On the Web

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National Center for Supercomputing Applications
University of Illinois at Urbana-Champaign
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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 past twenty 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. Today the center is recognized as an international leader in deploying robust high-performance computing resources and in working with research communities to develop the new computing and software technologies needed to take full advantage of the rapidly expanding national and international cyberinfrastructure.

The center focuses on three themes. Cyberenvironments will give research communities the means to fully exploit the extraordinary resources available on the Internet (computing systems, data sources and stores, and tools). NCSA’s cyber-resources ensure that 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. Finally, innovative systems research explores the path to petascale computing—testing and evaluating the performance of emerging computing systems for scientific and engineering applications.

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 the 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. 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.

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. For more information, see www.ncsa.uiuc.edu.

On the cover

Modeling the crystal structure of a given substance is the research focus of Julio Facelli and his team at the University of Utah. They predict structures for organic molecules that are frequently used in pharmaceuticals, fertilizers, and explosives. Shown on the cover is the comparison of the experimental and MGAC predicted (pink) structure of L-alanine.
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Merle Giles
Harnessing the power
page 04
Advances in networking and information technologies underlie most of the 10 flatteners that Thomas Friedman, in his book *The World is Flat*, asserts have leveled the playing field for 21st Century global, knowledge-based, economic competition. While the world may be flat, its landscape is not without spikes and occasional peaks—technological advances creating powerful spires of excellence for discovery, learning, and innovation and broadening participation.

Economic leaders will not only create the tallest spires of excellence, but will connect spires into effective distributed virtual organizations that assemble complementary expertise, distributed information, observatories, computational resources, and other unique facilities. Using the same “collaboratory” platforms to support not only discovery but also learning and rapid response to unexpected events will offer even further leverage and advantage.

National Science Foundation investments in cyberinfrastructure, cyber-enabled discovery and learning, and computational thinking are defining and pursuing a revolutionary vision of 21st Century discovery appropriate to leadership in a competitive, flat world with spires on its skyline. Collectively, outcomes are expected to produce paradigm shifts in our understanding of a wide range of science and engineering phenomena and socio-technical innovations that create new wealth and enhance the national quality of life.

Achieving this vision requires virtuous circles of interaction among three types of activity: 1) research, advanced development, and provisioning of shared and connecting cyberinfrastructure for supporting and bridging science and engineering, research, and learning; 2) transformative application of cyberinfrastructure to produce transformative research; and 3) identification and transfer of the relevant results of technological and social research into future generations of cyberinfrastructure.

First, cyberinfrastructure creation and provisioning are cross-foundational at NSF, but coordinated and catalyzed by an executive-level Cyberinfrastructure Council (CIC) and the Office of Cyberinfrastructure (OCI). The activities are organized around four themes: high-performance computing, data and data interaction, virtual organizations for distributed communities, and learning and workforce development. The creation of infrastructure, cyber or otherwise, is a long-term, socio-technical process to build diverse systems, nurture interoperability and consolidation among systems, build supporting institutions, conduct evaluation, and create enhancements.

Advanced cyberinfrastructure investments in leading-edge shared computational resources include the recent petascale (“Track1”) award to NCSA at the University of Illinois, and the continuing investment in interoperable computational resources (“Track2”) through the TeraGrid. The aggregate peak compute power for the Teragrid will soon be over 1.6 petaflops and is growing. Digital data are increasingly both the products of research and the starting point for new research and education activities. New investments address infrastructure for data curation, stewardship, interoperability, and interaction through a new solicitation for sustainable digital data preservation and access network partners (DataNet). Investments in cyberinfrastructure to support virtual organizations include international networking partnerships, middleware, portal, and workflow environments, as well as the practical applications of academic understanding of social architecture for collaboration in distributed teams. Learning and workforce activities address both learning about cyberinfrastructure and learning with cyberinfrastructure.

The second and third activity types—transformative application to produce transformative research and the regeneration of even more revolutionizing cyberinfrastructure—comprise the new NSF-wide initiative entitled “Cyber-enabled Discovery and Innovation” (CDI). CDI is intended to create revolutionary science and engineering research outcomes made possible by innovations and advances in cyber-enabled computational thinking. Computational thinking is comprehensively defined to encompass computational concepts, methods, models, algorithms, and tools. Applied in challenging science and engineering research and education contexts, computational thinking promises a profound impact on the nation’s ability to generate and apply new knowledge.
An Expert Opinion

In August 2007, the National Science Board approved a resolution authorizing the National Science Foundation to fund the acquisition and deployment of the world’s first sustained-petascale computing system for open scientific research at NCSA. Blue Waters, as the system is known, will be capable of sustained performance of one quadrillion calculations per second. It is expected to come online in 2011.

Blue Waters is a joint effort of the University of Illinois at Urbana-Champaign, NCSA, IBM, and the Great Lakes Consortium for Petascale Computation. This partnership is dedicated to encouraging the widespread and effective use of petascale computing to advance scientific discovery and the state-of-the-art in engineering, to increasing regional and national competitiveness, and to training tomorrow’s computational researchers and educators.

The details of the Blue Waters contract are now being finalized.

CDI seeks ambitious, transformative, multidisciplinary research proposals within or across three thematic areas: From Data to Knowledge: enhancing human cognition and generating new knowledge from a wealth of heterogeneous digital data; Understanding Complexity in Natural, Built, and Social Systems: deriving fundamental insights on systems comprising multiple interacting elements; and Building Virtual Organizations: enhancing discovery and innovation by bringing people and resources together across institutional, geographical, and cultural boundaries, perhaps in ways better than being there.

Congruent with these thematic areas, CDI projects will enable transformative discoveries that have the potential to identify patterns and structures in massive datasets; exploit computation as a means of achieving deeper understanding of natural and social systems; simulate and predict complex, stochastic or chaotic behavior; explore and model nature’s interactions, connections, complex relations, and interdependencies, scaling from sub-particles to galactic and from cellular to societal; and train future generations of scientists and engineers in the use of cyber-resources.

Creative, cyber-enabled, boundary-crossing collaborations, including those with industry and international partners, will contribute to advancing the frontiers of science and engineering, broadening participation in science, technology, engineering, and math (STEM) research, and educating an inclusive STEM workforce for the 21st Century.

Numerous community workshop and study panel reports contend that we have entered a nascent revolution through computational thinking in what, how, and who will be involved in future discovery and learning. These emerging cyber-enabled foundations will support the development of new and valuable technologies and services that will keep America globally competitive in today’s world, a goal to which NSF is fully committed.

Arden Bement
Director
National Science Foundation

Dan Atkins
Office of Cyberinfrastructure Director
National Science Foundation
Harnessing the power

NCSA’s Private Sector Program affords business and industry the opportunity to use the center’s resources. Merle Giles, director of PSP, talked with Access’ Barbara Jewett to explain how NCSA interacts with the business world.
Q: What is the Private Sector Program?
A: The Private Sector Program (PSP) is all about enabling companies to gain competitive advantage by leveraging NCSA resources.

Q: What companies can use NCSA?
A: We can work with companies of all sizes. Increasing demand for simulations means that many small companies that were using desktop computers to do their simulations now have datasets that are too large to run, so they need access to supercomputers. We have small entrepreneurial companies and we have very large companies and everything in between.

Once a company becomes a member—and that membership is simply a contract and paying a modest fee based on company size—that gets them into the house, so to speak. Then we can spend time together, dream together, talk about the opportunities—and that has value. They can talk with other business partners, hire our consultants, and access our resources. NCSA can also be a portal for them to the university. We've got many, many connections with other campus units and that is perhaps a little misunderstood or underestimated—what power this entire campus can give to a company simply by their coming to NCSA.

Q: Most of the private sector projects are proprietary, but are there any examples you can share that illustrate how you work with the PSP partners?
A: Every company will have some proprietary issues, absolutely. We are an open university, but we are set up contractually and with non-disclosure agreements to conduct business in a proprietary manner.

We have one company that uses us for consulting on code and chasing some things with the technologies that we have here and providing them some solutions, but then they run everything on their own supercomputers. There are others that use us for cycles on our machines. Another PSP partner was using eight and 16 processors on some clusters of their own. Some of these runs would take a week; they wanted to know how we could help them. We did a test, ran some code and simulations and found that sweet spot for this client in terms of number of processors, taking the run down from a week to about 10 hours. When industry is under time demands—under competitive bid situations, for instance—to be able to run a solution overnight is quite an advantage over taking a week to run it and then maybe having to run it again. So we will help this partner, and as they produce product for their clients they can be more responsive.

Simulation is also an area where we can help companies because of our computational capability. As the number of variables increase, the ability of the user to get increased fidelity grows phenomenally. For instance, if we had a simulation that involved statistical processes and sampling, the user would have to put together multiple samples to then try to extrapolate what an entire production line might look like. As computers get larger and we approach petascale computing, the ability to run more variables will mean that statistical sampling will be used less and less, and more variables will be run—could even run real time, perhaps—but also there will be huge runs with millions of variables to increase the fidelity and granularity of the results. So that will be a very exciting thing—to run an entire project without the need to rely solely on sampling. It's a huge impact to industry to be able to run a complex dataset and know exactly what an entire production would look like, and not just a piece of it. With petascale computing coming we'll have to dream even bigger and figure out how we can harness that kind of power.

Q: And isn’t that really what the PSP program is all about, helping businesses be more successful?
A: To be successful, to have quicker turnaround, ultimately to be more competitive and more profitable. But the ability to be more profitable, more competitive, can come in quicker turnaround or increased fidelity—there are two ways to really improve the product, and time to solution is one of them.

There was a fascinating article in The Wall Street Journal in July 2007 on how business has been through management-by-objective, and by TQM (total quality management), and the article claimed that it's time for the latest trend in business methodology: which is management by data. This is no surprise to NCSA partners—they've been managing by data for years.

Data drives decisions in many, many companies. The conversation I’ve had with partners is they have more data than they ever used to have and they’re trying to figure out how to analyze it. There’s valuable information in that data that may or may not change how they produce the product, but it may change how they run the business. So the very large datasets—terabytes every night that come into retail organizations, or off production lines—how does one manage that much data and get through it? Well, you do it with large computers. Data management, data mining, and data analytics are some of our strengths at NCSA. We deal with structured data, we deal with unstructured data. We have solutions for mass storage challenges, for large data sets—we have many tools and solutions we can offer.

More information: www.ncsa.uiuc.edu/AboutUs/Directorates/sp.html
Gimme structure
University of Utah researchers use parallel genetic algorithms to predict crystal structures for a variety of organic substances.

NCSA has helped Julio Facelli do his work for years, and that gives him an uncommon perspective on the impact that the center and others like it have had.

“I’ve been following [the National Science Foundation-supported centers] since the beginning,” says Facelli, “and they’ve done a tremendous job of encouraging new approaches to science. In the beginning, users were the traditional suspects. But now more and more people realize that they need computational simulation to understand their experiments. In every field, the centers have had an impact on the way people do science.

“Simulation science is becoming part of the mainstream toolkit of the experimental scientist. The NSF centers drove that.”

Facelli, director of the University of Utah’s Center for High Performance Computing and a biomedical informatics professor, uses NCSA’s Mercury cluster to predict crystal structures for organic molecules that are frequently used in pharmaceuticals, fertilizers, and explosives.

“Fifteen years ago, the drug companies wouldn’t think about talking to a guy like me,” he says. “But computational molecular science—numerical analysis—can now show them the promise of a good solution for their formulation problems.”

Supercomputing is part of the reason for this shift, but so is the method that he and his team have developed for calculating crystal structures. This method was featured in a 2007 *Journal of Chemical Theory and Computation* publication.

**Survival of the fittest**

Crystal structure refers to the identical pattern of atoms that repeats over and over to form the macroscopic material. The details of this microscopic duplication have a big impact on the substance’s macroscopic properties, influencing features like solubility, reactivity, and color.

Modeling the crystal structure of a given substance, Facelli and his team begin with nothing more than the atoms in the molecule and the nature of their bonds. They’re looking for structures with the lowest energies, which typically mark the molecules’ standard crystal structures or something very close. The problem is that this straightforward data and straightforward goal create billions of possible solutions. Just imagine finding the needle of the lowest energy in that haystack of possible structures.

Comparison of the experimental and MGAC predicted (pink) structure of L-alanine. The root mean square of the superposition is 0.30 Å, quantifying the close similarity between the experimental and the modeled results.
To narrow the search to more likely candidate structures, the team uses a parallel genetic algorithm called MGAC that they have developed over the previous six or seven years drawing on systems at NCSA and on TeraGrid.

"An exhaustive search is not feasible, so we have to have a way to direct the search," says Facelli. "[Genetic algorithms] are based on the principle of survival of the fittest. Trial solutions compete with one another in the population for survival and produce offspring for the next generation of tests. These algorithms offer excellent scaling properties, which make them good for large-scale parallel computing systems like those at NCSA and emerging computational grids like TeraGrid."

For example, an initial calculation on NCSA’s Mercury may run 20 simulations on 20 different processors simultaneously, calculating possible crystal structures for a given set of atoms and their bonds. The energies for these structures are compared. The 10 with the lowest energies are kept, and the features of those 10 are mixed and matched to generate the structures for another 10 possible structures. Energies are calculated again, comparisons are made, best candidates are kept, and the cycle continues.

The “mating operation,” as the mixing and matching is called, stagnates quickly, producing very similar structures over the course of thousands of generations. To combat this lack of variety, the genetic algorithm also introduces arbitrary mutations into the process, occasionally taking one variable from one of the best candidates and including a random number for that variable in the next generation.

**From billions to hundreds**

Even with a genetic algorithm greatly reducing the number of candidate structures and the amount of time it takes to find them, the researchers are still frequently left with more than a million possibilities. To narrow it down further, they find and remove the many structures that are the same physically but have very slightly different profiles numerically, “essentially getting rid of the rounding errors,” Facelli says.

Next, they eliminate candidates that are the same structurally but that have revealed themselves in different orientations. This post-processing, which is done automatically at Utah’s Center for High Performance Computing, eventually gets the number of candidates down to a couple of hundred.

Comparison of the experimental and MGAC predicted (pink) structure of 2-acetoxybenzoic acid (aspirin). The root mean square of the superposition is 0.29 Å, quantifying the close similarity between the experimental and the modeled results.
“It’s important to understand we’re not so much trying to predict the exact structure. There are dynamic factors influencing the crystal growth, which means that the experimental structure might sometimes be higher than the lowest energy,” Facelli says. Experts can compare those structures remaining and get it down to 10 or 20 that they want to test in the lab. “We take it from the billions of possibilities and say, ‘Here are the most probable.’”

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

Access Online: www.ncsa.uiuc.edu/News/Stories/gimmestructure

More information: www.chpc.utah.edu/~facelli/

Team members: Victor Bazterra
Julio Facelli
Marta Ferraro
Matthew Thorley

The blind test

Every few years—four times since 1999—the Cambridge Crystallographic Data Centre hosts a “blind test” for the crystal structure prediction world. About a dozen participating research groups are supplied the atomic and bond information for a handful of molecules. They then use their different simulation methods to determine the crystal structure of the molecules, while an independent crystallographer works in secret to determine the real-world structures experimentally.

Sure there are some bragging rights associated with determining the correct structure or coming the closest, but the real value of the event is the experience and the collegial atmosphere, according to the University of Utah’s Julio Facelli. “It’s a very open scientific meeting [when they get together to compare results]. We discuss different methods, issue joint publications, and set goals [for the field] for the next three or four years. We discuss our results and the future.”

Facelli’s team used NCSA’s Mercury system to complete their entry in the 2007 blind test. Most of the methods used by teams at the test treat only fixed conformations of the structures, looking at flexible conformations by running each of the possible conformations of the structures individually. Facelli and his colleagues, however, hope that their more comprehensive method will identify the structures of flexible conformations without that extra step.
The Weather Research and Forecasting Model (WRF) is used by thousands of researchers across the country and around the world to study the formation of dangerous hurricanes and tornadoes, shifts in climate, and air-quality issues. Many variables interact in these complex systems, and the model is not yet able to capture all of the small-scale features of interest to researchers—and current computing systems aren’t powerful enough to provide such fine resolution.

“When wind is blowing over the ocean, for example, that creates turbulence, and our computer models can’t see those swirls and eddies,” says David Nolan, a hurricane researcher at the University of Miami, Florida. Various approximations are used to account for the turbulence, and for other small-scale phenomena.

With petascale computing, researchers will be able to directly simulate phenomena down to a scale of 100 meters. By comparing these fine-grained simulations with current approximations, researchers will be able to determine whether those approximations are sufficient or, if they are not, how to improve the model to better capture what happens in the real world.

“We’ll be able to get much closer to reality,” Nolan says, which means understanding better where hurricanes will form and how their intensity can shift. “It simply comes down to better hurricane forecasting.”

Human beings have explored our planet’s icy poles, vast oceans, treacherous peaks, and remote jungles. But one frontier remains mysterious: the Earth’s interior. The depths of the mantle and core are, despite what Hollywood blockbusters claim, not hospitable to manned expeditions; instead, seismologists must rely on computational simulation.

According to Caltech seismologist Jeroen Tromp, there are two challenges that petascale computation will enable researchers to address.

“The first will require harnessing the entire machine to do very high-resolution simulations” of seismic wave propagation across the entire globe. “A machine like that should get us into the 1 to 2 Hz range,” which Tromp explains will provide unprecedented insight into the small-scale structure of our planet’s interior.

For example, where the liquid outer core meets the solid lower mantle, “all kinds of things appear to be happening at that boundary,” he says. The mantle appears to undergo a phase transition at this depth, changing its properties and behavior. “We would love to be able to really image that. “The fundamental question is: How does the planet work in terms of its physics and chemistry?”

The second grand challenge that petascale computing will enable seismologists to tackle is running many large simulations simultaneously for hundreds or even thousands of earthquakes in order to improve models of the earth’s interior, resolving smaller-scale structures. For this task, high-performance I/O will be critical, to ensure that massive quantities of data can be transferred, stored, and analyzed.

Petascale computing is on the way, and NCSA will play a key role in enabling scientists and engineers to take full advantage of this increased power. Drawing on years of experience and the expertise of its staff, NCSA will help researchers scale their codes to effectively use tens and hundreds of thousands of processor cores. And the center’s Innovative Systems Laboratory, in collaboration with colleagues at the University of Illinois, is exploring how new architectures like GPUs and FPGAs can take scientific computing to the petascale and beyond.
Proteins are the miniature machines that do everything in the human body,” says David Baker, a biochemist at the Howard Hughes Medical Institute at the University of Washington.

Understanding proteins—which ones perform which duties, how they operate, and what happens when they fail to function correctly—provides tremendous insights into the mechanics of life, the roots of disease, and how to better treat illness.

The determination of which amino acids are present in a particular protein, and in what order—the protein sequence—is proceeding at a rapid clip. But each amino acid string is folded and tangled into a complex three-dimensional structure; the unique structure of each protein gives it a unique function. Determining protein structures is lagging behind the generation of sequences.

Baker arrives at protein structure predictions computationally, using his Rosetta code to look for the shape of lowest energy among the possible forms the protein can take. “The bigger the protein is—the more moving parts it has, essentially—the larger the number of possible states,” he explains.

Baker likens the quest to searching for the lowest elevation on the planet. A single explorer would have to search and search and search and search and search. Multiple explorers can cover more ground in less time.

“More explorers increase your chances of success,” he says. Likewise, when it comes to protein structures “to really explore the space, you need a large number of processors. Each additional bit of computer power is more conformations that can be searched.” Making the leap to petascale computation will mean searching a much larger area much more efficiently, and therefore unlocking more of the secrets proteins hold.

High-performance computing is central to Boeing’s businesses. For example, the company uses tens of thousands of computational fluid dynamics (CFD) simulations to evaluate designs and systematically explore the possibilities of design improvements for its aircraft.

“Computational excellence is an enabler to our ability to lead aerospace technology and product innovation to the marketplace,” says Paul Fussell, senior manager of mathematical modeling for Boeing Engineering, Operations and Technology.

Using CFD to analyze the aerodynamics of the aircraft under certain conditions, like cruise or one-engine takeoff, is just the starting point. With petascale computing power, Boeing will be able to undertake much more complex simulations at much finer fidelity.

Petascale simulations could include more extensive aerodynamics and would enable optimization considering several physics, rather than just one. For example, simulations could include wing structure as well as aerodynamics in order to better capture the complex interplay occurring as the plane’s wing bends, influencing its aerodynamics, which affect the load and elastic response of the wing. With this computing capacity, Boeing could design better materials, consider structure and airframe, and study their response to dynamic loads.

“We always use all the computational capability on our machine room floors to solve the most significant challenges we face. And the bar is always rising; we always imagine how we’ll use the next increase in machine capability. We always know of more physics to consider or more design-spaces to explore,” Fussell says.

How will petascale computing advance science and engineering?

These researchers describe how their work will be transformed by the increased power that is on the horizon.

David Baker
University of Washington

Paul Fussell
Boeing
Small wonders

By James E. Kloeppep
Scientists tap NCSA resources to design a tunable semiconductor membrane that could be used for protein filtering or DNA sequencing.

A semiconductor membrane designed by researchers at the University of Illinois could offer more flexibility and better electrical performance than biological membranes. Built from thin silicon layers doped with different impurities, the solid-state membrane also could be used in applications such as single-molecule detection, protein filtering, and DNA sequencing.

“By creating nanopores in the membrane, we can use the membrane to separate charged species or regulate the flow of charged molecules and ions, thereby mimicking the operation of biological ion channels,” says lead researcher Jean-Pierre Leburton, the Stillman Professor of Electrical and Computer Engineering at the University of Illinois at Urbana-Champaign.

Leburton and postdoctoral research associate Maria Gracheva used high-performance computers at NCSA to simulate the operation of the semiconductor membrane at a number of electrostatic potentials.

“We have a huge grid of two million grid points that we have to simulate in 3D,” Leburton says. “It requires huge resources.”

Previously, Leburton and his collaborators had been using workstations to carry out their simulations, but “we were working at the limits of the capabilities of these workstations,” he explains. Moving their calculations to one of NCSA’s high-performance computing systems enabled the researchers to get their results more quickly and easily.

The team currently simulates each membrane configuration in sequence, with each one of the hundreds of configurations taking up to four hours to compute, even on NCSA’s powerful systems. Leburton says the team plans to parallelize their code in order to better leverage high-performance computing resources.

In the researchers’ model, the nanopore-membrane structure is made of two layers of silicon, each 12 nanometers thick, with opposite (n- and p-) doping. The electrostatic potential is positive on the n-side and negative on the p-side of the membrane.

“The use of p-type semiconductor material in the p-n membrane opens up additional possibilities for ion current and biomolecule manipulation,” Gracheva says. “With this membrane one can electrically block the current through the nanopore, even though the nanopore is physically open. One can also envision stretching biomolecules translocating through such a membrane.”

The nanopore has an hourglass shape, with a neck one nanometer in diameter and openings on each side of the membrane six nanometers in diameter. The “size” of the nanopore can be changed by changing the electrostatic potential around it.

By controlling the flow of ions, the artificial nanopore offers a degree of tunability not found in biological ion channels, said Leburton. The findings are reported in a paper accepted for publication in the journal *Nano Letters*. In addition to serving as a substitute for biological ion channels, the solid-state nanopore and membrane could be used in other applications, including sequencing DNA.

“Using semiconductor technology to sequence the DNA molecule would save time and money,” Leburton says. “By biasing the voltage across the membrane, we could pull DNA through the nanopore. Since each base pair carries a different electrical charge, we could use the membrane as a p-n junction to detect the changing electrical signal.”

James E. Kloeppel is a research editor with the University of Illinois News Bureau. Trish Barker, NCSA Public Information Officer, contributed to this article.

Support for this research was provided by the National Science Foundation and the National Institutes of Health.

More information: http://wwwbeckmanuiucedu/research/mensce.html
For more than 50 years, the University of Illinois, home to the National Center for Supercomputing Applications, has been a pathfinder, helping guide the impact that computing and information technology have had. The Nobel Prize winners who invented the transistor and the integrated circuit walked Illinois’ halls. The creator of the light-emitting diode still makes his home here. Some of the earliest supercomputers were born on the north end of campus. NCSA Mosaic, the first widely used graphical web browser, was built a few blocks away.

Here’s a look at some of that Illinois history.

**Past**

**1951-52** Illinois works with the U.S. Army to build ILLIAC and ORDVAC. ILLIAC is the first computer built and owned entirely by an educational institution.

**1956** John Bardeen, a physics professor, wins the Nobel Prize for his work, while at Bell Labs, on the transistor. Jack Kilby, a College of Engineering alumnus, will help invent the integrated circuit at Texas Instruments two years later. He wins the Nobel Prize in 2000.

**1977** Professor David Kuck and his co-workers introduce dependence graphs and analysis and transformation techniques for the graphs’ computation. This influential work enables many of today's optimization algorithms.

**1985** Construction begins on Cedar, a hierarchical shared-memory supercomputer. This system embodies advances in interconnects, parallelism, optimizing compilers, and parallel applications.

**Computer Science at Illinois**

**1951-52** Illinois works with the U.S. Army to build ILLIAC and ORDVAC. ILLIAC is the first computer built and owned entirely by an educational institution.

**1956** John Bardeen, a physics professor, wins the Nobel Prize for his work, while at Bell Labs, on the transistor. Jack Kilby, a College of Engineering alumnus, will help invent the integrated circuit at Texas Instruments two years later. He wins the Nobel Prize in 2000.

**1977** Professor David Kuck and his co-workers introduce dependence graphs and analysis and transformation techniques for the graphs’ computation. This influential work enables many of today’s optimization algorithms.

**1985** Construction begins on Cedar, a hierarchical shared-memory supercomputer. This system embodies advances in interconnects, parallelism, optimizing compilers, and parallel applications.

**Computer Science Today**

**Researchers study:**

- Computer architecture, run time systems, programming languages, and compilers for next-generation computers and computing components.
- Hardware and software aspects of parallel processing.
- Numerical techniques for approximating mathematical models of physical systems—like molecular systems, semiconductors, and solid rocket fuels—and algorithms for solving the resulting equations on high-performance computers.
- Machine learning and data mining techniques for the analysis of large data sets, including text and image processing.
1950s  David Muller helps develop Reed-Muller canonical networks, a standardized formulation of Boolean circuits that is still used today for testing circuit design.

1960s  PLATO, the first computer-assisted instructional program in the world, is built. Precursors of email and other forms of electronic communication propagate there.

1980s  Researchers lead the theory and implementation of fault-tolerant computing systems, issues that still loom large today.

1990s  Intel’s IA-64 microchips incorporate innovative technologies based on CSL’s work on compilers.

1983  University of Illinois professors send an unsolicited proposal for a scientific and engineering supercomputer center to the National Science Foundation, giving rise to the NSF supercomputer centers program two years later.

1987  NCSA Telnet, which allowed users to log in to other computers via the Internet, is released. By 1991, there are more than 100,000 users.

1993  NCSA Mosaic, the first widely used graphical web browser, is released. More than 5,000 copies are being downloaded per month in the software’s boom years.

1999  NCSA is the first NSF-sponsored center to provide more than one million normalized CPU hours of computing time to the nation’s scientists and engineers. By 2006, NCSA is providing 650 million hours per year.

**Coordinated Science Laboratory**

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**National Center for Supercomputing Applications**

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**CSL Today**

*Researchers investigate:*

- Integrated circuits, including reliability problems; low-power and high-performance integrated circuits for portable systems; and alternatives to bulk silicon for microprocessors.
- Physical electronics, including the use of carbon nanotubes for transistors and quantum dots for communication applications.
- Reliable computing, including foundational theory and practical techniques for ensuring reliability and security in high-performance computers, distributed networks, and mobile communications.
- Utility computing through the Trusted ILLIAC project, which is developing a large, demonstrably trusted cluster computing platform for on-demand computing.

**NCSA Today**

*The center provides:*

- Stable, robust computing resources, enabling the nation’s scientists and engineers to tackle their most demanding challenges. NCSA offers nearly 140 teraflops of computing capacity to the nation’s researchers and businesses.
- Cyberenvironments, which give research communities the means to fully exploit the extraordinary cyber-resources available.
- Innovative systems research, which evaluates the performance of emerging computing systems for key scientific and engineering applications.
- Advanced visualization technologies and expertise, which give critical insights into complex systems and bring the thrill of scientific discovery to the public.
Shining brightly

By James E. Kloeppele
Thin, lightweight panels could be used for residential and commercial lighting, and for certain types of biomedical applications. “Built of aluminum foil, sapphire, and small amounts of gas, the panels are less than one millimeter thick, and can hang on a wall like picture frames,” says Gary Eden, a professor of electrical and computer engineering. Eden is director of the Laboratory for Optical Physics and Engineering, a laboratory devoted to developing new sources and applications of coherent radiation in the spectral region below 500 nanometers.

Like conventional fluorescent lights, microcavity plasma lamps are glow-discharges in which atoms of a gas are excited by electrons and radiate light. Unlike fluorescent lights, however, microcavity plasma lamps produce the plasma in microscopic pockets and require no ballast, reflector or heavy metal housing. The panels are lighter, brighter and more efficient than incandescent lights and are expected, with further engineering, to approach or surpass the efficiency of fluorescent lighting.

The plasma panels are also six times thinner than panels composed of light-emitting diodes, says Eden, who also is a researcher at the university’s Coordinated Science Laboratory and the Micro and Nanotechnology Laboratory.

A plasma panel consists of a sandwich of two sheets of aluminum foil separated by a thin dielectric layer of clear aluminum oxide (sapphire). At the heart of each lamp is a small cavity, which penetrates the upper sheet of aluminum foil and the sapphire.

“Each lamp is approximately the diameter of a human hair,” says visiting research scientist Sung-Jin Park, lead author of a paper describing the microcavity plasma lamps in the June issue of the Journal of Physics D: Applied Physics. “We can pack an array of more than 250,000 lamps into a single panel.”

Completing the panel assembly is a glass window 500 microns (0.5 millimeters) thick. The window’s inner surface is coated with a phosphor film 10 microns thick, bringing the overall thickness of the lamp structure to 800 microns.

Flat panels with radiating areas of more than 200 square centimeters have been fabricated, Park says. Depending upon the type of gas and phosphor used, uniform emissions of any color can be produced.

In the researchers’ preliminary plasma lamp experiments, values of the efficiency—known as luminous efficacy—of 15 lumens per watt were recorded. Values exceeding 30 lumens per watt are expected when the array design and microcavity phosphor geometry are optimized, Eden says. A typical incandescent light has an efficacy of 10 to 17 lumens per watt.

The researchers also demonstrated flexible plasma arrays sealed in polymeric packaging. These devices offer new opportunities in lighting, in which lightweight arrays can be mounted onto curved surfaces—on the insides of windshields, for example.

The flexible arrays also could be used as photo-therapeutic bandages to treat certain diseases—such as psoriasis—that can be driven into remission by narrow-spectrum ultraviolet light, Eden says.

The team worked on the arrays as part of the university’s Technology Research, Education and Commercialization Center (TRECC) Accelerator Project. TRECC, funded by the Office of Naval Research and administered by NCSA, sought to accelerate the commercialization of outstanding emerging technologies by providing funding in order to fast-track technology development and commercialization. Eden’s project was also funded by the U.S. Air Force Office of Scientific Research.

“NCSA is one of the crown jewels in the university,” says Eden. His team frequently relies on NCSA computational resources to further their engineering advances.

James E. Kloeppel is a research editor with the University of Illinois News Bureau. Access’ managing editor Barbara Jewett contributed to this article.

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Researchers at the University of Illinois are developing panels of microcavity plasma lamps that may soon brighten people’s lives.

Researcher: J. Gary Eden
Sung-Jin Park
Andrew Price
Jekwon Yoon

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Getting down to details

By Trish Barker

Researchers at Scripps Institution of Oceanography develop fine-scale climate datasets using a novel numerical technique on TeraGrid systems at SDSC and NCSA.

Climate research—particularly studies aimed at management of water, energy, forestry, fisheries, or agriculture—requires fine-scale data over long time periods. But it’s nearly impossible to find data from multiple decades that is consistent, comparable, and of sufficient resolution.

To address this dearth of data, scientists turn to the process of reanalysis—integrating data from disparate sources within a numerical model in order to create a comprehensive dataset and to shed light on how and why climate has varied over the past half-century.

However, global reanalysis typically has a resolution that is too coarse for many application studies. Using compute resources at the San Diego Supercomputing Center (SDSC) and NCSA, Masao Kanamitsu, a research meteorologist at the Scripps Institution of Oceanography, and postgraduate researcher Hideki Kanamaru were able to carry out a fine-scale 10 km regional reanalysis of California covering 57 years, from 1948 to 2005 (CaRD10, for short). Their work is supported by the California Energy Commission Public Interest Energy Research program.

Kanamitsu and Kanamaru used a reanalysis technique called dynamical downscaling with the state-of-the-art Regional Spectral Model. They found that their reanalysis results compared well with observations and yielded more accurate wind and temperature data than other methods on all time scales, whether hourly or across decades. Their results, which will be published in the *Journal of Climate*, indicate that dynamical downscaling could be a reliable way to derive fine-scale regional detail from coarser analyses.

The data is being stored and made accessible to researchers who need detailed meteorological information through SDSC’s DataCentral service.

Experts at both TeraGrid sites were instrumental in helping the researchers get their simulations running smoothly.

Access Online: www.ncsa.uiuc.edu/News/Stories/climate

http://g-rsm.wikispaces.com/CaRD10
http://cec.sdsc.edu/

Team members: Hideki Kanamaru
Masao Kanamitsu

Near surface wind for a Catalina Eddy event on May 22, 1984. Shades are surface height (in meters) for each analysis. CaRD10 is the dynamical downscaling of California. The analysis using surface observation is shown on the right. Image courtesy of Hideki Kanamaru and Masao Kanamitsu.
CaRD10
10-km resolution
1500 UTC

North American Regional Reanalysis
32-km resolution
1500 UTC

Global Reanalysis
200-km resolution
1200 UTC

globe image courtesy of NASA Visible Earth
Power to the people
Scientific discovery used to rely on what could be observed under microscopes and through telescopes and what could be learned through experiments in the laboratory. But over the past two decades, computational simulation has emerged as a third powerful technique and is now integral to the scientific process. High-performance computers enable researchers to explore phenomena too big, too small, too fast, too slow, or simply too complex to be observed or contained within an experimental framework.

A national cyberinfrastructure of powerful computers and fast networks exists and is ever expanding to meet the needs of computational researchers. Thousands of scientists consume thousands of hours of compute time on systems across the country, many of which are linked through the National Science Foundation’s TeraGrid.

To get a slice of the computing pie, investigators submit proposals, which are peer-reviewed. This process works well for researchers who want time in the tens or hundreds of thousands of hours, but for researchers, educators, and students who may use just a handful of hours the barriers to entry are daunting—not just the need to write a proposal and wait for it to be reviewed, but the learning curve involved in tapping computing resources and the delays as submitted calculations await their turn on busy computers.

University of Utah chemistry professor Thanh Truong wants to break down those barriers to entry, making access to computational resources as simple as logging on to a website. In collaboration with NCSA, Truong’s team recently released a new version of CSE-Online (Computational Science and Engineering Online), a web-based framework for science and engineering disciplines as well as a science gateway that connects users with some of the computational resources of the TeraGrid.

Breaking down barriers

Prior to collaborating with NCSA, Truong’s Utah team spent three years developing CSE-Online with support from the National Science Foundation. From the outset, the goal has been to provide integrated, user-friendly access to a wide range of remote data stores, computational tools, and modeling and visualization resources for both research and education.

“We’re removing all of the hurdles, all of the technical difficulties, all of the barriers to entry,” Truong says. “The benefits of CSE-Online to the user are similar to the improvements offered by the Windows operating system over DOS.”

Supported in part by a summer fellowship with NCSA, Truong began work with NCSA in 2006, aiming to make it easier for researchers, educators, and students to access the TeraGrid’s powerful computing resources.

Previous versions of CSE-Online enabled users with their own TeraGrid allocations to run computational jobs on TeraGrid resources...
using their personal credentials for authentication. The version released in spring 2007 provides the same capability for users who have asked to become part of the community. These community users are authenticated and given access to TeraGrid resources by a community credential, which maps to a TeraGrid account that everyone in the community shares. Because an individual allocation isn’t needed, the TeraGrid is accessible to more research and education users.

To increase security, NCSA developed a restricted shell capability that limits the actions community users can take; this prevents malicious users from posing as legitimate community users in order to gain access to TeraGrid.

“Since creating the CSE-Online community we have doubled the number of registered users on the gateway,” Truong says. There are currently more than 600 registered users from countries around the globe, and nearly 4,000 jobs have been submitted to the TeraGrid. “People are using it every day.”

One of those users is Timothy Lippa, a research scientist at the Johns Hopkins University Applied Physics Laboratory. A part of his research looks at the fundamental physical properties of materials, and he has used CSE-Online to branch out into computational chemistry.

“I’m an experimentalist by training, but I’ve started to get interested in computation so CSE-Online has been a great tool for me,” he says.

As he dipped his toe into the computational waters, Lippa found the integration of multiple features and programs into a single platform particularly helpful.

“The way it’s all tied together really increases its usability” he says.

Computing in the classroom

Looking at the data on CSE-Online over the past several months, Truong believes that many of the thousands of often small jobs submitted may be coming from teachers and students. And that means his plan to broaden access to computational tools is working.

“These high-performance infrastructures are mainly used for research but can also be used for education,” he says. Truong points out that educating tomorrow’s scientists and engineers is a key first step in ensuring continued competitiveness and innovation.

Small institutions “don’t have the resources, they don’t have their own clusters, they can’t afford the software or IT professional to maintain the system,” he says. But with CSE-Online, “people can use it to learn computational chemistry. They can use it to teach undergraduates.” And they don’t need to invest in hardware, software, and the expertise required to keep both in operation.

NCSA provided CSE-Online users with a dedicated queue to the center’s Mercury cluster. This type of access enables educators
who use CSE-Online in the classroom to submit jobs and receive results in minutes, making it practical for instructors to introduce their students to high-performance computational science in the classroom.

Beta and beyond

NSF funding for the development of CSE-Online has ended, so now Truong’s team is courting support from industry and is focusing on meeting users’ needs for domain-specialized sets of integrated computational resources.

“Sustainability requires you to continually focus development on what is most relevant,” Truong says.

Work continues on refining CSE-Online, with the latest version—featuring a more user-friendly interface—planned for beta release by the end of the year. Truong intends to release an initial production version early in 2008.

“Although the environment that we have developed so far is extremely innovative, there are still some barriers to overcome,” he says. “But toward the end of the year when we release our beta version we are confident we’ll have removed those barriers.”

Access Online: www.ncsa.uiuc.edu/News/Stories/CSEonline

More information: http://cse-online.net

Team members: John Chuang Ly Le Sophia Han Hoa Nguyen Thanh N. Truong Yong Kim Lam K. Huynh. Priya Mahajan Jiangfa Xiao Suengkeol Choe Tom Cook Ha Pham Jihoon Choi Manohar Nayak
Following the International Computer Music Conference in Copenhagen last August, Ben Smith sat at his laptop on a stage in a darkened night club. As he and another performer began to work at their computers, flashes, streams of light, geometric shapes, and explosions appeared on the black screen behind them. As these visualizations danced and floated in the virtual space, their interactions created what Smith calls “MusiVerse,” an improvised, collaborative online symphony of images and sounds. Smith’s performance changed with every keystroke. Eerie and modern, the notes resonated throughout the room and the audience responded with applause.

Smith, a graduate student in the University of Illinois at Urbana-Champaign School of Music, developed an algorithmic computer music program that allows users to produce perfectly synchronized sounds and images with the ease of creating a website. Drawing upon the same technology that makes elaborate multi-person online games and virtual worlds possible, Musiverse creates visualizations.

“In the MusiVerse I go beyond superficial connections and try to create deeper relationships between the visuals and the music,” Smith explains. “Music itself is a result of carefully structured sounds and it is my hope that by carefully structuring the simultaneous generation of the graphics and music from a single source dataset, I can portray deeper connections and bring the audience into a new aesthetic experience.”

Smith recently took his music experience another step further with a performance at the university’s Krannert Center for the Performing Arts. The performance was similar to the Copenhagen debut, but with the addition of several other performers logged in to the MusiVerse portal from New York, Indiana, and Chicago. Smith says that although only 10 performers contributed to the Krannert performance, the server can theoretically support a few dozen performers (musical programmers) in the same online environment from anywhere in the world.

“I am very interested in reaching a bigger audience than this sort of music software usually reaches—making it a networked thing so people can share what they are creating,” he says.

Perfecting the art

The idea of using computers in performance arts is not new, but in the past most computer-generated music performances lacked visuals, leaving the audience to stare at the performer sitting at a computer while the music played. In the case of music program visualizers, the only connection between the sound and the visuals is the oscilloscope (the bouncing line that represents the audio waveform) so any actual alignment between them is coincidental and won’t repeat if you play the same song over and over.

Unsatisfied with this, Smith experimented with different online environments—like Secondlife.com—and found that visuals with music vastly increased his audience.

So you thought the visualizers on iTunes were entertaining? How about a live musical performance where digital artwork goes well beyond oscilloscopes and actually creates music in a real-time collaborative, interactive virtual world.

By Tracy Culumber
“I came to this idea after seeing results of what everyone else was doing, then rebelling,” Smith says. “What I see missing is the visual connection between the performer and the music, and how it is being played and produced; my focus is on the interaction between performers and computers.”

Audience members have mistaken Smith’s smooth improvisation for prerecorded material—a mistake that he considers a great compliment. But the development of MusiVerse is not without challenges. Although complications associated with large-scale, high-resolution graphics and computing pose the majority of challenges to his research, the settings engrained into the code for computer game software, such as gravity and terrain, are not optimal for his visualizations and difficult to remove. Also, game websites, or “toy simulations,” do not involve immediate interactions and they are not about collaborative immediate responses. He has spent the past year researching ways to avoid these problems and provide “online world-users” with fewer limitations on how they use computers to create art.

Although he still needs to walk others through the MusiVerse software initially, audience participants from the Krannert performance say they found the program easy to use once mastered. Smith’s goal for the technology is to make the creation of these visual-musical performances a reality for anyone with a computer.

Smith’s faculty advisor for the project is Guy Garnett, a professor of music and computer science and an NCSA Faculty Fellow; Smith also consulted on the project with NCSA researcher Robert McGrath. McGrath agrees that Smith’s research has great potential to become a household application. “I have visions of this being something that is easily available so people can sit down . . . and start jamming on the network,” he said.

**Cyberenvironment in action**

Smith says that his project is not the culmination of the technology, but rather a milestone that shows how online environment technology works.

“There is a shortage of people who are both interested in computing and talented in the arts, so we need to look for ways to change that situation and break down the barrier between the scientific side of campus and the arts side,” says Garnett, who is co-director of the Cultural Computing Program’s mWorlds initiative. CCP is a campuswide initiative at Illinois to foster creative activities, innovation, collaboration, and research that spans technology and the arts.

mWorlds are synthetic worlds focused on testing the limits of creativity, scalability, security, and flexibility in online, collaborative environments through art, science, research, education, and entertainment. The goal of the mWorlds initiative is to make the creation of and participation in these online worlds as easy as creating websites or browsing the Web. MusiVerse is a good representation of the endless possibilities of projects users can tackle in a synthetic world.

“We want to simplify and generalize the process of creating a virtual world and make it more flexible,” Garnett says. “The idea is to make this technology accessible on a desktop and ensure that the environment is collaborative and distributive—like Ben’s performance.”

Smith said in the near future he would like to use this interface to develop music that is not necessarily modern or “hard-to-listen-to” but music that people hear at a concert or on the radio.

“I want it to be music people are used to listening to in the clubs,” Smith says. “They would really freak out if they saw this with that music.”

**Access Online:** www.ncsa.uiuc.edu/News/Stories/Audiovisual
NCSA hosts PRAGMA events

In September, NCSA hosted PRAGMA 13, a meeting of the Pacific Rim Application and Grid Middleware Assembly. The 29 PRAGMA institutions meet twice a year at workshops hosted by member institutions around the globe. Founded in 2002, PRAGMA is an open organization in which Pacific Rim institutions collaborate more formally to develop grid-enabled applications and deploy the needed infrastructure throughout the region, and beyond, to facilitate data, computing, and other resource sharing.

NCSA was also the site of the first ever PRAGMA institute, a two-day slate of tutorials, speakers, and presentations on member institution-developed software and application technologies. This institute was sponsored by the Institute for Advanced Computing Applications and Technologies (IACAT) at the University of Illinois at Urbana-Champaign.

In addition to presentations, workshops, and speakers, participants in PRAGMA events were also afforded ample networking opportunities.
NCSA, FBI launch National Center for Digital Intrusion Response

NCSA and the FBI are collaborating to research, develop, and deploy new techniques and tools for cybersecurity. The new effort, called the National Center for Digital Intrusion Response (NCDIR), received $3 million from the FBI for its first two years of operation.

Digital intrusions are complex, often involving multiple hosts and organizations and crossing state and national borders. Tracking an intruder through that maze, and sorting the critical information from the noise, is difficult.

Through NCDIR, NCSA staff and FBI agents collaboratively tackle on-going FBI investigations. Working together on these cases helps the NCDIR team determine what new capabilities law enforcement officers need to more effectively respond to cyberattacks, ultimately providing investigators with the tools and knowledge they need to do their jobs more easily, quickly, and effectively without having to become technology experts.

More information is available online at www.ncdir.us.

RSSI’08 slated for July 7-10

NCSA will host the fourth annual Reconfigurable Systems Summer Institute at its facilities in Urbana-Champaign, July 7-10, 2008. RSSI brings together scientists and technology developers from industry and academia to present and discuss new research on high-performance reconfigurable computing.

RSSI’08 is sponsored by NCSA, the Center for High Performance Reconfigurable Computing, OpenFPGA, and the University of Manchester.

More information is available online at www.rssi2008.org or by contacting ask@rssi2008.org.

NCSA’s Xavier Llorà earns honors for recent work

Xavier Llorà, a member of NCSA’s Data Intensive Technologies and Applications division, recently received several honors for his research.

Llorà received two bronze Humies at GECCO 2007 (the Genetic and Evolutionary Computation Conference) in London in July. The Humies are awarded annually to recognize human-competitive results produced by genetic and evolutionary computation.

One was for work with NCSA faculty fellow Rohit Bhargava, a member of the University of Illinois’ bioengineering department, for “Towards Better than Human Capability in Diagnosing Prostate Cancer Using Infrared Spectroscopic Imaging.” The team used a novel genetics-based machine learning technique to diagnose prostate cancer.

The other was for work with co-authors Jaume Bacardit, Michael Stout, Jonathan D. Hirst, Natalio Krasnogor (all University of Nottingham), and Kumara Sastry (University of Illinois), for “Automated Alphabet Reduction Method with Evolutionary Algorithms for Protein Structure Prediction,” demonstrating that certain automated procedures can be used to reduce the size of the amino acid alphabet used for protein structure prediction from 20 to just three letters with no significant loss of accuracy.

With co-authors Sastry and David E. Goldberg (University of Illinois), Llorà earned a best paper award at GECCO 2007 for “Toward Billion Bit Optimization via Parallel Estimation of Distribution Algorithm,” which took on a major problem in the field of genetic algorithms.

Llorà and co-authors Goldberg, Noriko Imafuji Yasu (University of Illinois), and marketing researchers Yuichi Washida and Hiroshi Tamura also netted a best paper award at the International Conference on Enterprise Information Systems in June for “Delineating Topic and Discussant Transitions in Online Collaborative Environments.” The paper details a new algorithmic method for analyzing discussion dynamics and social networking in online collaborative environments.
The inside of a star at the end of its life may seem more than a galaxy away from a thunderstorm cell on Earth, but not to the University of Minnesota’s Paul Woodward and NCSA’s Chief Science Officer Bob Wilhelmson. The star interiors that Woodward studies at his Laboratory for Computational Science and Engineering and through runs on NCSA machines are analogous to an atmosphere, so he and Wilhelmson are working to adapt Woodward’s code to simulate severe thunderstorms, a research area of interest to Wilhelmson.

Woodward used a 2007 NCSA summer fellowship to work with an NCSA team and although they came close, Woodward says he still has some code debugging to do. “The rain doesn’t fall properly yet, but the code runs awfully fast and the cumulus cloud I made on my machines here in Minnesota looked pretty good,” Woodward writes in an email message. Their plan is to test the applicability of the new code’s structure, parallel implementation, and unusual multifluid advection algorithm for severe storm research.

Their hope is that this experimental code might run fast enough on NCSA’s machine Abe to make fully interactive storm simulation practical across a substantial portion of the machine at a reasonable level of simulation accuracy. They are also exploring scaling the code for a petascale application.

The image pictured here is Woodward’s previous work exploring what happens inside the central region of a star near the end of its life.