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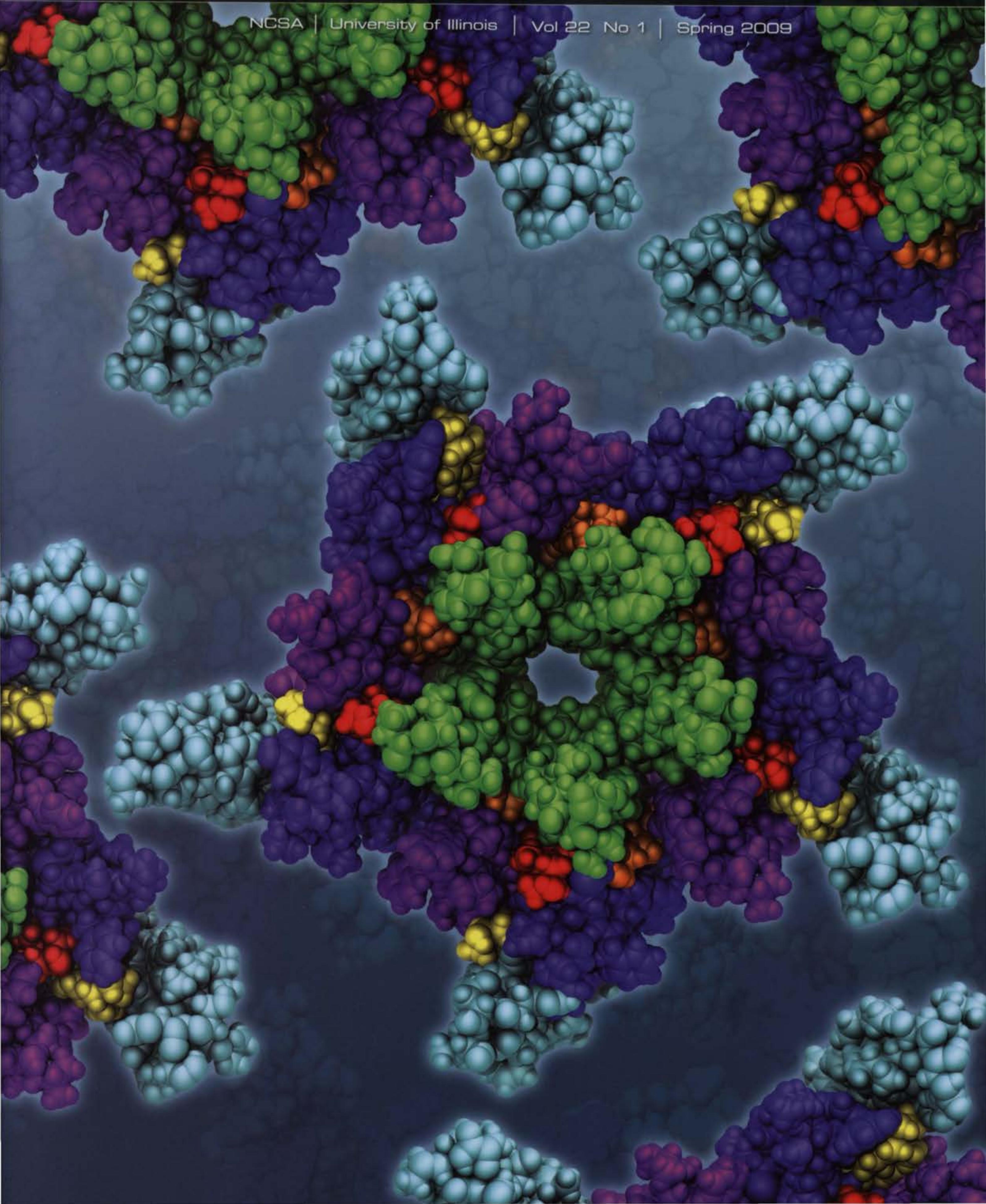

NCSA

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Vol 22 No 1 Spring 2009

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Who we are

The University of Illinois at Urbana-Champaign's National Center for Supercomputing Applications (NCSA), one of the five original centers in the National Science Foundation's Supercomputer Centers Program, opened its doors in January 1986. Over the years NCSA has contributed significantly to the birth and growth of the worldwide cyberinfrastructure for science and engineering, operating some of the world's most powerful supercomputers and developing the software infrastructure needed to efficiently use them.

That tradition continues as the center, Illinois, IBM, and their partners in the Great Lakes Consortium for Petascale Computation develop what is expected to be the first computer dedicated to open scientific research capable of sustaining more than one petaflop, or one quadrillion calculations per second. Called Blue Waters, the system will come online in 2011. It will be dedicated to massive simulations and data analysis projects that will improve our society, health, environment, and economic competitiveness. NCSA and the consortium will also work with research communities to create the new software technologies, scientific applications, and educational programs needed to take full advantage of this new system.

Blue Waters will benefit from NCSA's ongoing focus on cyberenvironments, cyber-resources, and innovative systems research. Cyberenvironments give research communities the means to fully exploit the extraordinary resources available on the internet (computing systems, data sources and stores, and tools). Cyber-resources ensure computing, data, and networking resources are available to solve the most demanding science and engineering problems and that the solutions are obtained in a timely manner. Innovative systems research involves testing and evaluating the performance of emerging computing systems for scientific and engineering applications.

NCSA also leads efforts to develop a secure national cyberinfrastructure. Through the National Center for Advanced Secure Systems Research, a project funded by the Office of Naval Research, critical cybersecurity and infrastructure needs and research requirements are addressed. In addition, NCSA is a key partner in the National Science Foundation's TeraGrid project, a $150 million effort to offer researchers remote access to some of the fastest unclassified supercomputers as well as an unparalleled array of visualization tools, application software, sensors and instruments, and mass storage devices.

The center also leaves its mark through the development of networking, visualization, storage, data management, data mining, and collaboration software. 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. Through its Private Sector Program, top researchers explore the newest hardware and software, virtual prototyping, visualization, networking, and data mining to help U.S. industries maintain a competitive edge in the global economy.

Support for NCSA is provided by the National Science Foundation, the state of Illinois, industrial partners, and other federal agencies. For more information, see www.ncsa.uiuc.edu.

On the cover

A team of researchers at the University of Pennsylvania's Center for Molecular Modeling is changing the way scientists view cholesterol in the nicotinic acetylcholine receptor (nAChR). For years, cholesterol was thought only to be in the outer membrane. Simulations conducted on NCSA's Abe demonstrated the possibility that the cholesterol, colored yellow, orange, and red, may actually bind to sites within the protein's transmembrane domain.

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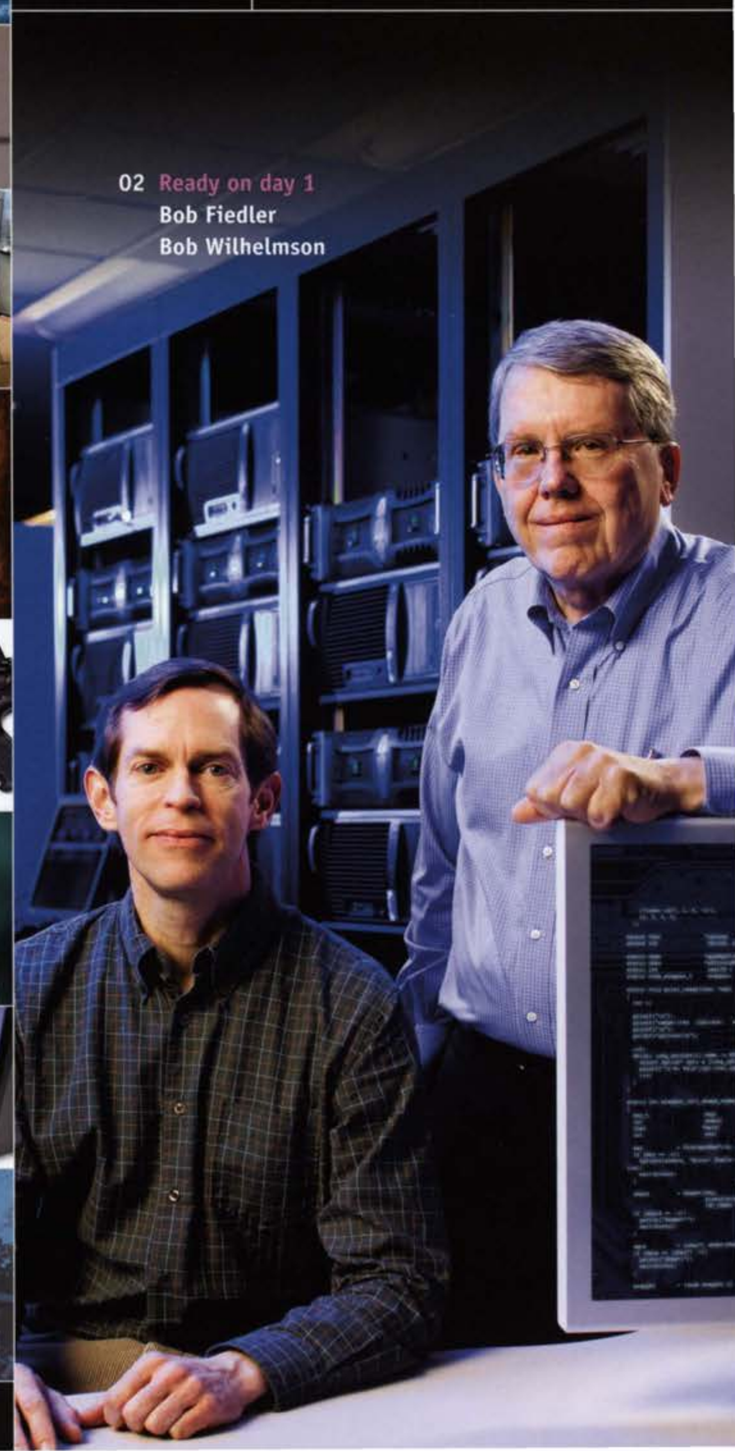
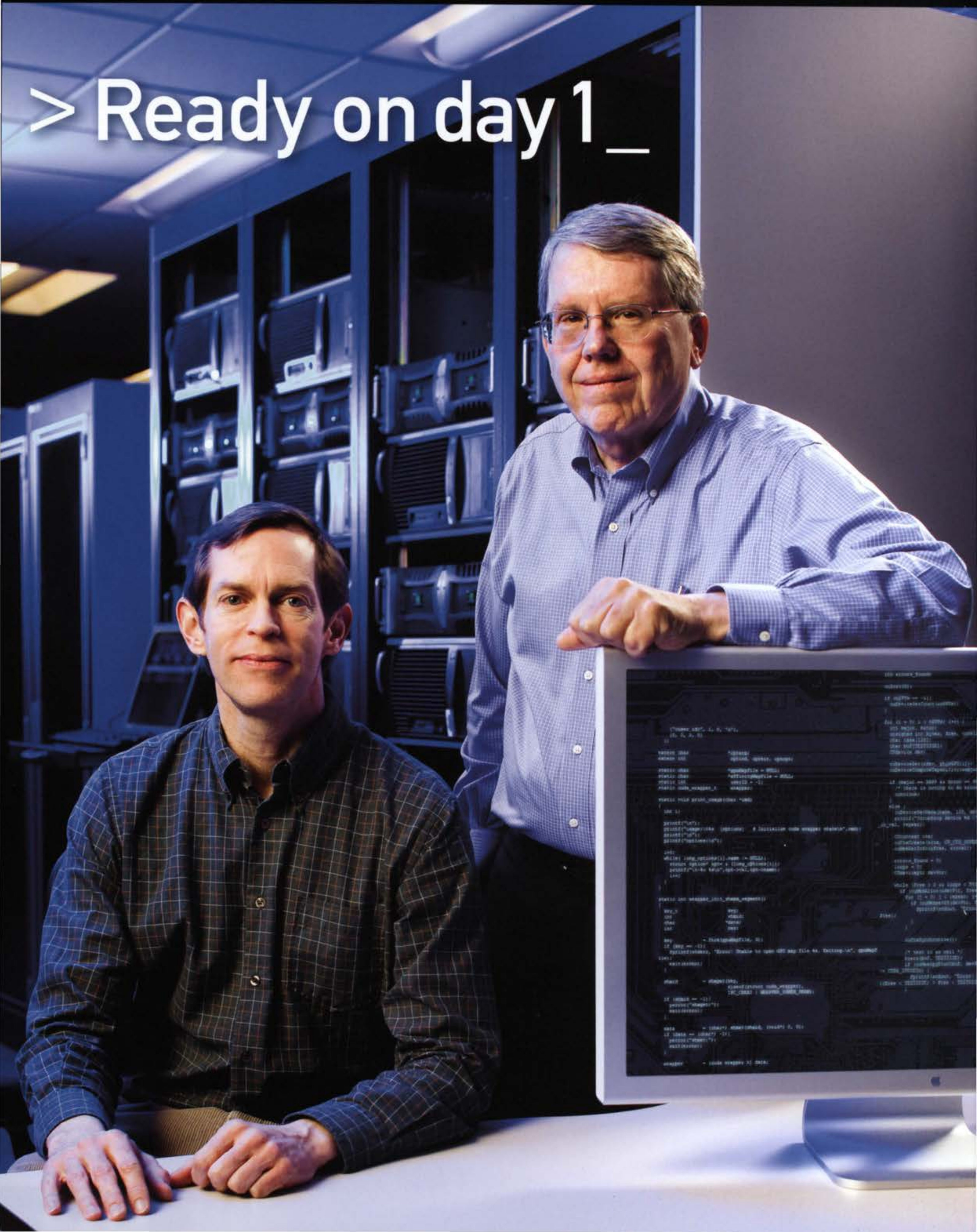


02 Ready on day 1
Bob Fiedler
Bob Wilhelmson

> Ready on day 1_



An Expert Opinion

TO ENSURE THAT scientists and engineers can achieve sustained petaflop performance on Blue Waters from day one, intensive work is under way now to port, optimize, and scale a range of applications to effectively use the system's more than 200,000 processors. Scientists and engineers who use these applications are working closely with computing experts, including staff from IBM, through Petascale Application Collaboration Teams (PACTs) to achieve this unprecedented level of performance.

The current PACTs focus on challenges in lattice quantum chromodynamics, biomolecular dynamics, and turbulent gas dynamics that were outlined by the National Science Foundation (NSF) in the solicitation that led to the Blue Waters project. You can learn more about these challenges and the current PACTs on pages 4 and 5 of this issue of *Access*. In each discipline, NSF has described a large-scale problem and specified a time to solution that represents a tremendous leap beyond today's capabilities. While we are both members of the turbulence PACT, we are also closely involved in other Blue Waters application development efforts.

Achieving the performance milestones is an intrinsic and vital part of the Blue Waters project. Our goal is not simply to build and deploy a powerful machine, it is essential for the machine and the targeted applications to work together to enable discovery and innovation.

Scaling to large numbers of processors requires techniques and approaches that are specific to each application. For example, it may be necessary to modify or change algorithms, use finer grained decomposition, eliminate replication of data structures and long critical paths, employ dynamic load balancing, etc.

To prepare the model problems for Blue Waters, they are being benchmarked on large processor counts on currently available systems with petascale peak speeds, such as the BlueGene/P at Argonne National Laboratory and the Cray XT5 at Oak Ridge National Laboratory. We are studying potential bottlenecks to scalability as they emerge, with code and algorithm modifications being implemented as needed.

In addition, the performance of modules in these codes on the level of a single Blue Waters compute node is being predicted using Mambo, IBM's application performance simulator for the POWER7 processor. Using these single-node predictions, the overall performance of applications running on the entire system, including the internodal communication network, is being estimated using BigSim, which was developed by a University of Illinois team led by computer science professor Laxmikant Kale, or using the analytical network modeling approach developed by Adolfy Hoisie and Darren Kerbyson at Los Alamos National Laboratory. In this way, we can make modifications that are needed to enable the applications to use the full capability that Blue Waters will provide when it becomes available in 2011.

While each PACT functions independently, members of the different teams also meet weekly in conjunction with performance experts from IBM to discuss issues and potential solutions. Lessons learned in optimizing one application will be applied to others as appropriate.

A solicitation is being prepared for one or two new PACTs to be formed soon, with more to follow each year, to prepare additional applications for Blue Waters. The codes on which these PACTs focus will:

- have a high potential for petascale-enabled scientific or engineering breakthroughs,
- already scale to thousands of cores,
- have the potential to effectively use the Blue Waters architecture,
- represent a broad range of science and engineering application types and algorithms,
- span a wide range of available programming models,
- have or potentially have analytic internode performance models.

If you are working on a code that fits these criteria, we welcome you to contact the Blue Waters Consulting Office: bwconsult@ncsa.uiuc.edu. □

Bob Fiedler
Blue Waters technical program manager for Science and Engineering Applications

Bob Wilhelmson
NCSA Chief Science Officer

A STIMULATING TEST OF ABILITIES

The National Science Foundation (NSF) outlined several science and engineering problems that a sustained petascale computer should address when it issued the solicitation for the machine. Blue Waters, the sustained petascale computer funded by NSF and being built at the University of Illinois through a partnership of Illinois, its National Center for Supercomputing Applications (NCSA), IBM, and the Great Lakes Consortium for Petascale Computation, will be ready on day one to focus on these problems, owing to the efforts of the Petascale Application Collaboration Teams (PACTs). These collaborative teams are working now to ensure that a range of applications can take full advantage of Blue Waters when it comes online in 2011.

Through the PACTs, scientists and engineers who use these applications are working closely with computing experts to address the specific challenges outlined by NSF, as well as other computational problems at this large scale. Lessons learned in optimizing one application will be applied to others as appropriate. Their efforts are outlined here.

PACT Information

One or two new PACTs will be formed soon, with more to follow each year, to prepare additional applications for Blue Waters. For more information on Blue Waters PACTs, please contact Bob Fiedler or the Blue Waters Consulting Office at NCSA.

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MILC Code

lattice QCD

Lattice quantum chromodynamics (QCD) is a method for studying quarks and gluons, subatomic particles that comprise some of the basic building blocks of our universe. In lattice QCD theory, physicists envision space-time as a crystalline lattice where quarks can be found only on vertices and gluons can travel only along lines connecting quarks. By simulating the evolution of the lattice system as the spacing between vertices changes, physicists hope to understand the behavior and interaction of these tiny, mysterious particles.

An application called MILC is being used to address the challenging lattice QCD problem described by NSF. MILC frequently passes many small messages and also requires frequent collective communication, during which all of the processors are communicating simultaneously. This communication load requires a network with very low latency. The lattice QCD PACT is working to increase MILC's scalability by increasing the amount of overlap between communication and computation operations. The PACT is also improving the efficiency of the conjugate gradient algorithm that is part of MILC in order to reduce the number of required iterations and will be exploring alternatives to this algorithm in order to make the code operate more efficiently.

PACT members include Greg Bauer at NCSA and Steven Gottlieb at the University of Indiana (one of the MILC developers).

NSF Challenge: Lattice-gauge QCD

A calculation in which 50 gauge configurations are generated on an 843x144 lattice with a lattice spacing of 0.06 fermi, the strange quark mass ms set to its physical value, and the light quark mass ml = 0.05* ms. The target wall-clock time for this calculation is 30 hours.

NAMD
molecular dynamics

Today's high-performance computers enable scientists to simulate systems as large as several million atoms, but this still falls short of capturing the full complexity and extended timescale of important biological processes. The NSF has outlined a molecular dynamics problem including 100 million atoms. At this level, biophysicists will be able to simulate the interactions of viruses with cell membranes and embedded proteins, ribosomes and the mechanism of protein construction, and the protein-folding problems that contribute to many diseases.

NAMD, the widely used parallel molecular dynamics program developed by Klaus Schulten's team at Illinois, is being used to solve the NSF molecular dynamics problem.

NAMD, written in C++ using the Charm++ parallel programming model, divides the computational domain into box-shaped patches, each containing varying numbers of atoms. Since the set of patches affected by pair-wise and bond interactions changes as the atoms move about, the dynamic load balancing capability of Charm++ is crucial to scalability, and improving load balancing is one focus of the NAMD PACT. The PACT is also working to overlap communication and computational work and reduce the code's memory usage.

PACT members include Sanjay Kale, Celso Mendes and Eric Bohm from the Charm++ group along with Schulten, John Stone, and Jim Phillips from the NAMD development group, all at the University of Illinois.

NSF Challenge: Molecular dynamics

Simulation of curvature-inducing protein BAR domains binding to a charged phospholipid vesicle over 10 nanoseconds simulation time under periodic boundary conditions. The vesicle, 100 nm in diameter, should consist of a mixture of dioleoylphosphatidylcholine (DOPC) and dioleoylphosphatidylserine (DOPS) at a ratio of 2:1. The entire system should consist of 100,000 lipids and 1,000 BAR domains solvated in 30 million water molecules, with NaCl also included at a concentration of 0.15 M, for a total system size of 100 million atoms. All system components should be modeled using the CHARMM27 all-atom empirical force field. The target wall-clock time for completion of the problem using NAMD with the velocity Verlet time-stepping algorithm, Langevin dynamics temperature coupling, Nose-Hoover Langevin piston pressure control, the Particle Mesh Ewald algorithm with a tolerance of 1.0e-6 for calculation of electrostatics, a short-range (van der Waals) cut-off of 12 Angstroms, and a time step of 0.002 ps, with 64-bit floating-point (or similar) arithmetic, is 25 hours. The positions, velocities, and forces of all the atoms should be saved to disk every 500 time-steps.

Pseudospectral method
turbulence

Turbulence problems are everywhere—from designing aircraft and automobiles to predicting the weather to understanding the lifecycle of a star.

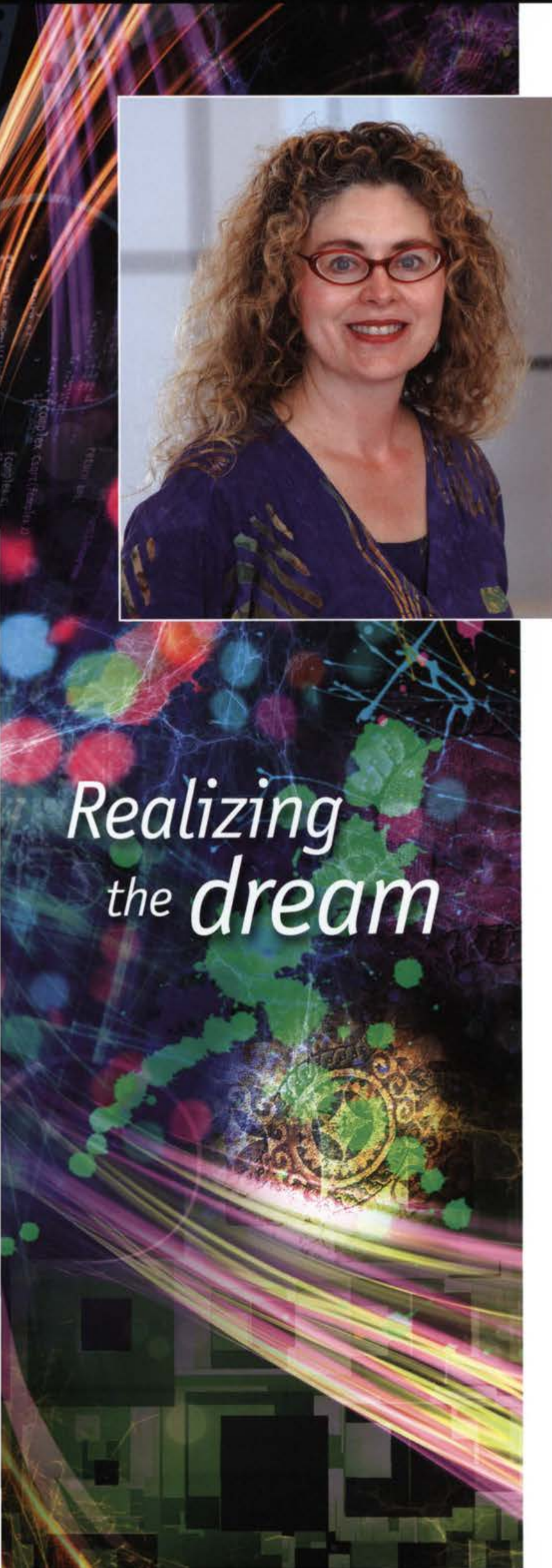
The NSF-specified turbulence problem requires the use of the pseudospectral method within a periodic box. Simulations at a higher resolution than ever used before and in this simple setting can be used to validate turbulence approximations made in other more complex simulation codes.

Various approaches and codes are being explored within the context of the specified problem, which requires over 30,000 one-dimensional Fast Fourier Transforms (FFTs) and transposes of multiple three-dimensional arrays for each of 10,000 time-steps. In addition to the need for high-performance transforms on a single core, high-performance data communication across the whole system is needed. The PACT also is looking at performance gains through overlapping FFTs and communication.

PACT members include Bob Fiedler, Bob Willhelmson, Mark Straka, Jeongnim Kim, and Jing Li at NCSA, and Adolfy Hoisie and Darren Kerbyson at Los Alamos National Laboratory.

NSF Challenge: Turbulence

A simulation of fully developed homogeneous turbulence in a periodic domain with 12,288-cubed grid points for one eddy turnover time with turbulent Reynolds number about 2000. The problem should be solved using a dealiased pseudospectral algorithm, a fourth-order explicit Runge-Kutta time-stepping scheme, 64-bit floating-point (or similar) arithmetic, and a time-step of 0.0001 eddy turnaround times. Full-resolution snapshots of three-dimensional vorticity, velocity, and pressure fields should be saved to disk every 0.02 eddy turnaround times. The target wall-clock time for completion is 40 hours.



Realizing the dream

The University of Illinois launched a new institute that will combine arts and technology. Called *e*Dream, the institute will be headed by NCSA's Donna Cox, who leads the center's Advanced Visualization Laboratory. Access' Barbara Jewett sat down with her and Kelly Searsmith, the institute's assistant director for planning and development, to learn more about the institute and digital arts media.

Q: Tell me about *e*Dream. What is the focus of this new institute, and how did it come to be?

COX: ***e***Dream stands for Emerging Digital Research and Education in Arts Media. This new Institute will help coordinate and converge the University's diverse activities in art and technology. Years ago the University of Illinois was well ahead in art and technology innovation in a lot of areas, and we prided ourselves on being number one. We pioneered computer music, for example, in the late 50s; we hosted experimental music/visual performances here in the 60s. Then in the 80s, we pioneered the convergence of art and science through scientific visualization. In the 90s university artists innovated web-based experimental art forms. Now we see this art and technology momentum across the world, having a very large impact in the creative industries, such as design and architecture, but also in other areas such as performance and interactivity. There've been hybrid PhDs in the arts growing up, primarily in Europe, around artists exploring technology. The ***e***Dream Institute will help to harness and promote Illinois innovations in these emerging digital arts. We are one of the top universities in engineering, and we have enormous computational capacity here through NCSA—and we will leverage that potential within the digital arts media.

A few years ago, the University formed the Seedbed Initiative to explore how art and technology could be synergized on campus. ***e***Dream grew out of this campus initiative to coordinate, synergize, and support interdisciplinary art, technology, and humanities creative research and education. Over a year ago I was asked to help institutionalize the Seedbed initiative exploring digital arts media. The provost appointed an advisory committee and we developed the ***e***Dream Institute, which was approved by the Illinois Board of Higher Education in December.

Q: Why all the interest in digital arts media?

COX: We've seen a global resurgence of what's possible with art, technology, and public engagement and outreach. An excellent example is the historic opening event of the 2008 Beijing Summer Olympics. Did you see? It was awesome! It expressed a cultural dynamic and astonished the world through its fusion of art and technology.

Illinois can also have important cultural impact by coordinating and leveraging our campus innovations in digital arts media. We will help Illinois participate in and lead a digital arts resurgence based upon our advances in technologies. Important technologies that have transformed this planet have come from this university, not the least of which is the Internet browser.

We'll help coordinate interdisciplinary activities, and help to build a whole new academic PhD in the arts and an online professional masters degree in digital arts media. We'll build upon our strengths and transfer this technology and this knowledge to upcoming generations.

Questions & Answers

Q: Is *e*Dream officially operating?

COX: We have five years to become self-funding and establish these degrees. And of course, we're taking this challenge on in some of the worst financial times we've ever experienced! But you know, Abraham Lincoln funded land-grant universities in the climate of the Civil War, and sometimes it takes those kinds of beliefs and passions to move forward in formidable times. The payoff will be great. Creative arts can come together with technology on this campus and create transformative public engagement. There are transformative technologies we've engendered at the university and at NCSA, and we know there's more transformation to be done.

SEARSMITH: The arts have traditionally been thought of as something that happens in a high cultural environment, like galleries or inside venues made for high culture. But there is a kind of ubiquitous art too, the idea of cultural informatics that breaks down the "boxing" of high art and makes it part of everyday life. So interested in the kind of art that's on the Internet, or impacting people on their cell phones, as well as things that take place in traditional arts venues.

Q: In tough economic times, some question the value of the arts.

COX: Art permeates and enriches our lives and has huge economic impact. The National Research Council released a report in 2003, "Beyond Productivity: Information Technology, Innovation, and Creativity," which noted that the creative industries—such as movie making, gaming, design, music, Internet, television, architecture, and advanced visualization—produce major economic opportunity wherever they thrive. They generate a massive global and cultural impact. At this time, creativity is a critical component in our university's strategic planning, as art, science, and technology are synergizing to drive the creative industries. And digital arts media now dominates the creative industries.

SEARSMITH: Times of crisis are also times when people are trying to reassess how they live and what their purposes are, and the arts is a cultural space that people turn to for that expression, for alternatives, to mainstream solutions. And one of the exciting things about digital arts media is that they are so participatory, they allow for more interaction and expression back.

Q: You've mentioned students and campus collaborations to develop public engagement—are those the target groups?

COX: And the community. I've had meetings with businesses, and business leaders, and various organizations in the community.

SEARSMITH: We're hoping to connect also with the national and international community. We're going to sponsor a biennial festival and symposium in digital arts media, bring in visiting scholars and artists, and take those communities we're engaging and hook them up with others across the U.S. and Europe who are doing these things as well, both audiences and practitioners.

Q: Back to education. When and how will that degree commence? And how many students?

COX: Through The Cyprus Institute we are already starting down this path, and we'll share some graduate students in the fall. We're putting together a new concentration of existing courses that students can remap to their current major; their degree would come out of an existing college, but they could take cross-college courses that would enable them to walk away with a concentration.

SEARSMITH: Creative media is a big draw within the arts. But there isn't enough of an applications focus on campus. Students who want to do creative work with an aesthetic technology, that's very much applications driven. One of the things that ***e***Dream hopes to do is partner with our local community college, Parkland, which is very interested in creating creative industries careers for their students. They have applications and technology focuses that benefit us, and they realize their students also need some of the research resources and research focus and the intellectual resources that Illinois has. We're hoping to create an undergraduate degree track that will be very complementary and use these community strengths to produce students who are competitive with those coming out of schools on the east and west coasts. And Donna is very committed to using all the industry contacts she has to lead to internship opportunities for these students.

COX: We will really try to give students the opportunity to work on creative productions such as a movie or digital gaming. The kinds of things that we do in our cinematic scientific visualizations have application in areas of special effects, as part of digital arts media education. The digital technologies designers and creative practitioners will learn here will be applicable in a lot of different disciplines, and some of these economic opportunities are emerging today.

The PhD in the arts is relatively new. Even big arts universities like UCLA do not have a PhD in the digital arts yet, although there is work to establish one there. There are design doctorates that have been offered in the U.S., but it's not exactly the same kind of focus we're talking of, which is really a very cross arts-humanities kind of PhD with a strong theoretical focus. For students who do want to stay in academia, having a PhD in arts informatics is going to be very important to them in the future—to get grants, to do research, and to publish.

It's all about perception. When people think of the arts, they think East Coast or West Coast. Illinois is passed over; we're not on the map. Maybe the Art Institute of Chicago, but that's private, not a state-funded, land-grant university. Forming ***e***Dream makes sense. Illinois may not be considered a coastal art mecca, but we are a tour de force in transformative innovation that will infuse our research and educational efforts in digital arts media. □

*e*Dream will officially launch on April 20, 2009, with a reception at the Krannert Center for Performing Arts on the University of Illinois campus at 5:30-7pm. This coincides with the Humanities, Arts, Science, and Technology Advanced Collaboratory (HASTAC) conference being held on campus April 19-21.

THEY LOVE A CHALLENGE

By J. William Bell

University of Illinois engineers use NCSA resources to score in an international data retrieval competition and to advance automatic speech and video recognition.

APPARENTLY, MARK HASEGAWA-JOHNSON and I are an object lesson in the challenges of automated speech recognition, his field of expertise. As we discuss his work, we frequently throw around the name "Barack Obama" as a phrase that might be parsed by the algorithms and software that his team creates. Just a name in the news that he can use to illustrate points to me.

We talk about the way that subunits in human speech are turned into sounds and how those sounds form words. We talk about how challenging it is to build an acoustic model of that process. And we talk about training a computer to use that model to identify words when accents vary so widely and when languages have a host of sounds that appear with varying frequency or not at all in other languages.

All the while, one of us is saying Bear-ack while the other is saying Buh-rock.

"The traditional model [for training a speech recognition system] is to provide 300 hours [of speech] exactly like what you're testing on and test it only on that. That's almost licked. You can get greater than 90 percent on a medium-sized vocabulary," Hasegawa-Johnson explains. "But if you change the conditions..."

His research team, made up of graduate students in electrical and computer engineering at the University of Illinois, works on the problems that surround those changed conditions. With colleague Tom Huang's students, they tackled the Star Challenge, a data retrieval competition hosted by Singapore's Agency for Science, Technology, and Research in October 2008.

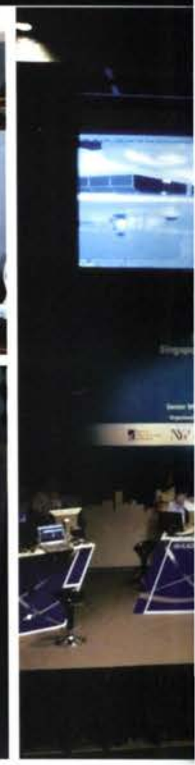
Nearly a year of planning and algorithm and software development went into the Star Challenge's three preliminary rounds and grand final, as well as nearly 50,000 hours of compute time on NCSA's recently retired Tungsten supercomputer.

Members of the Illinois team included Yuxiao Hu, Dennis Lin, Xiaodan Zhuang, Jui-Ting Huang, Xi Zhou, and Zhen Li.

The teamwork was exceptional among these electrical and computer engineering students. "My students work together but not to this extent. It was a very intense experience," Huang told *Synergy*, a publication that highlights work done by faculty at Illinois' Beckman Institute.

The challenge

The Star Challenge tested their speech and video recognition systems' abilities under conditions that varied not only in terms of accent but also in terms of language. For the final round, for example, they had to find eight 30-second snippets of video and audio in about 15 hours of footage from Singaporean television news. The footage was in English, Mandarin, Malay, and Tamil—the four official languages of the southeast Asian city-state and four languages that weren't revealed until the competition was underway.



Images courtesy of Yuxiao Hu and Dennis Lin

The team's speech recognition software considered that footage in 10 millisecond segments, comparing the segments to a dictionary of words and trying to identify snippets that matched the terms they had been tasked with finding. It also kept track of as many as 200 preceding words that it had already identified and used that information to improve the likelihood of getting a correct match. Prior words provide hints on what a word or sound might be. In a given language, particular sounds tend to follow other sounds and certain words tend to go together.

For the qualifying rounds, those comparisons meant running more than a thousand jobs at a time on Tungsten over the course of 48 hours. The team used the best algorithms it could find, using existing software and building new, developing approaches in-house and borrowing techniques developed elsewhere.

The result was a speech recognition system that is multilingual. It can search media in different languages based on the sounds that are produced instead of being focused on a single language's particulars. For the Star Challenge, the Hasegawa-Johnson team trained it in 12 languages.

The payoff

After leading throughout the qualifying rounds, the Illinois team ultimately came in third. But Hasegawa-Johnson expects that the speech recognition system built for the Star Challenge will serve as a testbed for their work for the next few years.

"Language-independent speech recognition is something we have less of a handle on," Hasegawa-Johnson says. But that's the direction his team is headed.

Language-independent speech recognition systems move researchers away from systems that are trained for a single language. This, in turn, can be used to improve the operation of systems that today are easily tricked by varying accents or noise—like automated telephone systems that ask you to say the name of the party you are trying to reach or to say "two" for Spanish.

Their work is also being applied to speech recognition software for people with disabilities. A study underway in Hasegawa-Johnson's group considers software for those with cerebral palsy, who often can't use keyboards due to the impact the condition has on their muscles and motor control and whose speech is often slurred. They're using data from 20 speakers with cerebral palsy and similar conditions, statistically modeling both the small and large impacts they can have on speakers.

By creating a dictionary of words customized to a speaker with cerebral palsy, researchers can improve the performance of contemporary speech recognition systems. One member of the study, for example, is understood only six percent of the time by a human listening to her and transcribing what she says. Using an automated speaker-independent system, accuracy drops to two percent. Using a custom dictionary, trained on her speech, accuracy rockets to 75 percent for the automated system, according to findings from the Hasegawa-Johnson team.

The problem is that custom dictionaries are expensive, time-consuming, and difficult to create. Language- and speaker-independent speech recognition systems may someday overcome that hurdle, understanding or automatically adapting to the nuances of that speech.

"We would like to make it possible to start from a speaker-independent system and adapt it gradually—or with relatively little training data—to the speech of a talker with cerebral palsy. Similar to the way that dictation software usually adapts to the speech of talkers with less unique characteristics, but using algorithms that are aware of the particular kinds of distortions that can happen in the speech of talkers with cerebral palsy," Hasegawa-Johnson says.

"It would, I think, give us the chance to improve accuracy. A lot, I hope." □

Project at a glance

Team members

Mark Hasegawa-Johnson
Yuxiao Hu
Jui-Ting Huang
Tom Huang
Heejin Kim
Zhen Li
Dennis Lin
Harsh Sharma
Xiaodan Zhuang
Xi Zhou

Funding

National Science Foundation
National Institutes of Health

More information

www.ifp.uiuc.edu/~hasegawa/
hlt.i2r.a-star.edu.sg/starchallenge/

Access online

www.ncsa.uiuc.edu/News/Stories/Challenge

A*STARing role

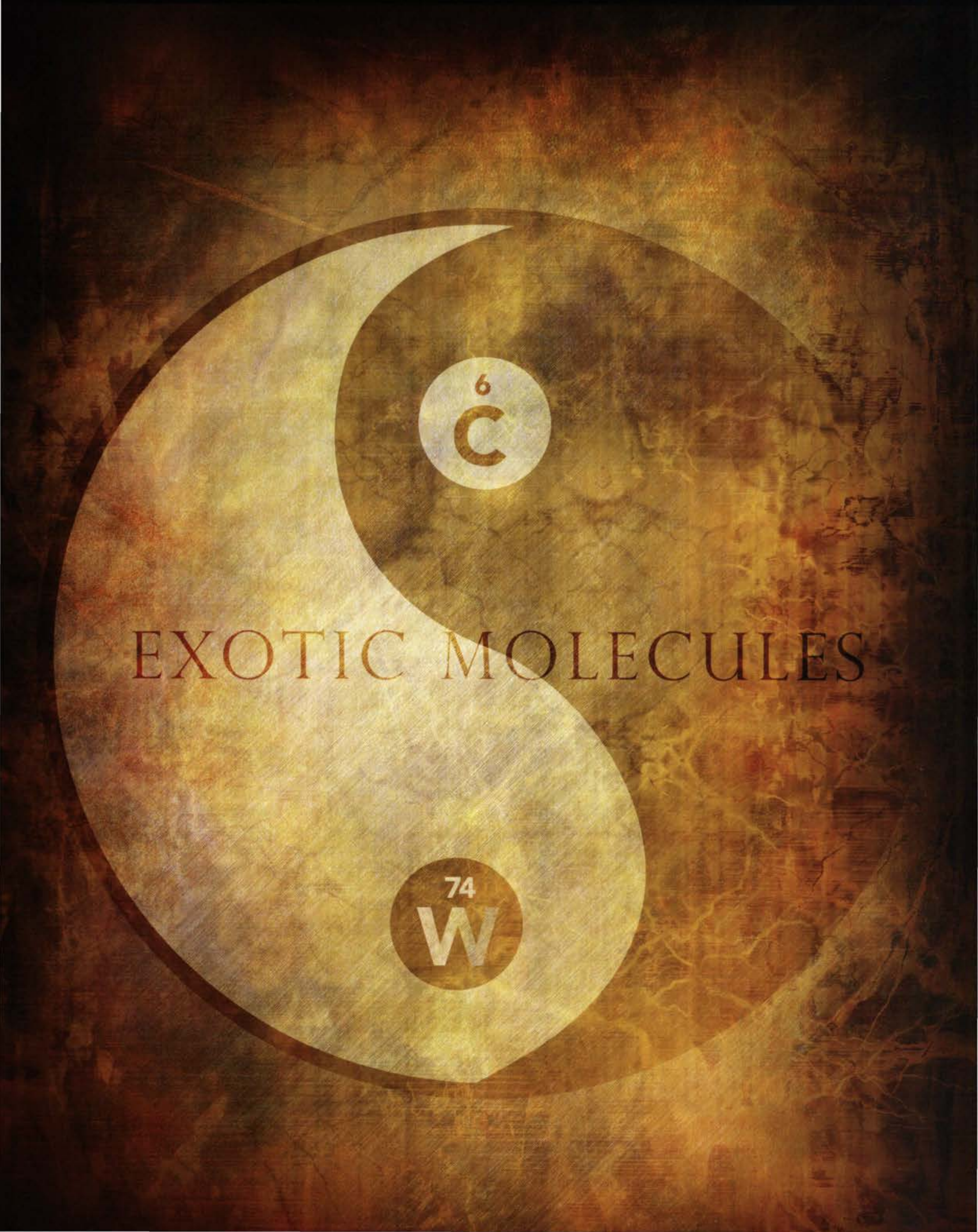
Entry into the Star Challenge isn't the University of Illinois' only connection to Singapore's Agency for Science, Technology, and Research (A*STAR). In October 2008, the university also announced that the two organizations are establishing a major research center in Singapore. The Advanced Digital Sciences Center (ADSC) will be focused on breakthrough innovations in information technology that are expected to have a major impact in transforming human beings' utilization of information technology.

The center's signature project will be the Human Sixth Sense Project—research to develop information technology infrastructure and human-machine interfaces enabling people to interact naturally with the digital world, giving them information they want, when, where, and how they need it. The Human Sixth Sense Project will be led by Illinois' College of Engineering.

A*STAR, which has research collaborations and partnerships with universities and industries worldwide, will provide $50 million of renewable funding for ADSC over the next five years.

"I'm really excited that ADSC and the Human Sixth Sense Project offer Illinois and Singapore the opportunity to work together on a problem of global significance," says Ravi Iyer, the vice chancellor for research at Illinois. "Imagine being able to provide timely, relevant and accurate multimedia information anywhere and everywhere."

— from the University of Illinois News Bureau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EXOTIC MOLECULES
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By Barbara Jewett

Understanding of the chemical bonding of many elements has been fundamentally changed by chemists at the University of Virginia, who rely on NCSA resources to verify their results.

ZAP. ZAP ZAP. Z-A-A-A-P.

That's the sound of chemist Lester Andrews and his team at work at the University of Virginia. They use a pulsed laser to create unusual, one-of-a-kind small molecules. Their work has fundamentally changed the understanding of chemical bonding in many elements, providing key insights for generations of chemists to come.

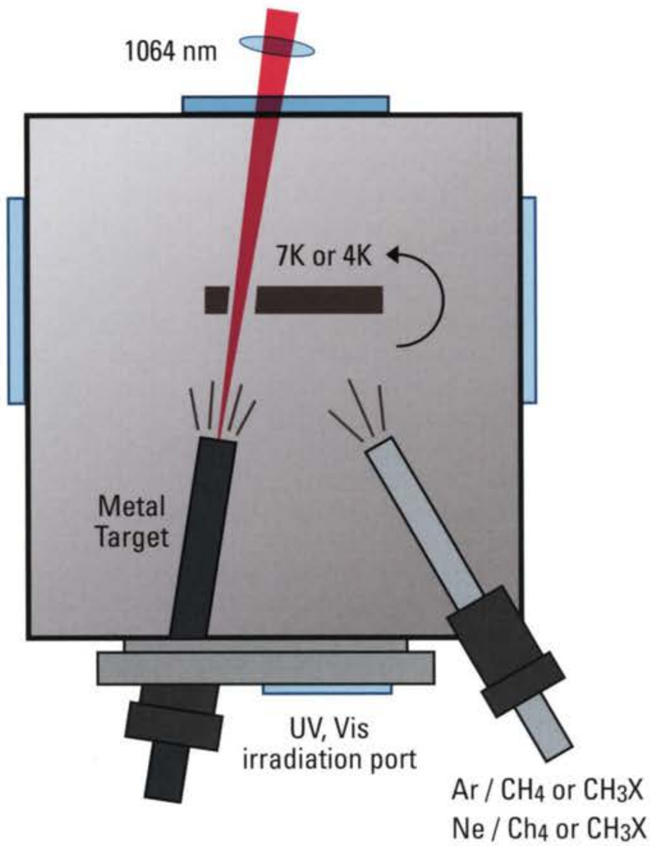
Andrews recently retired from teaching but is continuing his research. He is well known in the global chemistry community for his 40-plus years of matrix-isolation spectroscopy research, an experimental method of studying the individual molecules of chemical compounds at very low temperatures. His current work is "kind of an exotic corner" in the organometallic area, he says. Organometallic chemistry studies chemical compounds containing bonds between carbon and a metal.

Employing a method developed by Andrews and his group over the last two decades, the team uses a focused, pulsed laser to vaporize material from a solid sample and direct it toward a cryogenically cooled reaction window (four to seven degrees Kelvin) for co-deposition and reaction. Andrews notes that this method exploits two advantages of the process. First, the ablated atoms contain excess energy, which can activate reactions with small molecules. Second, collisions with matrix atoms during the condensation process relax the energetic product molecules and allow them to be trapped in the solid matrix for infrared spectroscopic study. Each chemical bond in a molecule vibrates at a frequency that is characteristic of that bond. These infrared spectroscopic studies compare vibrational energies within related chemical species, providing conclusions about the bonding in these newly observed chemical intermediates.

Andrews says the team tries "to pick things we think are going to have interesting chemical properties." During his career he has worked with every non-radioactive element in the periodic table.

Exploring the unexpected

It was an unexpected experimental result that led Andrews to his current research path. A few years ago the team reacted tungsten and methane, confident that tungsten would insert into the methane C-H bond to make a methyl metal hydride. But the reaction went



further, and transferred two more hydrogen atoms from the carbon onto the tungsten to make $HC\equiv WH_3$, which contains a carbon-tungsten triple bond. "We didn't expect this," says Andrews.

This bond is unique in that it is not supported by large ligands, just the smallest element, hydrogen; the carbon-tungsten triple bonds in the organometallic literature are stabilized by ligands or substituents. Ligands are like armour, necessary protection to shield the bond and ensure that it holds. But ligands are also extra baggage, increasing a molecule's size and weight and making it difficult for researchers to examine the molecule at precise levels.

With the unexpected creation of a simple carbon-tungsten triple bond, Andrews says the team realized they had a way to make some fairly exotic simple molecules by using appropriate laser ablated metal atoms and small molecules. Their work with small exotic molecules further advances the understanding of chemical bonding and has been published in numerous journals, including the *Journal of the American Chemical Society* in 2008 and *Organometallics* and the *Proceedings of the National Academy of Sciences* in 2007.

Verifying through computation

A significant advantage of these small, simple molecules is that their small size lends them well to computations, enabling them to be modeled at a reasonably accurate level with straightforward approximations. Over the years the team has used Cobalt and other NCSA machines and the Gaussian 03 software. Andrews says his team likes computing at NCSA because the center keeps the Gaussian 03 software supported and updated so their jobs "sail right through." Quick job processing keeps their research moving forward, as the computations are of critical importance to understanding the chemistry.

"We make molecules, we measure spectra, we try to figure out what they are, then we do calculations to model what we think we have," says Andrews, noting that when you can figure out what you've got chemically and spectroscopically before you do modeling calculations, you have a stronger scientific case. Then, of course, the case is even stronger when experiment and computation agree on the spectroscopic properties of the new molecule.

Top: A schematic diagram of the laser-ablation matrix-isolation apparatus. It is used for reacting transition-metal atoms and methane, methyl halides, or other small molecules, and trapping the products in solid argon or neon for infrared spectroscopic and photochemical investigations. The metal laser ablation target is on the left side and the cold sample window where the ablated metal atom reactions take place and the products are trapped is in the center.

Bottom: The two degenerate π bonding molecular orbitals that make up part of the triple bond, carbon-tungsten, $HC\equiv WH_3$ (left pair), and silcon-tungsten, $HSi\equiv WH_3$ (right pair), have similar shapes and bond strengths.

$HC\equiv WH_3$

"Our work is considerably stronger coupled with the calculations we do on NCSA's computer than it would be without NCSA's computer," he observes. "And obviously the theoretical community is interested in what we do, in part because of the calculations."

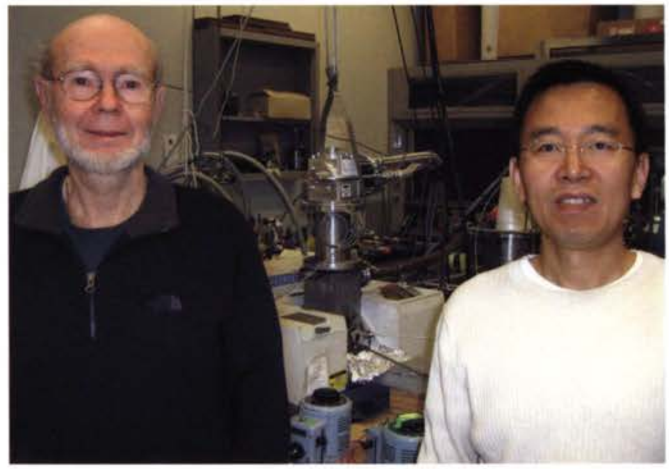
New molecular species

One of the exotic small molecules created by the Andrews team is an extension of the tungsten-methane work. "If we can make a carbon-tungsten triple bond, why not make a silicon-tungsten triple bond?" says Andrews.

So they did. Andrews said previous research by others yielded triple bonds, but they required a significant number of bulky ligands. He was able to make his molecule viable with one hydrogen atom on the silicon and three on the tungsten, which gives $HSi \equiv WH_3$ a simple molecular compound. Making the molecule in this manner, says Andrews, is the most straightforward way, but it also leaves the molecule in the most vulnerable situation. By trapping the molecule in an argon bed at seven degrees Kelvin, it can be measured spectroscopically, and its properties can be studied in detail computationally. But as the temperature warms, the molecule diffuses around and reacts with other molecules in the sample.

"The advantage of our work is that we have a very simple molecule. The disadvantage is that it is not chemically stable at room temperature and you can't play with it in a bottle in your hands," Andrews explains. "You can't use it for catalytic reactions and other things that the organometallic people like to do."

Andrews' research has transformed the fundamental understanding of chemical bonds. "Silicon is an exotic element. We have helped understand the bonds silicon makes. Somebody else might figure out a way to use that knowledge. There's where you'll get into new applications," he says. "Someone else will take it and add ligands, and they might use that on the way to making a better computer chip." □



From left to right: Lester Andrews, laser-ablation matrix-isolation apparatus, and Xuefeng Wang.

Project at a glance

Team members

Lester Andrews
Xuefeng Wang
Han-Gook Cho

Funding

National Science Foundation

More information

www.virginia.edu/chem/people/faculty/andrews

Access online

www.ncsa.uiuc.edu/News/Stories/Exotic

$HSi \equiv WH_3$

Smart searching

By Erika Strebel

To address the need for faster, more targeted searching on the Web, the Army and private companies teamed up with NCSA researchers.

THE SURFACE WEB is a vast ocean of millions of pages. People search the surface Web every day by putting keywords into search engines like Google or Yahoo! Search.

But when an Army trainer needs to quickly find information to put together a training session, a simple keyword search isn't always the most efficient way to navigate the surface Web. A search for "arms" would pull up everything from 19th century firearms to adjustable rate mortgages. A similar image search turns up a melee of pictures of octopus tentacles, family coats of arms, and human appendages. It could take hours to refine a search—hours that a trainer may not have.

To address the need for more focused, faster searching, the Army and private companies teamed up with NCSA researchers.

NCSA's Alan Craig and graduate research assistant Yunliang Liang created a Web crawling system that allows users to create a searchable database of relevant pages and websites, search within that database, and choose how to rank the results of that search. NCSA researcher Andrew Wadsworth oversaw the project and aided in designing both the search system and program user interface.

Getting started

In October 2007, the U.S. Army and Vertex Solutions, a software engineering company that specializes in training software, approached NCSA with a proposal involving the creation of an information database for an Army training software prototype called Training Assistant.

"We evaluated several universities and other not-for-profit research groups," says Vertex representative Amanda Palla. "The combination of demonstrable expertise in the area of Web crawlers, the collaborative attitude of NCSA staff, and the proximity to Vertex's Champaign office made working with NCSA an easy decision for us."

Creating the crawler

Craig had previously worked on a surface Web mining project called VIAS, a Linux-based system that automatically created databases. The Army wanted to work in Windows and Craig wanted to work with fresh technology, so the NCSA team decided to create a new system based on open-source software rather than modify VIAS.

To begin creating the database of surface Web content, a user needs to provide some keywords, keyword combinations, and several URLs as a starting point for the crawler. From there, the crawler can start searching the surface Web.

"Our goal was to present a much more focused database of information that we knew would be very pertinent to the needs of the Army trainer," says Craig.

The team started with a list of terms and URLs collected by Anna Cianciolo, researcher with Command Performance Research, Inc. She worked with Army personnel to define the key terms used to limit the database. The Army supplied websites and other examples of databases so the NCSA team could define exactly what the Army wanted.

The process of limiting the database seems straightforward, but it was one of the more difficult parts of the project. "Deciding what goes in or out of the database is a hard question," says Craig. "What goes into the database depends on who you talk to."

Eventually, they decided to create two databases: one with tighter parameters and one with looser parameters. That way, if a relevant page doesn't make it into the tighter database, the crawler will eventually find it.

The team also spent time tweaking the crawler's search functions to make sure irrelevant data didn't somehow slip into the databases. And they examined the pages within the database, looking for irrelevant pages or relevant pages not included, and determining what other terms needed to be added or excluded from the database parameters.

While the crawling system makes searching the surface Web faster and easier, it also observes online rules and etiquette. Instead of bombarding a relevant website with continuous hits, the crawler has been programmed to return to a website periodically to collect information.

"These Web crawlers need to comply to a set of rules and etiquette so it doesn't disturb any Web server out there and cause them to go crazy," Wadsworth says. "They can see what's hitting them."

In addition, the crawler works within parameters of the robot.txt file each website has. The file tells crawlers which website directories they may and may not access.

More than crawling

But the NCSA system is more than just a crawler—it also analyzes the results it produces. The crawler has its own ranking system that the user can modify. It uses special algorithms to rank results so the best results come back.

Unlike Google and other commercial search engines, the crawler allows a user to define how results are ranked. They can choose to rank results by date, relevance, key term and domain name. In the case of the Training Assistant, the crawler can place results from .mil on a higher priority than those from a .com site.

"The goal is to make it easier for the Army trainers so that they didn't have to go to Google and sift through 9 million results," says Craig.

Putting it all together

The NCSA team's Web crawler was integrated with the user interface that Vertex had designed.

Also, because the Army expressed an interest in mining the deep Web—the databases, live newsfeeds, and data hidden behind form searches that makes a large segment of the data available online—Craig suggested collaboration with Cazoodle, a software company launched by former NCSA Faculty Fellow Kevin Chang, a professor in the University of Illinois computer science department.

"Alan immediately realized, 'Why reinvent this? Let's go and see what (Cazoodle) has,'" says Wadsworth. "It was so beautiful, we couldn't ask for more."

By combining Vertex's interface with the two Web searching systems within Teaching Assistant, Army trainers using the software can copy text and images from search results of various databases within a single program.

"That's what was so golden about this, the ability to lift information right from the results," says Wadsworth.

Moreover, the different systems multitask during each search. The programs are integrated to allow various components of the Training Assistant to talk to each other and process a user's query. Thus, the Training Assistant can automatically refine a user's search and filter results.

Liang worked with Cazoodle programmer Paul Yuan to ensure that the search systems were compatible with each other and with the final Training Assistant program.

"It's not just a computer program talking to a human," says Craig. "While a human starts the process, there is a lot of integration of various systems to combine the results, rank them, and present them to the user."

Crawling in the future

While the new surface Web crawling system was specifically made for the Army's Training Assistant, Craig wants to make the system more generally accessible.

The NCSA team is working on creating a user-friendly interface for the Web crawling system. Their goal is to create an interface so researchers can easily define their database limits and ranking heuristics without having to know detailed computer programming. They also are working on creating a friendly interface for accessing the resulting databases.

"What we want to do is generalize what we've built and make it broadly applicable to different NCSA communities and a resource for other projects," says Craig. □

Project at a glance

Team members

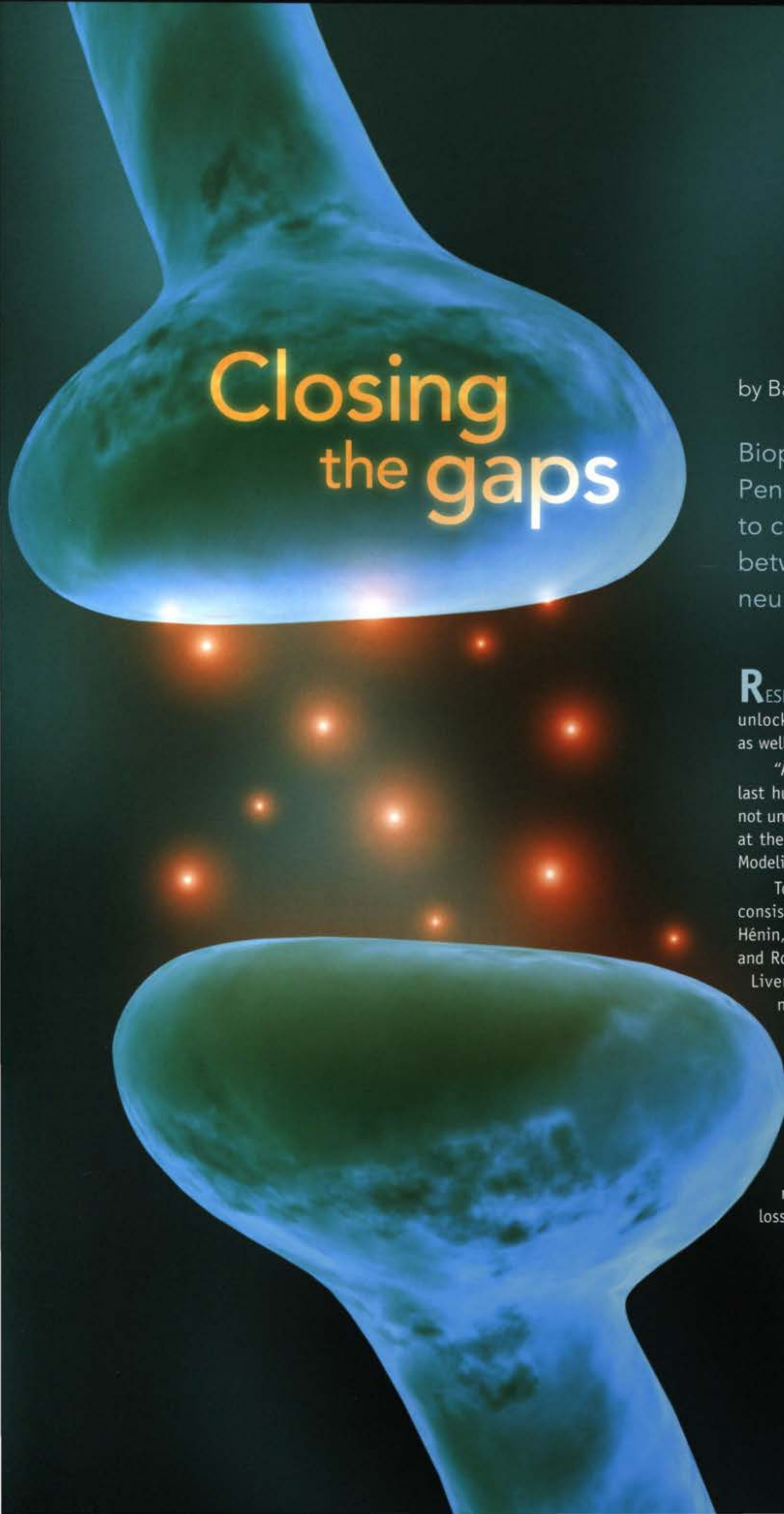
Kevin Chang
Anna T. Cianciolo
Alan Craig
Yunliang Liang
Amanda Palla
Andrew Wadsworth
Tim Wentling
Paul Yuan

Funding

United States Army

Access online

www.ncsa.uiuc.edu/News/Stories/Crawler



Closing the gaps

by Barbara Jewett

Biophysicists at the University of Pennsylvania used NCSA's Abe to clarify a mysterious interaction between cholesterol and neurotransmitter receptors.

RESEARCH INTO HOW anesthesia works may eventually unlock not only that mystery but dozens of others as well.

"Anesthetics have improved significantly over the last hundred years, but the mechanism of anesthesia is not understood at all," says Grace Brannigan, a researcher at the University of Pennsylvania's Center for Molecular Modeling (CMM).

To gain insight into how anesthetics work, a team consisting of Brannigan and fellow researcher Jérôme Hénin, University of Pennsylvania professors Michael Klein and Roderic Eckenhoff, and Richard Law of the Lawrence Livermore National Laboratory, is focusing on the nicotinic acetylcholine receptor (nAChR).

This receptor, found in both brain and muscle cells, is a ligand-gated ion channel. The channel opens or closes in response to binding with a chemical messenger (ligand) such as a neurotransmitter, like acetylcholine. When the channel is open, ions can cross the membrane. Anesthetics are believed to close the channel, thus reducing sensations and possibly causing the memory loss associated with being under general anesthetic.

Structural gaps

The basic nAChR structure consists of five protein subunits symmetrically arranged. Cryo-electron microscopy examination of the structure by British and Japanese researchers revealed more particulars about the receptor's structure than previously known, including holes (gaps) in the protein's density that were thought to hold water.

The CMM team looked at those holes, however, and realized they were the perfect size and shape for cholesterol. Knowing that cholesterol is essential for brain function, and that nAChR can only do its job properly if cholesterol is nearby, the team decided to explore the relationship between the gaps and cholesterol.

As nAChR is also involved in inflammation, Alzheimer's disease, Parkinson's disease, schizophrenia, and epilepsy, the team's findings could lead to increased understanding of these health issues as well. In addition, the team's results likely apply to closely related receptors, such as the GABA receptor. These related neurotransmitter receptors are involved in regulating mood and sleep.

Modeling the hypothesis

Since modeling and simulation is the domain of the Center for Molecular Modeling, the team directed their expertise to their hypothesis that the nAChR protein density gaps were occupied by cholesterol rather than by water.

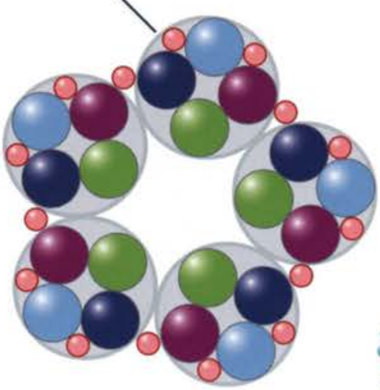
The CMM team used the basic shape of the nAChR transmembrane domain as revealed by electron microscopy (EM) structure 2BG9. Improvements in EM allow researchers to observe specimens in their native environment, affording more accurate observations and better data to use in computer modeling and simulations. The team then calculated potential binding sites (colored yellow, orange, and red in **B**) within the protein's transmembrane domain. This was done by carefully examining the receptor using advanced visualization software, identifying holes, and then relying on their chemical intuition as to where to place cholesterol, as well as using an automated docking program that found holes and inserted cholesterol.

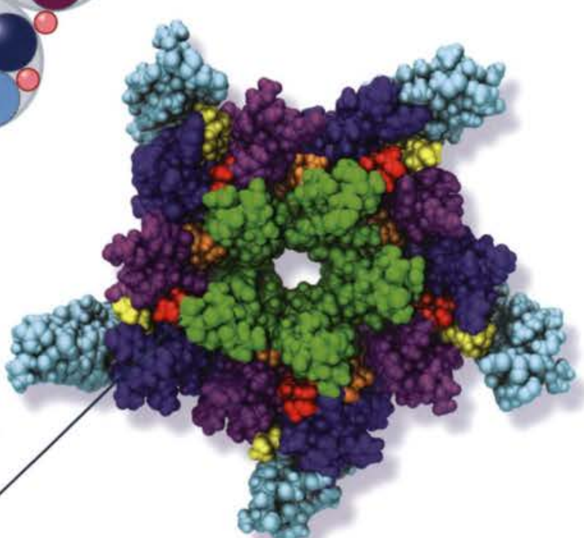
The researchers say their proposed sites for cholesterol that are colored orange and red contradict the 1993 publication of hypothetical binding sites for cholesterol for nAChR. The earlier research primarily considered cholesterol in the interface with the surrounding membrane only (**A**). This new research shows that cholesterol can be deep within nAChR.

Using the prior data, the researchers utilized the Nanoscale Molecular Dynamics (NAMD) code on NCSA's Abe cluster to test their theory. Running four simultaneous jobs requiring 800 processors each, the team simulated more than 230,000 atoms for 100 nanoseconds (**C** and **D**).

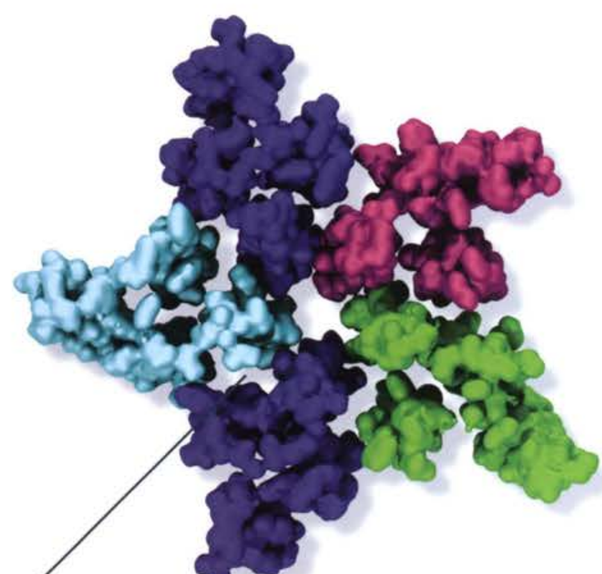
They observed that after 25 nanoseconds in the control simulation, the protein significantly redistributed its density, with gaps closing because of the collapse of individual subunits (**D**). Placing cholesterol in the gaps reduced the number of subunits collapsing.

A 1993 proposed binding sites for cholesterol (shown in red) on the surrounding membrane only.

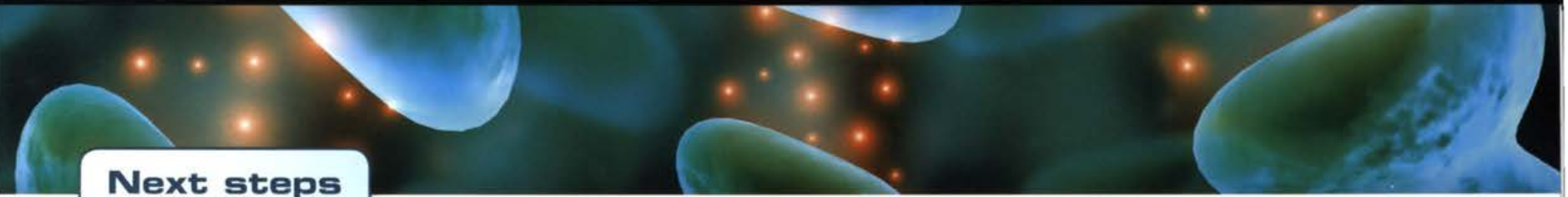




B Currently proposed cholesterol binding sites (colored yellow, orange, and red) within the protein's transmembrane domain.



C Beginning of the protein simulation showing the open gaps.

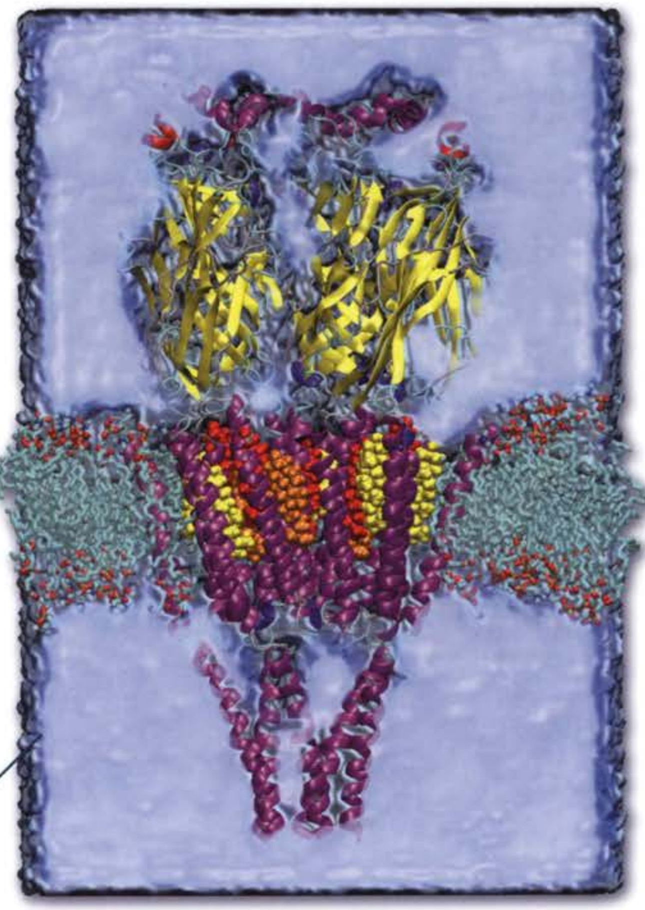


Next steps

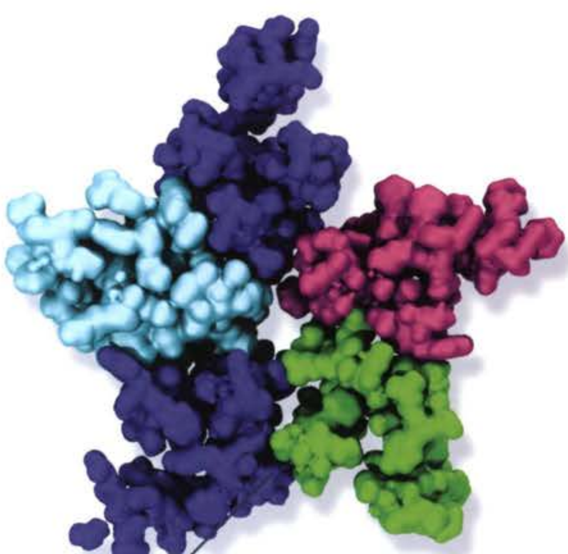
The molecular dynamics simulations supported the team's hypothesis that the published experimental structure is consistent with cholesterol molecules buried within the receptor. Their findings were published last September in the *Proceedings of the National Academy of Sciences*. Although the findings need to be confirmed by experimental researchers to become accepted scientific fact, the simulations will aid the team in the next phase of their anesthetics research.

"There are several next steps, but the most important in the framework of this project is to now actually start looking at how small anesthetic molecules are going to interact with the protein," says Hénin. "And now we know that when we do these simulations, we'll need to include cholesterol molecules at the places where we think they are interacting (**E**). We think that is going to be more of a multiple interaction. Not just a protein-anesthetic interaction, but also a protein-cholesterol-anesthetic interaction."

The researchers hope their work leads to improved drug design. "You could fine-tune the properties of the drug if you could understand how the mechanism works," says Brannigan. "For instance, by understanding how anesthetics work, you could design new anesthetics that could be more powerful yet maybe wouldn't have some of the side effects that current ones do." □



E



D

25 nanoseconds into the simulation showing the collapse of the protein's subunits due to lack of cholestrol at the binding sites.

Project at a glance

Team members

Grace Brannigan
Jérôme Hénin
Michael Klein
Roderic Eckenhoff
Richard Law

Funding

National Institutes of Health
National Science Foundation

Access online

www.ncsa.uiuc.edu/News/Stories/Gaps

BUILDING TOWARD

BLUE WATERS

NCSA has several systems that are being used as stepping stones for the sustained-petaflop system that will come online in 2011.

The Blue Waters project faces an interesting challenge: The IBM POWER7 hardware on which that sustained-petaflop supercomputer will be based doesn't exist yet. Because there is much application development work and other research to be done in preparation for Blue Waters and for other future systems, NCSA has installed four systems to help with these critical tasks. These systems are available to project team members and collaborators who are working on application enhancement, system software development, and education projects for Blue Waters.

An IBM POWER575+ cluster nicknamed BluePrint serves as a testbed where NCSA can validate the performance of compilers, the development environment, monitoring and management tools, and other elements of the software environment that IBM will provide for Blue Waters. BluePrint is composed of 120 POWER5+ nodes, each having 16 cores and 64 GB of memory. The AIX operating system is installed, with Linux to be available for specific projects.

Two IBM POWER6 systems are an important part of the development of the Blue Waters archival storage environment and are also being used as a platform for application development. In order for scientists and engineers to be able to productively use Blue Waters from day one, those researchers are working closely with computing experts to port, optimize, and scale applications to effectively use the system's more than 200,000 processors. These Petascale Application Collaboration Teams (PACTs) are using the POWER6 platform for development and testing.

Another important tool for the PACTs is the IBM system simulator environment (called Mambo). This software, which runs on an x86-compatible system, allows the Blue Waters team to simulate the performance of the POWER7 processor. This sneak peak at the Blue Waters' processor is essential to understanding how codes must be adjusted to use the architecture most effectively.

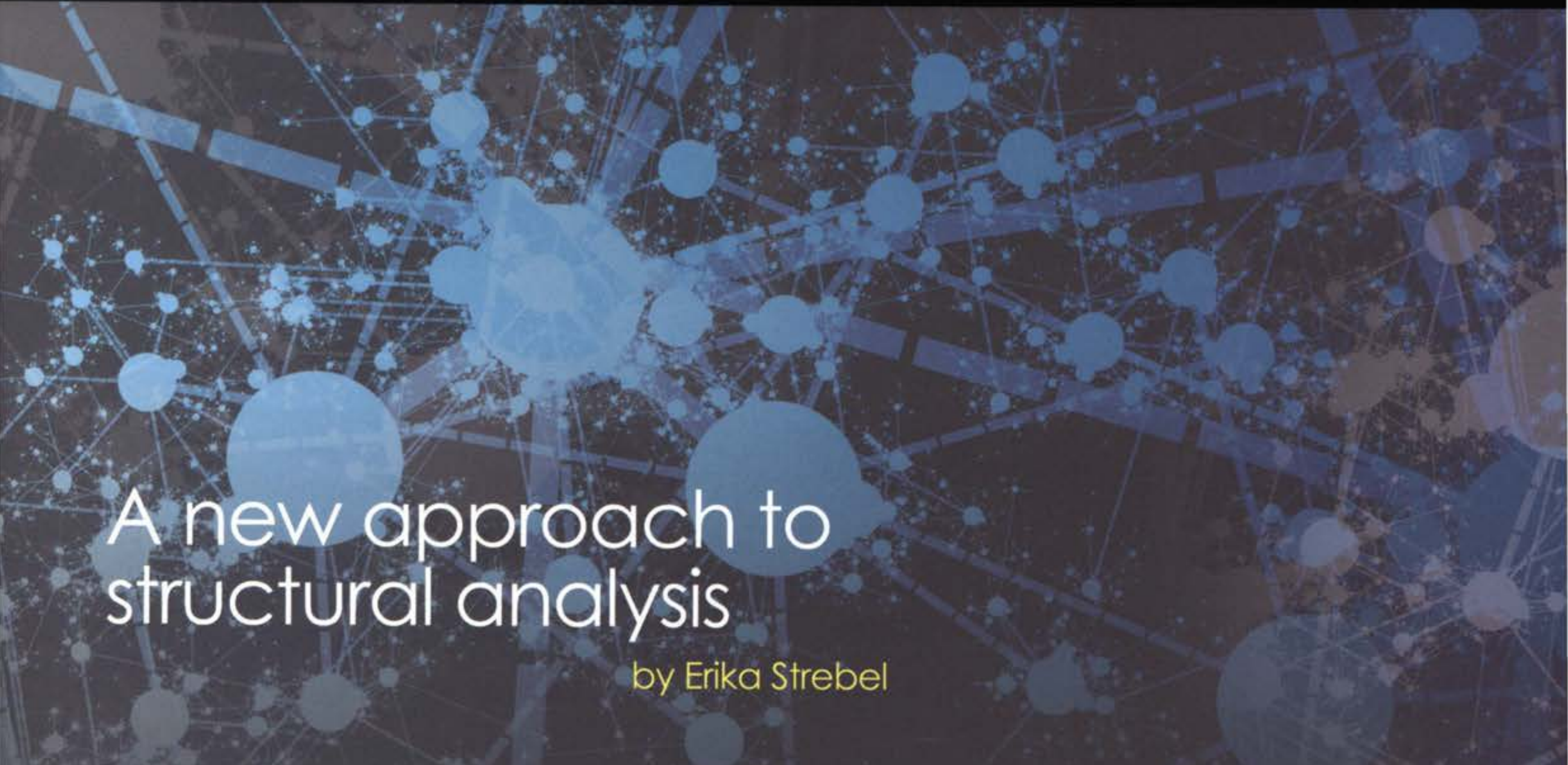
"You can see clock tick by clock tick what will happen inside the processor," says NCSA's Mike Showerman.

Details of the POWER7 architecture and the simulated performance are still confidential at this time.

NCSA's Innovative Systems Laboratory (ISL) also has an accelerator system with 16 nodes, each featuring two dual-core 2.4 GHz AMD Opterons, four NVIDIA Quadro 5600 GPUs, and one Nallatech H101-PCIX FPGA accelerator. This cluster is used for collaborative projects in which ISL staff work with scientists and engineers to adapt their applications to run more quickly on these specialized architectures, which may be a key feature of future petascale systems.

The cluster is also used for classes offered at the University of Illinois, for workshops, and for summer schools offered by the Virtual School of Computational Science and Engineering, which helps prepare the current and next generation of scientists and engineers to use leading-edge computer systems.

Work is under way to double the number of compute nodes on this development cluster. □



A new approach to structural analysis

by Erika Strebel

WHEN ENGINEERS want to build a structure like a plane or a car, they create prototypes based on existing materials and test them, making adjustments and modifications.

This trial and error method works, says Harry Hilton, "but it's a question of efficiency more than anything else."

Hilton, professor of aerospace engineering at the University of Illinois at Urbana-Champaign and NCSA's senior academic lead for structural and solid mechanics, has developed a radical approach to designing material structures. Rather than relying on existing, "off-the-shelf materials," Hilton's approach, through various calculations and equations, determines the properties of materials that would best suit a particular structure.

For example, instead of trying to create the best mouse trap based on available materials, Hilton's design analysis determines what material properties would make the best mouse trap. Present structures, says Hilton, are either overdesigned or not as good as they can be.

While Hilton's approach is formulated to analyze flight structures, it can also be used to analyze parts of structures like doorframes and wings, or even parts of wings.

Hilton's way of looking at structural analysis and design is unique in that it defines materials that have yet to exist, laying out what attributes those materials should have to produce the optimum results.

"Rather than putting in values for the materials, I'm looking for how the materials should behave," Hilton says. "It doesn't always mean you can make them. I'm leaving that to the chemists."

But Hilton's take on analysis and design does more than just calculate the properties of an ideal material. It also takes into account practical constraints engineers have when creating a structure; the formulas let a designer input variables like cost and weight.

Hilton and members of his team, including graduate students Craig Merrett and Daniel Lee, have tested the equations and formulas on a non-parallel scale, making calculations for simple structures like beams and plates, which only require a dozen or so calculations.

But Hilton is aiming for something bigger. The team is broadening the approach to encompass areas beyond structural analysis, like aerodynamics, flight stability, servo controls, and viscoelasticity. As a result, there are 600 million unknown parameters a computer would need to determine in order to define the optimum material and aerodynamic properties.

The sustained-petascale Blue Waters machine that will come online in 2011 could best handle that load of calculations, he says. Therefore, Hilton and his team are developing a theory for deploying his approach on Blue Waters. Currently, the group is not ready to test the approach on any large-scale simulators.

Over all, Hilton's approach would simplify the analysis and design process for engineers. Instead of making lots of small calculations, engineers would simply make one calculation for any given specifications. □

Project at a glance

Team members

Craig C. Merrett	Sarah E. Fullmer
Daniel H. Lee	Abdul Rahman A. El Fouly

Funding

Office of Naval Research
NASA

NCSA launches staff recognition awards program

TO RECOGNIZE and thank a few of the remarkable people behind NCSA's ongoing success, the center instituted the NCSA Employee Recognition Awards last year. The inaugural winners of these awards were honored in December 2008 for their outstanding contributions to NCSA's core mission of driving science and engineering through high-performance computing. In addition to a certificate, honorees received a $500 individual award and a $500 award for each recipient of group (up to a $2000 maximum award). The student recipient received a $250 gift certificate to the campus bookstore.

Student of the Year: August Knecht

August is a senior in computer engineering at the University of Illinois. He joined NCSA's Cybereducation group when he was a sophomore in high school. He has developed many new tools for use in NCSA education programs, and currently leads nine other interns as they work on various education projects. August is also working on an interactive website linking the LEAD portal to a set of LEAD-to-learn educational modules.

Administrative Excellence: Susan Vinson

Susan has worked in administrative support at NCSA for more than 20 years. She's recently taken on a host of new responsibilities under the Blue Waters project. Day after day, Susan projects her positive attitude and often goes beyond what is asked of her to ensure the success of the people and projects she supports.

Best team player: Jeremy Enos

Jeremy's been instrumental in bringing up the Blue Waters interim systems (see story on page 22). He also played a crucial role in transitioning Abe into a dual boot system, giving NCSA's industrial partners access to the Windows HPC Server environment at a large scale. When he's not helping the corporate partners, he's rolling up his sleeves with the academic partners, helping users of the GPU cluster avoid the time-consuming details of running an experimental system and so they can focus on their science.

Best Collaborative Effort: The MAEviz team
Team members: Terry McLaren, Shawn Hampton, Chris Navarro, Jong Lee, and Nathan Tolbert.

MAEviz is a tool NCSA and the Mid America Earthquake Center created to provide detailed predictions of the damage resulting from an earthquake. Which bridges, roads, and buildings would sustain damage, and how much? What impact would a quake have on gas, water, and electric services? How much, and for how long, would traffic be disrupted? The information is presented visually so it's intuitive to understand, easily giving planners and policymakers a comprehensive view.

Outstanding Contribution: Donna Cox

Donna has been wowing NCSA and the world for more than two decades. Visualizations and animations by Donna's team in NCSA's Advanced Visualization Lab have been nominated for Academy Awards. They've been shown on planetarium domes across the country, and on PBS, the Discovery Channel, and the National Geographic Channel. She's a true renaissance woman and, fittingly, in 2006 was named a "modern-day Leonardo da Vinci" by Chicago's Museum of Science and Industry. More recently, she's been tapped by the University of Illinois to start a new institute dedicated to research and education in the digital media arts (see story on page 6).

Outstanding Contribution: Rob Pennington

A leader in developing innovative systems, Rob led NCSA's effort to win the National Science Foundation's Track 1 competition. When Blue Waters comes online in 2011, it will be the world's most powerful supercomputer for open scientific research.

Construction begins on petascale facility

Construction of the Illinois Petascale Computing Facility on the campus of the University of Illinois at Urbana-Champaign is underway. Work on the 88,000 square foot facility began in October 2008, and was commemorated with a ceremonial groundbreaking on November 5.

Over 100 people took advantage of the unseasonably warm November day to recognize not only those involved in the building project but also the efforts of all involved in winning the nod from the National Science Foundation to build Blue Waters, the machine that will be housed in the building. Blue Waters will be the world's first sustained petascale computer for open scientific research when it comes online in 2011. Blue Waters is a joint effort of NCSA, the University of Illinois at Urbana-Champaign, IBM, and the Great Lakes Consortium for Petascale Computation.

You can follow the building's progress through the live webcam at: timelapse.ncsa.uiuc.edu

Video of the groundbreaking ceremony is available at: www.ncsa.uiuc.edu/News/Video/2008/groundbreaking.html

PSP program adds new members

A company that spun off from the University of Illinois' Center for Simulation of Advanced Rockets is the latest member of the Private Sector Program (PSP) at NCSA.

IllinoisRocstar, based in Champaign, Illinois, uses the Rocstar simulation software suite to analyze fluid flows, combustion, materials, structures, and their interactions while solving engineering and scientific problems for commercial clients and government agencies. Access to the high-performance computing systems at NCSA will enable IllinoisRocstar to perform these complex calculations more quickly and efficiently.

Waterborne Environmental, Inc., an environmental modeling and risk assessment company, also joined PSP and will collaborate with the NCSA informatics research group led by Peter Bajcsy. Bajcsy's Image Spatial Data Analysis group aims to automate information processing tasks that can be repetitive, laborious, and tedious and to build user-friendly decision-making systems that are fully or semi-automated.

Another new PSP member is Nimbis Services Inc. NCSA will collaborate with Nimbis to increase the high-performance computing capabilities and enhance the productivity of leading companies and their suppliers. Nimbis will connect its clients to the compute resources and commercial application software at NCSA, lowering the risks and effort for these companies to access high-performance computing.

NCSA's Private Sector Partner Program puts the center's expertise and technological innovation to work on the real-world challenges faced by business and industry, enabling companies to reap the benefits of early access to breakthrough technologies. NCSA's partners include Boeing, Caterpillar, John Deere, Microsoft, Motorola, Rolls-Royce, and State Farm. For more information, go to industry.ncsa.uiuc.edu, or contact Merle Giles (mgiles@ncsa.uiuc.edu or 217-244-4629).

LEAD enhances meteorology education

The Linked Environments for Atmospheric Discovery (LEAD) portal makes meteorological data, forecast models, and analysis and visualization tools available to interactively explore the weather as it evolves, from one convenient access point.

The LEAD education initiative focuses on the means to integrate data, tools, and services used by researchers into undergraduate meteorology education to provide an authentic and contextualized environment for teaching and learning. The LEAD education team designed interactive, integrated, instructional pathways within a set of learning modules (LEAD-to-Learn) to facilitate, enhance, and enable the use of the LEAD gateway in the classroom.

Educators, educational specialists, and students from meteorology and computer science backgrounds collaborated on the design and development of learning materials, as well as new tools and features, to enhance the appearance and use of the LEAD portal gateway and its underlying cyberinfrastructure in an educational setting.

Undergraduate meteorology students from Millersville University, led by Sepi Yalta, and NCSA Cybereducation computer science interns, led by Edee Wiziecki, collaborate on a regular basis across geographic locations via the Access Grid to discuss, design, and test the tools.

The development of educational materials has centered on promoting the accessibility and use of meteorological data and analysis tools through the LEAD portal by providing instructional materials, additional custom designed tools that build off of Unidata's Integrated Data Viewer, and an interactive component that takes the user through specific tasks utilizing multiple tools. This collection of materials, demonstrations, interactive guides, and customized tools available to the educator and student through the LEAD portal gateway can serve as an instructional pathway for a set of phenomenon-based exercises (e.g. fronts, lake-effect snows, etc.).

LEAD was developed through a multi-disciplinary effort involving nine institutions, including the University of Illinois and NCSA, and funded by the National Science Foundation. More information can be found at portal.leadproject.org.

IACAT hires first professor

The Institute for Advanced Computing Applications and Technologies (IACAT) at the University of Illinois is well underway, having established initial research themes and projects involving campus faculty in computer science, engineering, the sciences, the humanities, and the arts. IACAT will make the most of emerging approaches to simulation- and analysis-based research, and transfer advances from that research to the larger academic community.

A number of new faculty appointments are intended as part of IACAT's continuing growth. Recently, the first new faculty appointment was made. Athol Kemball joined the Department of Astronomy and IACAT as associate professor. His research focus is on the application of advanced computing in radio interferometry, particularly for instruments and astrophysical problems that demand computation and data processing at extreme scales. He currently leads the calibration and processing efforts within the U.S. Technology Development Project (TDP) for the Square Kilometer Array, a next-generation radio telescope with petaflop or higher computational demands. The TDP project, led by Jim Cordes of Cornell, is funded by the National Science Foundation through 2011. In his research, Kemball has also applied advanced computing to a number of other problems in astrophysics, including the theory of interferometry and image formation in radio astronomy, the study of late-type evolved stars in data-intensive observing campaigns, and the analysis of gravitational lensing.

Learn more about IACAT at: www.iacat.uiuc.edu

William Kramer joins Blue Waters team at NCSA

William Kramer has joined NCSA as a deputy project director for the Blue Waters project. Formerly general manager of the Department of Energy's National Energy Research Scientific Computing Center (NERSC), he'll assist in managing the NSF-funded project to build the world's first sustained petaflop computational system for open scientific research.

During his career, Kramer has led the acquisition, testing, and introduction of more than 20 high-performance computing and storage systems. He was instrumental in managing the paradigm shift from vector computing to massively parallel systems and was one of the primary contributors to Lawrence Berkley National Laboratory's (LBNL) Science Driven Computer Architecture initiative. He introduced project planning and metrics, negotiated multi-million dollar contracts, and led the effort to re-engineer LBNL's computer support system. Kramer was named one of HPCWire's "People to Watch" in 2005 and chaired SC05. At NASA Ames, he put the world's first UNIX supercomputer into production.

For more information on the Blue Waters project, visit: www.ncsa.uiuc.edu/BlueWaters

Workshop helps researchers prepare codes for Blue Waters

Last fall, more than 40 researchers from around the country participated in a workshop at NCSA that addressed issues researchers may face when modifying their codes for deployment on Blue Waters.

The workshop is part of a larger plan to prepare for Blue Waters before it comes online in 2011. According to Bob Wilhelmson, NCSA's chief science officer, it usually takes three to five years after the arrival of a machine for its user base to mature. But, he says, it is more practical to complete the porting or modification of codes in advance so applications are ready to run as soon as the machine is available.

The workshop addressed topics such as challenges in efficiently scaling applications, strategies for debugging, and details on IBM hardware. Speakers working on different projects shared how they solved problems relating to those topics.

Reimagining performance

THEY CURL DOWN and then up, lunging, swaying, swinging arms and legs. Others stand and watch, some drawn into what is happening before them. Then the onlookers move on, only to encounter more curling, lunging, swaying bodies around the next corner.

It's not an altercation on a busy downtown street. It's what happens when visionary artists set out to break through the imaginary "fourth wall" that separates audience members from performers.

The audience for "Dance: Re-Imagining the Proscenium" roamed from the lobby to the nooks and through the crannies of the University of Illinois' Krannert Center for the Performing Arts, ultimately finding themselves on a theater stage. Throughout the journey, dancers executed choreographed and spontaneous dances to music composed by New York-based composer James Lo. It was all part of the November 2008 modern dance performance showcasing the area's reliance on the Mahomet Aquifer that flows deep beneath the ground.

"I am interested in large phenomena like bird migration and aquifers—the systems that quietly surround us on a scale that is almost unknowable. When I knew I was coming to Illinois I started to research environmental issues and concerns, and water issues came up on my radar; there was some concern that ethanol production

Parting Shot

could have a lasting impact on water levels. As I started to learn about the aquifer I became fascinated with how vast as well as how invisible it is. I had a romantic notion of some vast underground lake with pure glacier water hundreds of thousands of years old, but as I researched it I realized how much more complex a phenomenon it is," explains the performance's creator, Illinois dance professor Jennifer Monson.

This distinctive dance experience was executed with the assistance of numerous collaborators, including some from NCSA's Advanced Visualization Lab (AVL). Jeffrey Carpenter, Robert Patterson, and Stuart Levy created visualizations like the one showing behind the dancers here. The visualization depicts a persistent ground of dark, shimmering sand perpetually in motion, evoking the opaque and porous substrates of the aquifer through which water moves and from which it is drawn. Slowly an isomorphic image of the aquifer rises and turns to open, inviting viewers to move within the exposed mystery of its negative space. Gradually a graphic representation of the aquifer resolves until it is superimposed across the three-dimensional outlines of the aquifer. The images linger only a short time until the reality of the aquifer—dense, dark, and subterranean—is reasserted. The visualizations were projected not just on the rear wall of stages and rooms, but around corners as well, surrounding and immersing the dancers and the audience, expanding their experience into new dimensions.

In creating her dances Monson is working from the systems of the body—the fluid, skeletal, and muscular systems, engaging what she calls "the imaginative state of the body" to evoke something that contains a multiplicity of potential meanings.

"By bringing the audience through the space I offered them the opportunity to understand the dance through their own kinetic, sensory experience of movement combined with the sound score and visual element," she says.

In addition to expertise of the AVL staffers, Monson collaborated with her students; fellow dance professor John Toenjes and his students; Krannert Center technicians; Cultural Computing Lab director Guy Garnett and research programmer Mary Pietrowicz; and Illinois State Water Survey scientists H. Allen Wehrmann and George Roadcap.

The performance was part of the Institute for Advanced Computing Applications and Technologies (IACAT) Creativity and Computing research theme, which is exploring, among other things, the use of new technology for creating innovative performances. □

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