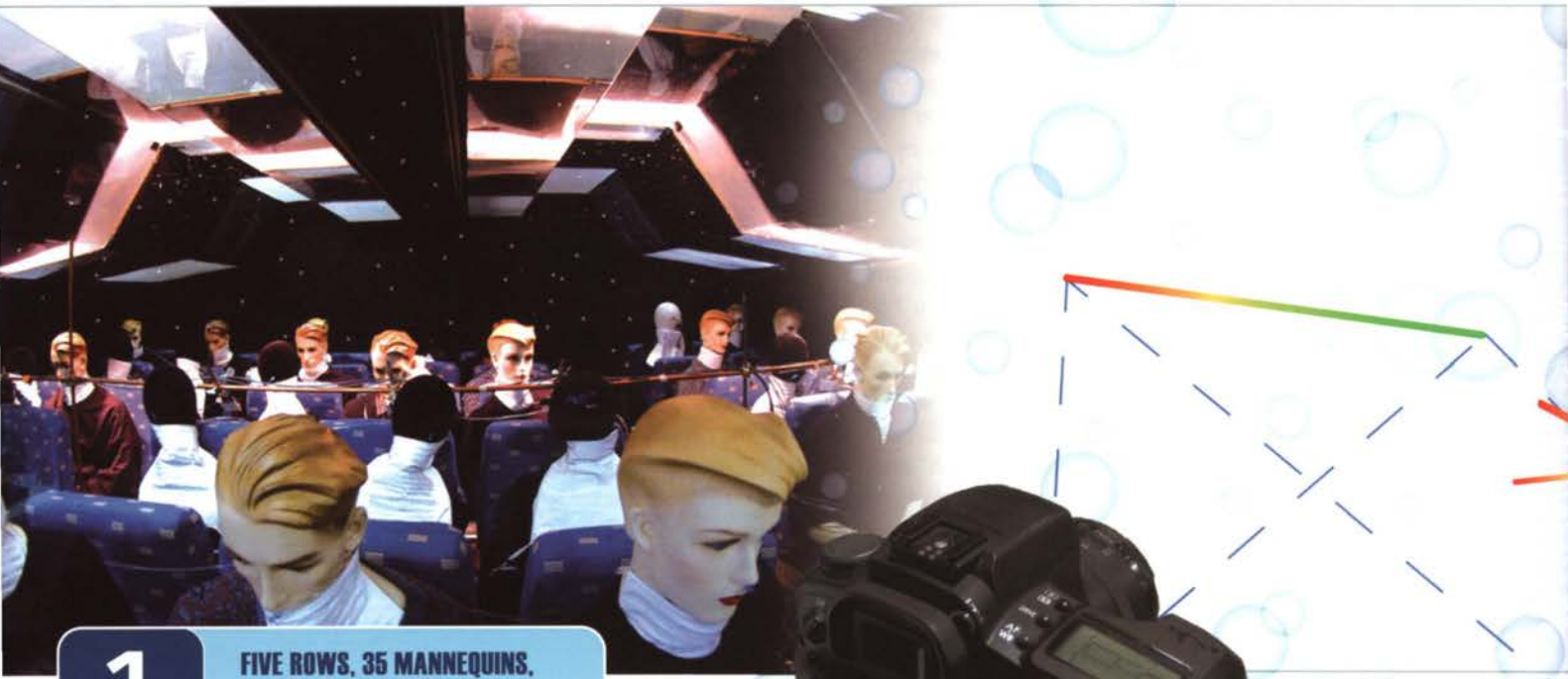
MORE THAN JUST MUSCLE

After years of using NCSA's supercomputers, Yuanhui Zhang's team works with the center's Faculty Fellows Program to get a new view of airflow in airplane cabins.

Story by J. William Bell
Infographic by Blake Harvey

Professor Yuanhui Zhang, of the University of Illinois at Urbana-Champaign's Department of Agricultural and Biological Engineering, has computed with NCSA for almost a decade. His team analyzes data from experiments that track airflow in enclosed spaces such as livestock barns and office buildings. This year the efforts expanded to include visualization of those airflows in virtual environments. Collaborating with NCSA's Alan Craig and Kalev Leetaru through the center's Faculty Fellows Program, the Zhang group tracks, analyzes, and visualizes the transportation and fate of pollutants in airplane cabins for the Centers for Disease Control and Prevention.

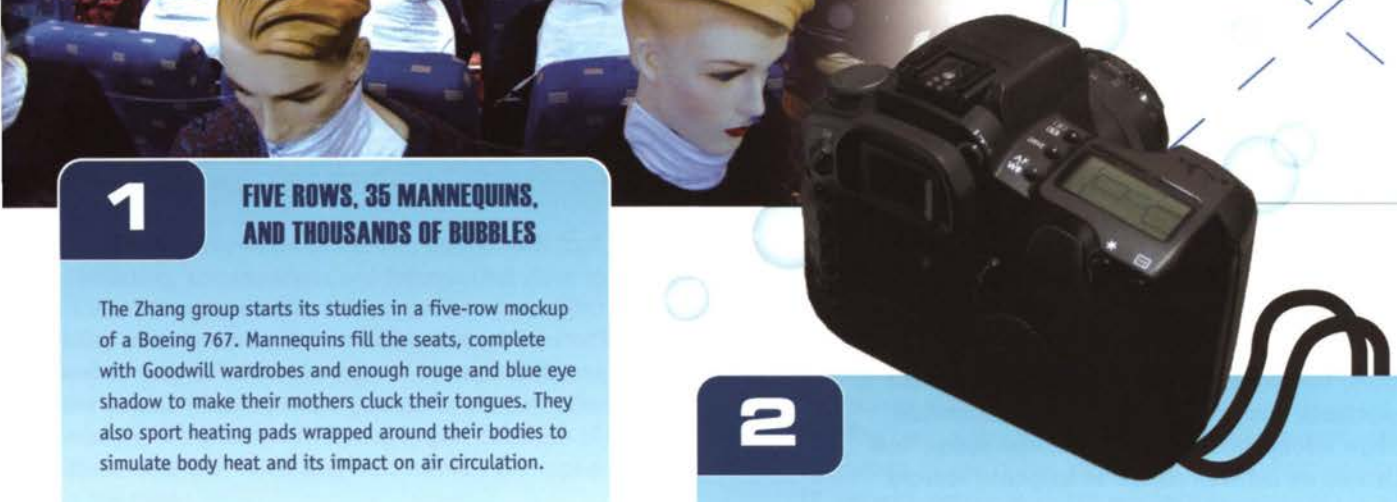
"We're very fortunate to have NCSA on our campus," Zhang says. Previously, "it's all been about the muscle" that NCSA's systems provide. That continues to be important, but "we're now getting lots of interaction. We've always wanted to have visualization to help with our public education efforts. It is an important part of our job."



1 FIVE ROWS, 35 MANNEQUINS, AND THOUSANDS OF BUBBLES

The Zhang group starts its studies in a five-row mockup of a Boeing 767. Mannequins fill the seats, complete with Goodwill wardrobes and enough rouge and blue eye shadow to make their mothers cluck their tongues. They also sport heating pads wrapped around their bodies to simulate body heat and its impact on air circulation.

Tiny helium-filled soap bubbles are pumped into the cabin. The airplane's ventilation system whirs, and the neutrally buoyant bubbles swoop about the cabin to expose the space's air currents. It "looks like a snowy room. Chaotic," Zhang says.



2 VOLUMETRIC PARTICLE TRACKING VELOCIMETRY

To hack through the chaos, Zhang and his team use what they call volumetric particle tracking velocimetry (VPTV). Two cameras at the front of the cabin take snapshots every few seconds. These snapshots record the bubbles' trajectories. By combining paired images from the two positions, the cameras allow for depth perception; 2D becomes 3D, just as it does with your own pair of eyes.

Sophisticated algorithms, developed by the team over the years and run on a succession of NCSA supercomputers, play the part of the brain. They clean the images, match individual particles from pairs of the 2D images, combine the 2D images into 3D images, and produce vector data for each bubble.

INTRODUCING SHADOWLIGHT

With vector data in hand, work with NCSA's ShadowLight begins. Previously used heavily in a faculty fellows project with the U of I architecture department's Joy Malnar, ShadowLight allows users to draw and create objects on the fly in the CAVE virtual environment. It also works in smaller-scale environments such as stereoscopic display walls.

Aijun Wang, a PhD student on Zhang's team, designed a 3D visualization of the airplane cabin's geometry in the VRML2 format on in-house machines. They are able to import and make changes to the visualization using ShadowLight, easily navigating through the space and adding new objects as necessary.

3

VECTORS NOW INCLUDED

That gives them a view of the environment, but what they really want is a view of the airflows from the vector data. Leetaru and Craig developed a plug-in for ShadowLight for those data. The vector viewer was a straightforward exercise because ShadowLight was designed to be very extensible and because Leetaru and Craig recently worked with a similar tool created by Valparaiso University as part of a collaboration with NCSA.

4

Back to reality

"Boiled down, there's never been a good quantitative way of measuring" the air's velocity and trajectory profile in a full-scale room, according to Zhang. Traditionally, anemometers or laser Doppler devices capture data at one physical point. VPTV gives researchers the massive amounts of experimental data–vectors for individual particles over time across the space–that they need. Those data allow them to develop and validate simulation software, which in turn can be used to model airflow in enclosed spaces more easily and inexpensively.

The combination of experiment and modeling allows engineers to bring their work back to reality–to model the conditions in a space, whether it's a barn or an airplane cabin, and explore methods of improving those conditions. "The fundamental information is flow patterns," Zhang says. With that, "we build a healthy, better environment for everybody."

Funding information

This research is supported by the Centers for Disease Control and Prevention, The Boeing Company, and NCSA/UIUC Faculty Fellows Program.

For further information

http://www.age.uiuc.edu/bee/

Team members

Alan Craig
Kalev Leetaru
Dongning Li
Yiangng Sun
Aijun Wang
Yuanhui Zhang

NCSA takes on Cyber Trust

NCSA's Security Research Division was recently awarded a three-year grant of $400,000 from the National Science Foundation's Cyber Trust program to support the development of tools for computer and network security.

The explosive growth of the Internet has been accompanied by growing concerns about computer and network security. Fortunately, various computer and network logs provide information and opportunities to diagnose and prevent problems. Organizations could benefit from sharing their log information with one another, but are reluctant to release such sensitive data. The capability to anonymize log information would make information-sharing more secure and would allow organizations and individuals to collaborate comfortably.

Current tools for log anonymization are primitive—they lack the ability to anonymize at different levels that correspond to the different degrees of trust between organizations. The anonymization process strips away some information that could be useful, so trade-offs must be made between anonymization and security on the one hand and information and utility on the other. Therefore, log anonymization becomes an optimization problem: How can you achieve both utility and security? The goal of NCSA's project is to create an anonymization framework that allows users to customize anonymization, creating the optimal level of security and utility for their specific needs.

NCSA will also play a key role in the University of Illinois at Urbana-Champaign's new Trustworthy Cyber Infrastructure for the Power Grid center, which is part of UIUC's Information Trust Institute and is also supported by the Cyber Trust program.

HDF spins out into non-profit corporation

The Hierarchical Data Format group has spun off from NCSA as a non-profit corporation supporting open source software and non-proprietary data formats.

The HDF Group

"This is another example of how technologies created and developed at NCSA can empower science, engineering, and business communities and can drive economic development," said NCSA Director Thom Dunning. "We're proud of what the HDF group has created at NCSA and of the plans they have for the future."

At NCSA, a team led by Mike Folk has developed and supported HDF software and file formats for the management of scientific data and other large datasets, including tools for analyzing, visualizing, and converting data, clearly defined data formats, and I/O libraries. These freely available tools are used by an estimated 2 million users in fields from environmental science to the aerospace industry and by entities including the U.S. Department of Energy, NASA, and Boeing.

The new non-profit corporation, called The HDF Group (THG) is dedicated to the sustainable development of HDF technologies and the ongoing accessibility of HDF-stored data. THG will continue to make the open-source HDF software freely available to commercial and non-commercial users. It plans to draw revenue from grants, service and development contracts, and training and support activities.

"We had no idea that that HDF would spread to nearly every country in the world and be used in hundreds of scientific, commercial, and public applications for managing huge amounts of data," says Mike Folk, who has guided HDF development at NCSA for 17 years. "Our mission at THG is to ensure that those who depend on HDF will be able to access their data for centuries into the future, and that current users of HDF have the best support we can provide."

Record allocation for Tungsten system

In the September 2005 round of allocating supercomputing time, 800 million normalized units (NUs) were meted out on supercomputing systems around the country that are supported by the National Science Foundation. This is more than the total NUs allocated in 2004's four allocation rounds combined.

More than 377 million units were made available on systems at NCSA. About 162 million units were allocated on NCSA's massive Tungsten cluster. User requests for Tungsten were almost double that number, far exceeding the number available. This made Tungsten the most requested and the most allocated system in NSF's arsenal in September.

Of the 800 million total units, more than 410 million NUs were allocated on systems supported by NSF CORE funding. The balance was on systems supported by the NSF's Extensible Terascale Facility or TeraGrid.

The Large and Medium Resource Allocation Committees (LRAC and MRAC) peer review proposals for time on these systems.

tupelo

Tupelo now available

NCSA's Digital Library Technologies group has released a new version of Tupelo, a data and metadata archiving system. Earlier versions of Tupelo were previously available as part of the NEESgrid software distribution.

Tupelo is designed to support archiving and configuration management for complex metadata objects and files. Objects and files can be created, updated, organized into semantic networks, and secured. In addition, metadata objects can be searched and retrieved based on the values of arbitrary, user-defined attributes. Tupelo supports the description of metadata ontologies in RDF-OWL and secure, remote access using Grid Services and GridFTP.

The Digital Library Technologies group is currently working with a pair of teams at NCSA and the University of Illinois at Urbana-Champaign to use Tupelo to archive molecular dynamics simulation data and digital music collections.

For information on Tupelo, go to http://tupeloproject.org/.

User wins Presidential Early Career Award

This summer Neil Kelleher received the Presidential Early Career Award for Scientists and Engineers. Kelleher is an associate chemistry professor at the University of Illinois at Urbana-Champaign and a member of the university's new Institute for Genomic Biology. Fifty-eight young researchers were honored this year.

Kelleher's research team works on a "top-down" approach to identifying and characterizing proteins, which they hope will become a more standard and widespread method for the collection and interpretation of proteomic data. To analyze the large amount of mass-spectrometric data produced by this approach, they used supercomputing resources supported by the National Science Foundation's Partnerships for Advanced Computational Infrastructure program. NCSA's Ian Brooks helped them port the analysis code and get it up and running. With new, larger mass spectrometers coming to the U of I campus, the demands for processing yet-larger amounts of raw data are set to increase markedly as top-down mass spectrometry matures into a mainstream approach.

Kelleher's work appeared in NCSA's Access magazine in 2003: http://access.ncsa.uiuc.edu/CoverStories/topdown/.

The Kelleher team in 2003.

NSF awards new TeraGrid funds

The National Science Foundation has made a five-year, $150 million award to operate and enhance the TeraGrid. As a provider of significant TeraGrid resources and leadership, the NCSA will receive more than $14 million of this award.

TeraGrid—built over the past four years—is the world's largest, most comprehensive distributed cyberinfrastructure for open scientific research. Through high-performance network connections, TeraGrid integrates high-performance computers, data resources and tools, and high-end experimental facilities, making these resources accessible to researchers and educators across the country to accelerate advances in science and engineering.

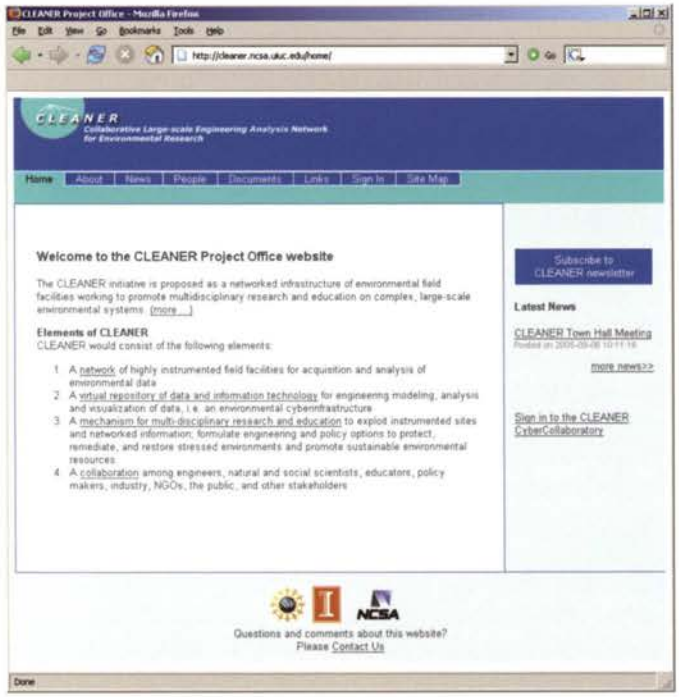
NCSA offers TeraGrid users access to two high-performance computing systems, Mercury and Cobalt, that together provide more than 16 teraflops of computing power. The center also contributes personnel to coordinate TeraGrid development and production services, to maintain and support the computational resources provided at NCSA, to assist users, and to enhance and advance the usability and utility of the TeraGrid. A special focus of NCSA's user support is partnership with TeraGrid scientific communities to architect high-end database solutions on NCSA's SGI database server, Charon, running Oracle 10g.

TeraGrid™

NCSA technologies that have been incorporated into the TeraGrid include: the account management software AMIE; CluMon, a tool to facilitate cluster monitoring; MyProxy, which allows users to manage grid credentials; VMI, a middleware communication layer; UberFTP, an interactive GridFTP file transfer client; POPS, which enables proposal submission, review, and administration; and a ticketing system that provides a standard, easy-to-use method for reporting and responding to problems.

For more information about TeraGrid, please see http://www.teragrid.org/.

NCSA leads CLEANER project office



NCSA will lead a two-year intensive effort to develop a roadmap for CLEANER, the Collaborative Large-scale Engineering Analysis Network for Environmental Research. The goal of CLEANER is to transform and advance the scientific and engineering knowledge base in order to address the challenges of complex, large-scale, human-stressed environmental systems, such as managing and protecting our nation's water supplies, restoring altered ecosystems, preserving endangered species, and tracking harmful agents. The vision for CLEANER includes multiple distributed, networked sites where sensors and instruments will gather data, as well as cyberinfrastructure for sharing, storing, managing, analyzing, mining, visualizing, and drawing fresh insights from that data.

Over the next two years, the CLEANER project office will coordinate planning efforts, including refining the key science questions and grand challenges to be tackled by CLEANER, developing a unified vision for the facilities and sensor technology required, understanding the cyberinfrastructure requirements, determining how social scientists and economists can be involved in CLEANER, and outlining strategies for the educational component of CLEANER at the K-12, undergraduate, and graduate levels.

"This project is immensely important to the national environmental research community," said Barbara Minsker, a co-director of the CLEANER project office and also the leader of NCSA's Environmental Engineering, Science, and Hydrology group and an associate professor of Civil and Environmental Engineering at UIUC. "We will be defining a research and education agenda and supportive infrastructure that have the potential to dramatically advance our understanding of complex environmental systems."

Partner institutions include Carnegie Mellon University, Drexel University, Duke University, Howard University, Humboldt State University, Rensselaer Polytechnic Institute, Resources for the Future, Texas A&M University, the University of California, the University of Iowa, and the University of Michigan.

Berkeley Lab and NCSA build Geophys

Members of NCSA's expert cluster computing staff recently traveled to Lawrence Berkeley National Laboratory (LBNL) to help the Department of Energy center install a new high-performance computing cluster. When they returned to Illinois, they brought with them LBNL-developed cluster management software, Warewulf, which they will use to speed the performance of NCSA clusters.

The NCSA/LBNL team installed a Dell system—a Linux cluster of 256 Intel Xeon processors—in a six-day marathon at LBNL. Named Geophys, the system will be applied to solving large-scale geophysical problems in computational seismology and electromagnetic imaging. In 2004, NCSA installed a similar system dubbed T2.

Earlier this year, LBNL's Greg Newman had the opportunity to run his geophysics code on NCSA's T2 and was so impressed with the performance that he wanted to acquire a similar system for the Earth Sciences Division at LBNL. NCSA helped speed the process, leveraging its strong relationship with Dell, an NCSA Private Sector Partner, to work out many of the implementation details so that LBNL could essentially duplicate the T2 system on a smaller scale in a shorter amount of time.

Five In Focus

Cyberenvironments will provide a broad range of capabilities to scientists and engineers. They allow researchers to execute, monitor, and analyze simulations. To combine and search distributed databases. To extract notable features from data streams. And to interact with colleagues and information around the world all the while.

Research communities' needs will drive these cyberenvironments; it's the only way they will advance science to its next discovery. Here are five examples of NCSA community partnerships, as they work together to design the overall architecture of the cyberenvironments and prototype and deploy their necessary elements.

1. CLEANER. The Collaborative Large-scale Engineering Analysis Network for Environmental Research will create a network of instruments for the acquisition of expansive environmental data, as well as a repository for that data and the tools to analyze and visualize it, so that researchers from a variety of fields can collaborate and formulate engineering and policy options.

2. LTER. The Long Term Ecological Research program represents many different ecosystems and means of monitoring them.

3. LSST. The Large Synoptic Survey Telescope will produce about 15 terabytes of raw data a night and 130 terabytes of processed products from those data. This will produce a series of challenges in archiving and processing the resulting data and distributing it to the astronomy community that will investigate it.

4. GridChem. To serve large communities of researchers in addition to the biggest individual users, GridChem supports computational chemists who require modest, but difficult-to-obtain, resources. It also makes those resources much more accessible to experimental chemists who can benefit from easy-to-use computational tools.

5. MAEviz. MAEviz is a single interface for performing seismic loss assessment and analysis. It integrates a variety of data sources and types, so that earthquake engineers and policy makers can understand the physical, social, and economic ramifications of the next temblor.

2. A sound plan

Professor Stuart Gage of Michigan State University (MSU) believes that recording, storing, and interpreting an area's soundscape represents valuable scientific data and that long-term acoustic monitoring can tell us a lot about how an ecosystem changes over time. Since 2003 Gage and his collaborators have monitored the sounds of several locations in the U.S., including California's Santa Margarita Ecological Reserve, Michigan's Haymarsh Reserve, the W.K. Kellogg Biological Station near Kalamazoo, Michigan, and suburban residences in Okemos, Michigan, and Fort Collins, Colorado. Microphones record samples for 30 seconds every 30 minutes. The data are automatically labeled, transferred to a computer at MSU, converted to a sonogram image, and stored.

The Kellogg Biological Station in Michigan is just one of 26 sites in the National Science Foundation's Long Term Ecological Research program, which represent many different ecosystems and means of monitoring them. An LTER site in Alaska monitors the dynamics of boreal forests and how they are influenced by climate change. The Plum Island LTER site focuses on how human land-use and climate change impact the complicated foodweb in marine estuaries, while another studies the Moorea Coral Reef near Tahiti.

Working with MSU, the NSF Middleware Initiative's GRIDS Center, and the LTER Network Office, NCSA built a pilot cyberenvironment for the program around Gage's acoustic monitoring. It allows Gage and colleagues to search data files' metadata in a catalog and then move the data requested from its storage site to NCSA computational resources for listening and analysis.

The comprehensive LTER cyberenvironment that this project demonstrates would ultimately facilitate the sharing of ecological data, compute resources, sensors, and instruments, models and analytical tools, and provide a collaboration environment for the wider ecological community.

Stuart Gage with an experimental solar panel that powers a remote acoustic monitoring station.

A long way in all directions:
20 years at NCSA

NCSA opened its doors to the national scientific computing community in January 1986. Since then, the bottom line has always been helping researchers get their work done and propel science toward its next discovery. In celebration of that 20 year history, NCSA has assembled a timeline of the center, its users, and the accomplishments they've made together.

To relive these years, go to: http://www.ncsa.uiuc.edu/20years/

National Center for Supercomputing Applications
University of Illinois at Urbana-Champaign
1205 West Clark Street
Urbana, IL 61801

http://www.ncsa.uiuc.edu