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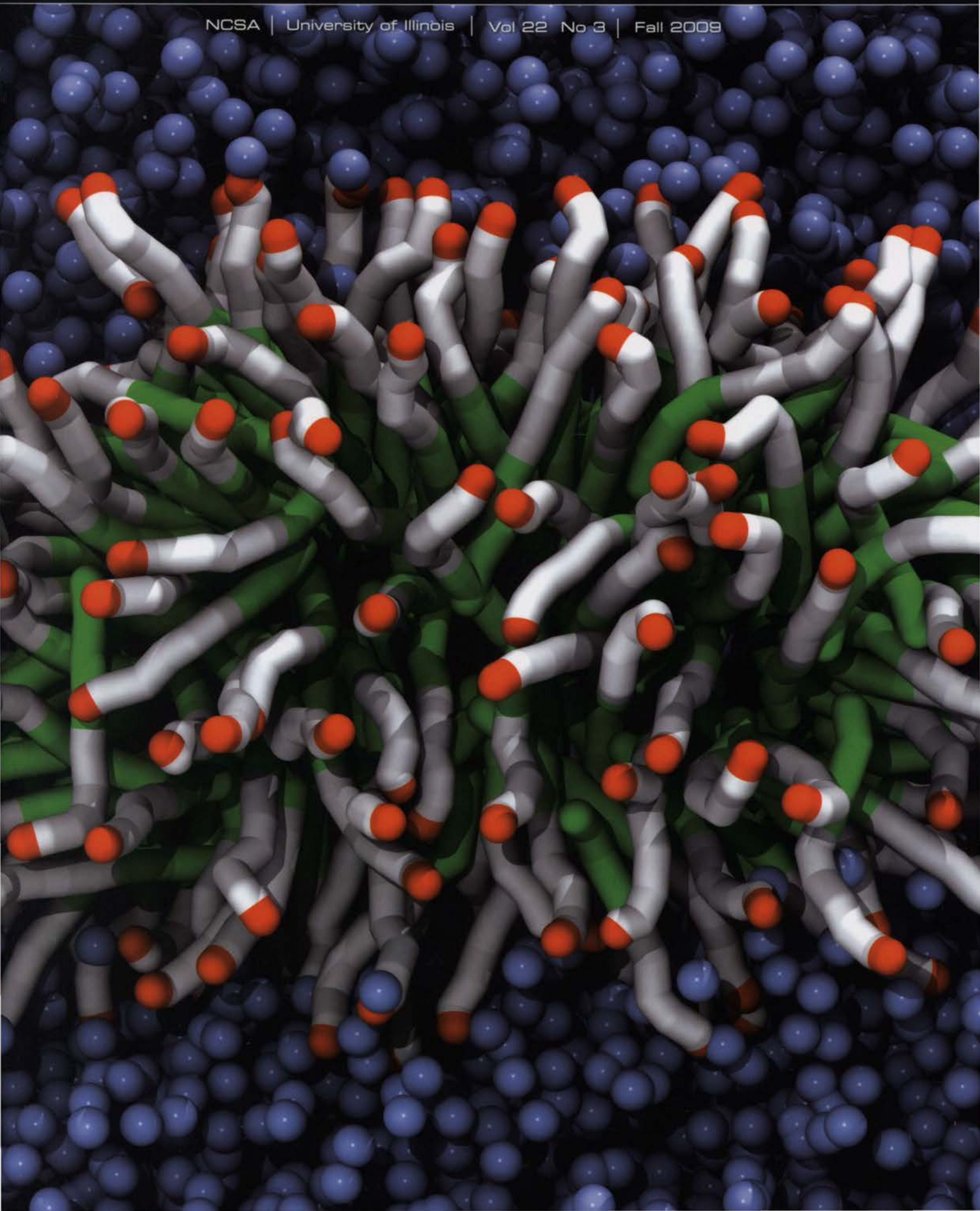

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Executive Editor
J. William Bell
jbell@ncsa.illinois.edu

Managing Editor
Barbara Jewett
barbaraj@ncsa.illinois.edu

Art Director
Blake Harvey
bharvey@ncsa.illinois.edu

Copy Editor
Trish Barker

On the Web

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www.ncsa.illinois.edu

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

Who we are

The 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.illinois.edu.

On the cover

Snapshot of a self-assembled elongated micelle of non-ionic surfactant molecules (penta-(ethyleneglycol)-dodecylether, $C_{12}E_5$) in water from a coarse grain molecular dynamics simulation. These sorts of molecules are used in everything from detergents to drug-delivery systems. Structures like micelles and vesicles form and can trap or protect other materials. Researchers at Temple University model these structures on NCSA's Abe and Lincoln supercomputers. Learn more on page 9. This image was created using VMD from the University of Illinois' Theoretical and Computational Biophysics Group, and it was rendered with the embedded Tachyon renderer.

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contents

02 Details of Blue Waters start to emerge
William Kramer
Deputy Project Director, Blue Waters

Details of Blue Waters start to emerge

WHEN I WAS ASKED to write the editorial for this issue of Access, I realized that I joined the Blue Waters project a year ago. It has been an amazing, intense, and rewarding year for me, and the project, as we transitioned from mostly planning to the execution of all the project components. I came to Blue Waters with nothing more than the information that was public at the time—which means, precious little—and a great deal of anticipation. Once I was able to see the details of the base Blue Waters system and the entire project, I was excited to see the Blue Waters system align so well with the philosophy and goals I used in deploying and running 19 previous high-performance computing (HPC) systems to serve the general science community.

The computational science and engineering community requires five attributes from the systems they use and the facilities that provide those systems. These attributes deliver systems that efficiently and productively enhance the scientists' ability to achieve novel results. They are performance, effectiveness, reliability, consistency, and usability (which I refer to as the PERCU method). This is a holistic, user-based approach to developing and assessing computing systems, in particular HPC systems. The method enables organizations to use flexible metrics to assess the features and functions of HPC systems and, if they choose to purchase systems, assess them against the requirements negotiated with the vendor.

Blue Waters epitomizes a project and a system design dedicated to providing those five attributes to the widest range of science and engineering areas. A key, and in many ways unique, aspect of Blue Waters is that the entire project is focused only on sustained performance for a wide range of science problems. This translates to Blue Waters being dedicated to time to solution as a way to assess the productive work potential for an arbitrary large set of applications. While the sustained performance will be measured on several petascale benchmarks that represent yet unsolved problems, we are confident that sustained-petascale performance will be achieved for a broad range of applications that scientists and engineers use every day.

Recently, many details of the POWER7 chip, the computational heart of the Blue Waters system, were presented by IBM at the August 2009 Hot Chips conference. You can learn more about those on page 7. Looking at the chip, one can see a number of new features that will make the processor itself the highest performance, most general processor of its time. Beyond the common measures of clock speed and multiple simultaneous operations, the processor will have significant new advantages in the memory hierarchy that enable the POWER7 processor to match memory performance to processor performance. The presentations also hint at another critical area, admittedly not well defined at the moment: the high-performance and balanced way the processors will be integrated together for petascale systems.

The Blue Waters staff is now working with about 20 large science teams to start revising their application codes to take full advantage of the Blue Waters features. Much of the work will enable codes to run well and at large scale on Blue Waters, but the work

can also be applied to other systems in the future. We are doing this with simulation of the machine itself, application and system performance modeling with premier modeling groups, and early access to prototype systems and software. Over time, we will engage with other science areas as they are allocated time on Blue Waters.

In summary, I am particularly pleased to report to you that the Blue Waters project is well on-track and moving to deliver a world-class resource for science and engineering. Over the next nine months, much more information about the technology in Blue Waters, particularly the innovations on the interconnections, will become available. Further, starting at SC09, we will be sharing more of the information about the base software features, and importantly the "value added" software features the Blue Waters project is developing or enhancing. All this will culminate in the arrival of the system components and its use by the science teams in 2011. □

William Kramer
Deputy Project Director, Blue Waters
NCSA

DOING THE BEST

Since the National Science Foundation gave the nod to build Blue Waters—a sustained petascale computer for open scientific research—NCSA, the University of Illinois, IBM, and partners around the country have been collaborating on the machine and a facility to house it. Building the two simultaneously has afforded unprecedented opportunities for synergy between machine and facility. Access' Barbara Jewett chatted with IBM Fellow Ed Seminaro, chief architect for Power HPC servers at IBM, about this synergy as well as some of the unique aspects of the Blue Waters project.

Q: IBM is collaborating with NCSA and the University of Illinois on the Illinois Petascale Computing Facility (PCF) as well as the Blue Waters hardware that's going into it. Is collaborating on the building something you normally do?

A: We do, but not necessarily to the degree that we've done it here. It's not often that you get in on the ground floor and that you start before the building has even been drawn up on blueprints, so we were able, in fact, to design some of the server racks to accommodate this specific facility. It's likely a lot of things we're doing here will become more standard practices, but we were able to do some things that are unique in this situation.

As one example, we actually have the system laid out on a raised floor to take up all the available area from side to side; there's almost no wasted space whatsoever. The aisles on both sides of our cabinets are about the minimum you'd want them to be. If a room is constructed ahead of time or plans are drawn up ahead of time you're usually not able to achieve that.

The Blue Waters system is completely water-cooled. You really have to plan up front for that. What we've been able to do with the help of EYP, the building architect, is position the machines directly over the cooling main lines so we have no extra plumbing whatsoever for feeding water to the parts of the machine. We were able to do very similar things with how we distribute power to the machine.

Q: Talk about the cooling strategy for Blue Waters.

A: By putting the water almost in contact with the chips that are dissipating the power, it literally conducts the heat directly out without having to move any air around. That allows the electronics to run cooler, which causes them to dissipate less power. Less power dissipated, means less power or energy is used.

During a large part of the year we'll run with what's called free cooling. With the outdoor water-cooling tower, the water won't be any cooler than the outside air temperature but during a large portion of the year the weather is cool. So we'll literally circulate the water through the electronics, outside through a big radiator with a fan blowing through it, and right back into the building. The only energy we have to provide is the energy for the fans to help cool that radiator outside and to pump the fluid around.

Q: Does the water have to be a particular temperature to effectively cool?

A: For maximum efficiency, you want to be able run the water at the warmest possible temperature because that will capture the most free-cooling days. The coldest the water can be is to just above freezing, but the water is moving at a good enough pace that it never gets quite that cold. The warmest the water can be, in our case, is a temperature of about 68 degrees Fahrenheit or so. We're actually investigating trying to run the water even warmer to use free cooling more months.

We have a metric we use in the industry, power usage effectiveness or PUE. What that refers to is you have power coming into the building at some voltage and you have energy used by the machine, and you take the ratio of the energy used by the IT equipment versus the energy consumed by the entire building. If that ratio is 1.00 that means there wasn't any energy wasted in the building infrastructure prior to getting to the machine. What would that wasted energy be used for? It would be used to reduce the voltage down to a voltage the machine could use, to transmit power, and there are some losses, the biggest being the energy it takes to move the heat from the IT equipment out to the outside environment. And when the outside temperature is higher than you would like the room to be, you would also have to cool the heat transfer mechanism, which is typically water.

With PCF and Blue Waters, we will achieve a PUE in the neighborhood of about 1.18. To give you an idea of how good that is, a typical well designed data center will be 1.4. The lower the PUE, the more efficient the building. If we can gain additional free cooling days that number will be even lower because we'll save more energy.

Q: Do you ever worry about water leaks in the machines?

A: Bringing the water right to the electronics means there is more potential for leaks, but we really haven't seen any in our Power 575 systems that are presently cooled this way. In order to guard against it, we use very high-quality components within the cabinet, and also in each cabinet we have a completely self-contained water-cooling system. In our present product, it's about seven gallons. But the machine would sense a leak and shut off long before we lose seven gallons of water.

Q: What other technologies are employed to increase energy efficiency?

A: After you get past cooling, the next thing is power delivery to the product itself. In the world of power delivery, the higher the voltage the more efficient the power transmission. So the best thing is to always use the highest voltage you can.

In PCF, we'll run directly off line from 480 volts, which is the standard AC voltage in North America. The ability to do that really depends on how good the IT equipments' immunity is to power line disturbances, and Blue Waters' cabinets have exceptional immunity to power line voltage glitches. In the case of PCF, it was a very high-availability environment before we even started, so we took the infrastructure that was there and routed that right into the building. The machines will literally run directly off the voltage that comes out of the substation transformers in the building. By doing that, we only lose about 2 percent in power conversion efficiency, which is an extremely low number.

Q: I've heard you refer to new metrics in computing. What are they?

A: In the world of what most people refer to as enterprise computing—which is really any type of computing done in very large scale—you generally have a lot of equipment and your goal is to get a lot of throughput [a lot of work through the machine]. The higher throughput you need, the more compute power you need. Throughput per watt or throughput per amount of power used is one of the prime metrics in designing the server. Because, of course, not only is it environmentally friendly to have the most throughput per watt, it also saves money, especially with the rising cost of energy.

Also, throughput per the amount of space used is a very important metric, especially when a new building is being constructed. The smaller the space we can put the computer in, the lower the cost of the building will be. Last, another important metric is how much building infrastructure we need in a facility to accommodate a server. How do we transfer the power coming into the building, which is typically high voltage, down to the voltage the machine can use; how do we transfer the heat from the machine out to the outside ambient environment while at the same time keeping the inside ambient environment at some temperature limit we establish? The more lax we're able to make those requirements of the data center, again, the lower the cost of the facility.

Q: What are the common mistakes people make when building a data center?

A: One of the most common mistakes I see is designing the data center to be a little too flexible. It is easy to convince yourself that, when you build a building, you really want to build it to accommodate any type of equipment, but this is at the cost of power efficiency.

Today the best efficiency is to run high-voltage power directly to an IT cabinet, directly water cool like we're doing with Blue Waters. Of course, not every piece of IT equipment is equipped to be directly connected in that fashion. So if you want to be more flexible, you might want a center that is air cooled with some water-cooling capability, and the capability to bring low-voltage or high-voltage power to the cabinets.

Another mistake I see is shorting space. It starts out that a customer has a lot of space, usually because they're replacing some very old equipment with more modern equipment that is inherently smaller for the amount of work that's done. So they convert the extra to meet other company needs and then have no room to add more hardware later. If you need more power and more cooling there often are solutions, but when you're out of space, you're out of space.

Q: What do you see as data center trends?

A: Centralization, consolidation. I see more and more of that. I see companies that had many smaller data centers considering consolidating to two very, very large centers. Most of the time people will want more than one so they have some disaster recovery capability, and they'll be separated by a fairly large distance. But the idea of some very, very large companies wanting to go down to just two data centers, that's definitely a breakthrough.

Another is cost of building construction. Some people spend enormous sums, but really, it gets back to can you design the IT equipment so that it doesn't require too much special capability. And what that really means is that you don't have to build a very special facility, you just have to be able to build the general power and cooling capabilities you need and a good sturdy raised floor. This can save a phenomenal amount of money.

There's a thought that one way to really achieve the same thing is with an approach called container computing, where you actually take a tractor trailer, retrofit it with computing hardware, and then roll that entire trailer on site. And in a similar fashion to what I mentioned they put electricity and water to it. The space is basically the space in the parking lot where you park the trailer. Or the container can be within a facility for those who like the data IT equipment under their roof.

A single Blue Waters rack in itself will be a breakthrough in the industry of medium- to large-scale computing. A single rack containing server, networking and storage capability can replace a small data center and can be placed in a small 11' x 16' (175 square foot) room. All that is needed to power and cool this system is two small water lines and a standard 480 power panel. A second rack will double the compute power, and fits in a 15' x 16' (240 square foot) room.

Imagine fitting an entire data center of today in a room the size of a bedroom. The need to pack a tremendous amount of Blue Waters compute power in an area of just 10,000 square feet in PCF has inherently yielded an architecture that makes housing data center equipment far more economical.

Q. What's been the biggest challenge for you with the Blue Waters/PCF project?

A: The biggest challenge when you are doing something like this is to do it cost effectively. With government contracts the money is lean in the first place because you are trying to do an awful lot with the money you have. This is something all of us who are in the throughput computing arena deal with on a daily basis. A lot of times the way we get by is by using commodity hardware because at least you do have a good understanding of what the costs likely are.

Here, we're doing this with leading-edge, very custom hardware to try to achieve the best energy efficiency and the highest compute density. Having to invent on a schedule, and having to do it extremely cost effectively, is very difficult. That has positively been the biggest challenge. And it's nothing completely unique to the National Science Foundation and to NCSA. Generally, in all these type of large-scale projects this is what you see. Possibly not quite to this degree, I'll say.

But that's been a challenge—trying to do everything the best and to do it cost effectively. □

BLUE WATERS

MORE THAN A FAST, GENERAL PURPOSE PROCESSOR

BLUE WATERS will be based on IBM's multicore POWER7 processor. The machine will employ 200,000+ processor cores and will provide more than 800 terabytes of memory. The POWER7 processors will be packaged in clusters of four, forming standalone SMP nodes called multichip modules (MCMs) that have 32 cores in a module.

Blue Waters is projected to have as much as 500 petabytes of archival disk storage and much more than 10 petabytes of usable disk space. IBM's General Parallel File System (GPFS) and HPSS will be combined into a managed file systems using the GPFS-HPSS Interface (GHI) software. So the apparent disk space a user will have direct access to will be higher by at least an order of magnitude than anywhere today, with corresponding bandwidth increases. The file system and archive will be substantially larger, faster, more reliable, and easier to use than similar systems on today's platforms.

The file system will automate many storage and data transfer tasks done manually by users today. Researchers will have a simplified and easily searched view of their data. They will be able to set lifetime information-management (ILM) policies that establish where their data are stored, how long data are kept in the faster-access file system instead of the tape-based archive, and how the data are backed up and retrieved. This is markedly more efficient than current systems where researchers must log into multiple systems, manually transferring their data, keeping track of where those data are stored, and confirming that transfers have been completed successfully. Blue Waters is also enhancing HPSS by adding Redundant Array of Inexpensive Tape functions to increase resiliency while still fully automating all data storage.

NCSA is testing the GPFS-GHI-HPSS managed file system on interim computing systems and other testbeds.

Blue Waters will be housed at the new Illinois Petascale Computing Facility; the facility's network will be capable of transferring 100 to 400 gigabits of data per second. □

POWER7 AT A GLANCE

Blue Waters will be based on IBM's multicore POWER7 processor. Each POWER7 processor will:

- Include eight high-performance cores, with each core providing 12 execution units.
- Feature simultaneous multithreading that delivers four virtual threads per core.
- Have three levels of cache—private L1 (32KB) instruction and data caches, private L2 (256KB) cache and L3 (32 MB) cache that can be used either as shared cache or separated into dedicated caches for each core, reducing latency.
- Combine the dense, low-power attributes of eDRAM with the speed and bandwidth advantages of SRAM for optimized performance and power usage.
- Have two dual-channel DDR3 memory controllers, delivering 100GB/sec of sustained bandwidth.
- Employ new IBM interconnect technology, providing a high-bandwidth, low-latency interconnect that scales to hundreds of thousands of cores.
- Have six fabric bus interfaces to connect to other cores and groups of cores, providing improved reliability.
- Provide an eight-channel memory subsystem, to enable the solution of memory-intensive problems.
- Provide 32 or more gigabytes of memory per SMP and 2 or more gigabytes of memory per core.
- Support 10 or more data streams.
- Offer vector multimedia extensions on each core with four or more floating-point operations per cycle.

Get in the game

By J. William Bell

The graphics processing units in NCSA's Lincoln cluster speed molecular dynamics simulations that drive the development of detergents and drug-delivery systems.

A FEW YEARS AGO, a graphics processing unit had one job: Thrill videogamers by throwing as many pixels up on the screen as fast as possible. Let them see through their sniper sight in more detail. Reduce the lag between when they press the key on the controller and when their swords clash.

Seeing the processors' power and blazing speeds, researchers have begun moving some scientific work to these processors, which are often called GPUs. In fact, after years of working with scientists on experimental GPU-based systems, NCSA launched the Lincoln supercomputer in 2008. Lincoln includes NVIDIA GPU units, as well as traditional Intel CPUs. GPUs, in other words, have moved into the supercomputing game.

'You use them all the time'

A team from Temple University is already harnessing those GPUs in their daily research. At Temple's Institute for Computational Molecular Science, they use the Lincoln cluster to model surfactants. Surfactants are used in common household products like detergents and shampoo. Researchers are also exploring another class of surfactants as a way of controlling the delivery of drugs in the body and improving their impact.

"These are molecules that you use all the time, but you don't see them," says Axel Kohlmeyer, the institute's associate director. "You can use them to change the properties of liquids. In practice, that means if you have something dirty on your clothes, the surfactant can attach to it and mix with water, so you can wash it away."

By modeling surfactants on a computer, researchers can also wash away expensive and slow laboratory work as they design new products.

But mixtures of surfactants, water, and other molecules are exceptionally challenging to model. They aggregate themselves into micelles, vesicles, and other structures that can trap materials. The self-assembly process takes place at the micrometer scale over the course of hundreds of nanoseconds, and it often includes hundreds of millions of atoms.

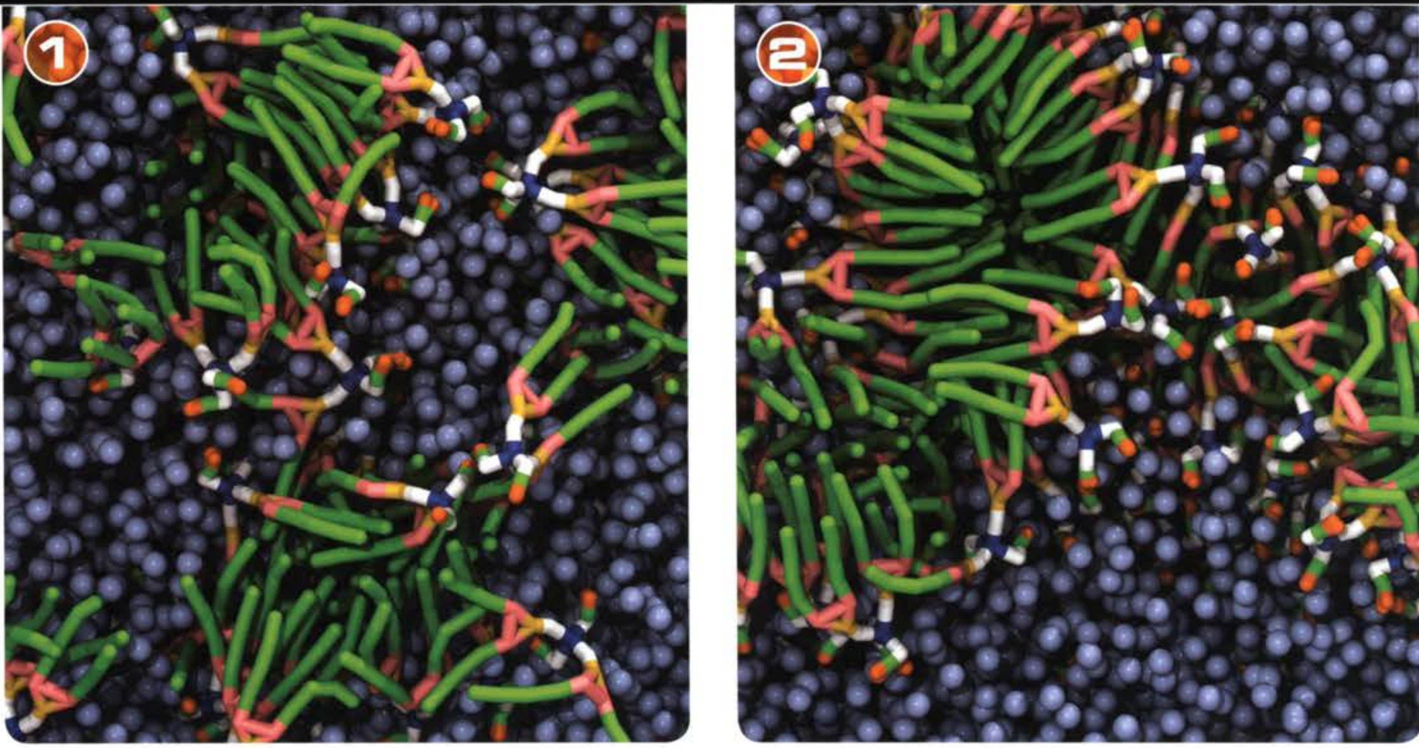
To capture this complicated and long (relatively speaking) activity, the team relies on a clever approach and a powerful simulation code.

'Just a fun summer project'

The approach is known as coarse-grain molecular dynamics. With this strategy, molecules fragments are modeled as spherical "pseudo-particles," dramatically reducing the number of particles and thus the number of particle interactions that must be computed. Three water molecules, for example, might be represented by a single sphere in coarse-grain calculations.

"A natural way to model it is to break a molecule into pieces by their chemical properties, and then sum up the interactions of the fragments into one pseudo-particle each," Kohlmeyer says. Some details are lost, but how the molecules self-assemble and how they interact with other molecules can still be determined with high fidelity.

Self-assembly of non-ionic surfactants (octa-(ethyleneglycol)-docecylether, $C_{12}E_8$) in water from an initial random configuration into a hexagonal structure of spherical micelles by coarse-grain molecular dynamics. These polyetheleneglycol (PEG) surfactants can be used in household products like detergents. They also help crystallize membrane proteins for X-ray structure analysis and to form liposomes for drug delivery. All images in this story were created using VMD from the University of Illinois' Theoretical and Computational Biophysics Group, and they were rendered with the embedded Tachyon renderer.



Self-assembly of a bilayer structure of dendrimeric amphiphiles in water. This simulation demonstrates how the structure of the monomeric molecules can determine the final configuration of the self-assembled structure. The initial configuration was set up with an even distribution of monomers and water. The monomers quickly assemble into "hands" in image 1, then combine into a larger three-dimensional structure in image 2. This structure finally rearranges into a flat bilayer in image 3. This whole process happens in only 20 nanoseconds of coarse-grain molecular dynamics.

The team from Temple published results using this approach in the *Journal of Chemical Theory and Computation* in 2009.

Recently, the group began testing a new simulation code called HOOMD-blue. HOOMD, for short, is a molecular dynamics code written for use on GPUs. It was created in 2007 by the University of Michigan's Joshua Anderson while he was a graduate student at Iowa State University. About a dozen developers around the country, including Anderson, now contribute to the open-source application.

"When I started out, it was just a fun summer project," Anderson says. A new software development kit for GPUs, called CUDA, had just been released by NVIDIA, "and I just wanted to play with it."

Within a couple of months, he had code running 30 times faster on a single GPU than it did on a single traditional processor. Since then, algorithm improvements and a new generation of GPUs have sent that performance number to more than 60 times faster. That "new" generation of GPUs is already more than a year old and the announcement for another performance-doubling hardware generation is expected soon.

A scripting language in HOOMD makes it very extensible and adaptable. In fact, it allowed the Temple team to easily create a parallel version of the code and run on multiple processors simultaneously.

"I didn't envision taking [parallelism] to the level that Axel has done, but I wanted that functionality to be available," Anderson says.

"HOOMD uses many modern techniques of portable and flexible programming, yet keeps it simple and easy enough for people to add functionality quickly and consistently. I wish more scientific software projects would spend that much effort on these fundamental issues. My life would be much easier," Kohlmeyer adds.

'It still blows my mind'

Validation runs of the coarse-grain method on NCSA's Lincoln supercomputer have shown tremendous speedups.

"The outcome is quite spectacular...With two GPUs we can run a single simulation as fast as on 128 CPUs of a Cray XT3," Kohlmeyer says. And with HOOMD, they have a straightforward way of running hundreds of those simulations in tandem.

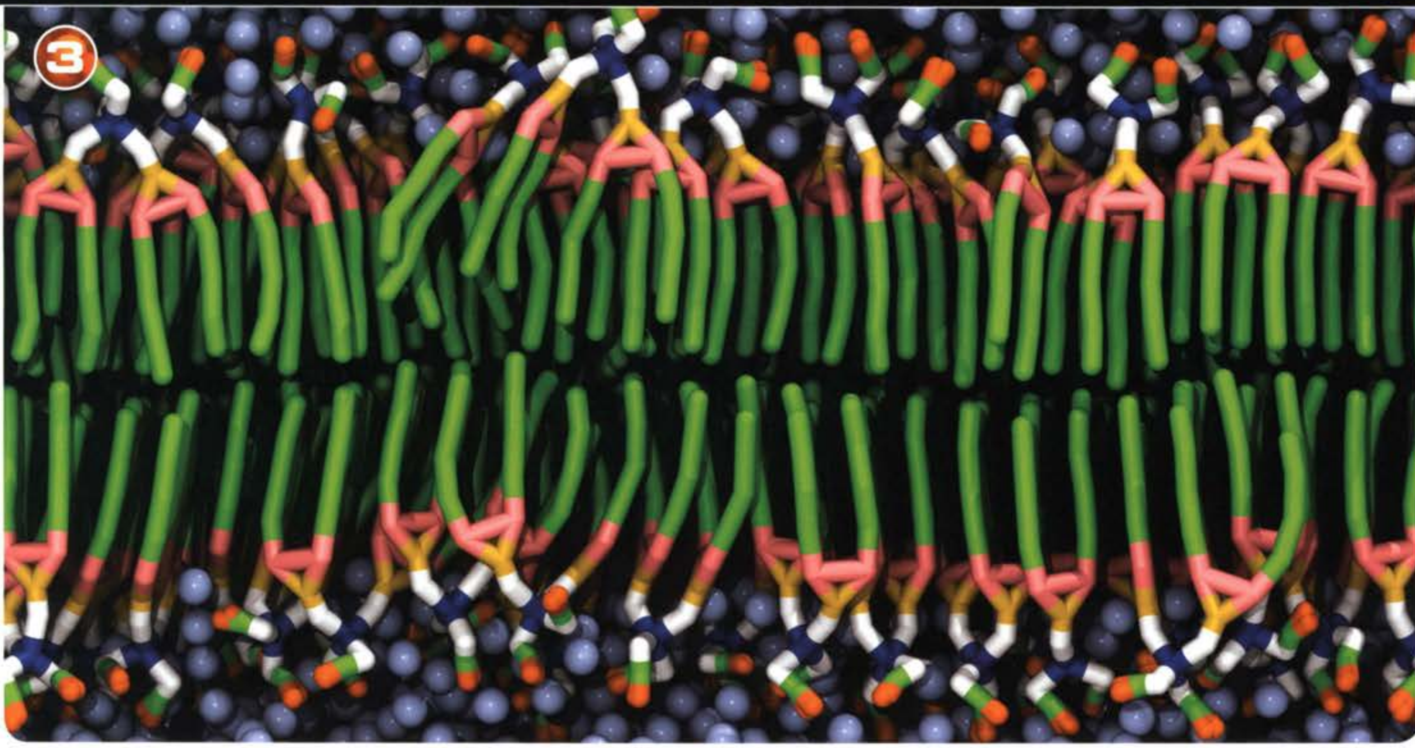
What's the Temple team doing with this approach and computing power? Getting real science done, and gearing up for even bigger simulations.

Using NCSA's Abe supercomputer and partnering with a team of experimental chemists at the University of Pennsylvania, they're simulating self-assembling dendrimeric molecules that can be tailored to particular shapes and properties. Ultimately, these molecules could be used to build customized "containers" for drugs. Self-assembled capsules would be built around the drug, which might otherwise be destroyed as it made its way through the body.

The team plans to move those simulations to Lincoln soon.

"We will be able to screen potential modifications to the individual molecules on the computer and save people tons of hours and money in the lab," Kohlmeyer says. "A machine like Lincoln is perfect for that, as one would need to run many variations at the same time."

"We can try things that were undoable before. It still blows my mind." □



Project at a glance

Team members

Russell H. DeVane
David LeBard
Benjamin Levine
Axel Kohlmeyer
Wataru Shinoda
Christopher J. Wilson
Joshua Anderson
Alex Travesset
Rastko Sknepnek
Carolyn Phillips
Trung Dac Nguyen
Michael Klein

Funding

Department of Energy
National Science Foundation
National Institutes of Health
Procter & Gamble

For more information

www.temple.edu/cst/icms
codeblue.umich.edu/hoomd-blue
www.nvidia.com/object/cuda_home.html

Access online

www.ncsa.illinois.edu/News/Stories/get_game

Not just for graphics anymore

Graphics processing units (GPUs) aren't just for graphics anymore. These high-performance "many-core" processors are increasingly being used to accelerate a wide range of science and engineering applications, in many cases offering dramatically increased performance compared to CPUs.

But many questions surround the use of GPUs. Here are answers to some of the most common ones. You can learn more about GPUs and the GPU resources offered by NCSA and the Institute for Advanced Computing Applications and Technologies at www.ncsa.illinois.edu.

How is a GPU different from a CPU?

CPUs have few (two to eight) large, complex cores, while GPUs have up to a few hundred small, simple cores. Unlike CPUs, GPU cores are not general purpose. They are focused solely on computation, with little support for I/O devices, interrupts, and complex assembly instructions.

What advantages do GPUs offer?

GPUs can deliver up to a teraflop (1 trillion calculations per second) of computing power from the same silicon area as a comparable microprocessor using a small fraction of the power per calculation. That means high performance in a smaller footprint, for a lower cost, and consuming less power.

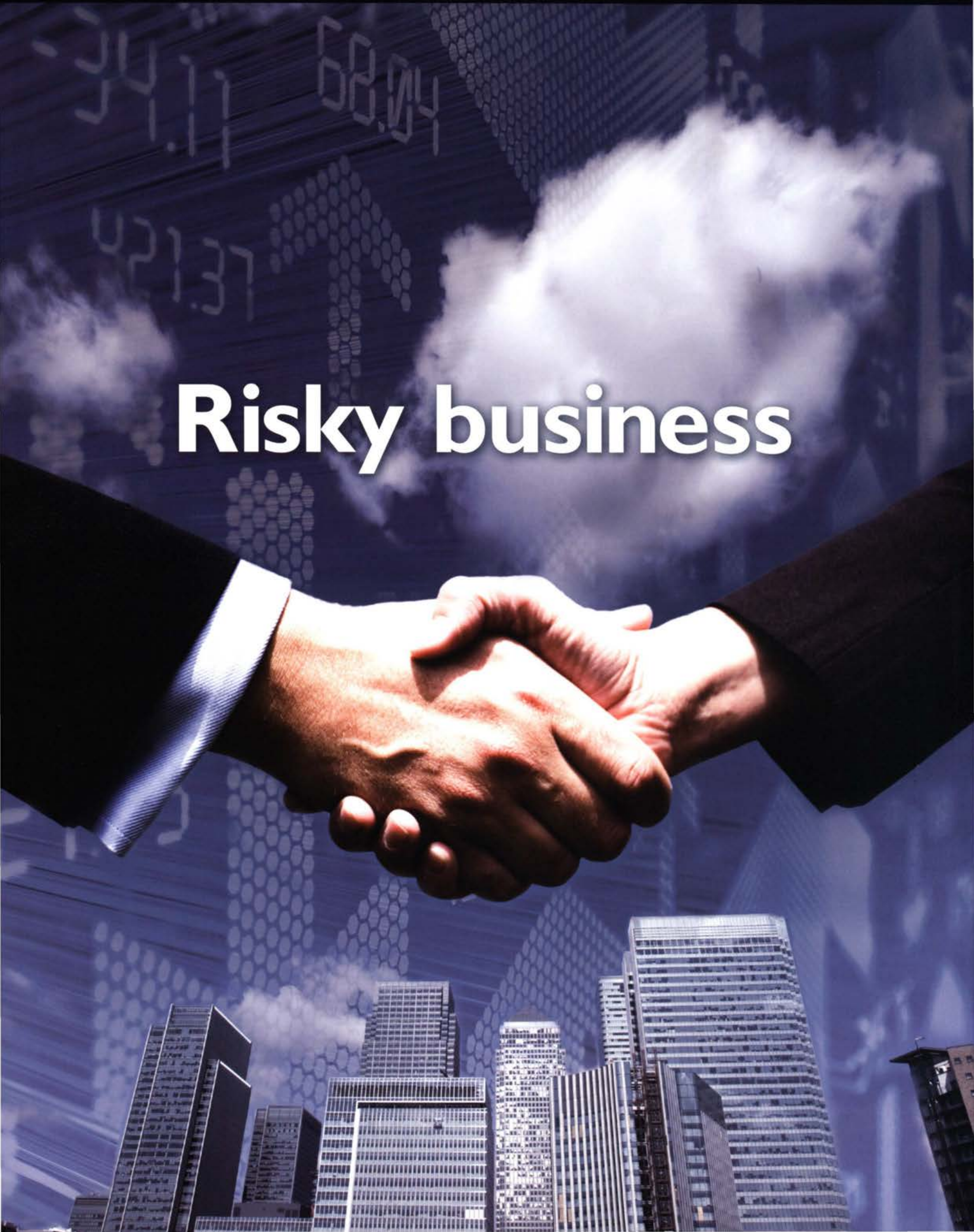
So are CPUs obsolete?

No, because GPUs still require CPUs to access data from disk, to exchange data between compute nodes in a multi-node cluster, and other tasks. CPUs are very good at executing serial tasks and every application has those. And as more and more cores are combined on a single chip, CPUs are becoming parallel as well.

What is the downside of using GPUs?

GPUs are not right for every application. Only applications that have a substantial amount of parallelism can benefit from GPUs. GPUs also require a fresh approach to programming.

Risky business



By Vince Dixon

University of Illinois professors use NCSA computers to study how the economic environment and financial institutions influence entrepreneur behavior.

BEFORE STARTING a software company in Texas, Pat Sullivan discussed with his wife the possibility of opening the firm. His wife feared the risks of starting a new business.

Sullivan reassured her by telling her that in Texas, they can't take your house away, they can't take your last car, and they can't take your kids.

Sullivan was later named Entrepreneur of the Year by *Inc.* magazine and made millions off the business. Stefan Krasa and Anne Villamil, professors of economics at the University of Illinois at Urbana-Champaign, use Sullivan's story to explain their ongoing study of the effects of economic environments and financial institutions on small firms.

The project pinpoints the risks budding entrepreneurs face when starting their businesses and why some entrepreneurs are willing to bear these risks. The professors also wanted to understand the roles financial institutions and credit play in such decisions.

"One question is, why do so many of these entrepreneurs who don't choose to be incorporated not try to protect themselves more?" Krasa says.

Modeling the question

Using NCSA resources, Krasa and Villamil developed a model in 2005 to help understand the answer to this question. With Jamsheed Shorish of the Institute for Advanced Studies in Vienna and the University of Illinois, the researchers have recently extended the model to include the effects of the banking sector.

Understanding how the environment—which includes bankruptcy policies, protections, and rules—and access to credit affects small firms is important in recognizing the overall significance small firms have in an economy, the researchers say.

In the United States, these firms are responsible for more than 50 percent of Gross Domestic Product (GDP) and 45 percent of total private payroll. Small businesses also create 60 to 80 percent of net new jobs annually, including high tech "good jobs."

"Small firms are a very dynamic part of the macro-economy because some people start out small and they eventually become big," Villamil says. "If these firms are not healthy and hiring, that's going to affect [the economy]."

The first half of the project centered on how the economic environment influences entrepreneur behavior. Countries and states have different policies that affect small businesses. Depending on the risks involved with the policies, entrepreneurs in one area may find it easier to start businesses than entrepreneurs in other areas. U.S. institutions favor risk taking, Krasa says. New business owners like Sullivan take advantage of it and find the risks of starting a new business in the U.S. manageable.

Krasa and Villamil use the contracting model to quantify such risks. The model was "computationally intensive," taking 10,000 hours to complete on the NCSA Copper supercomputer. Information on how a firm raises money, the size of the firm's loans or interest rates, and the amount of protection granted by legal codes were included in the model's parameters.

"A real virtue of a computable model is you can look at different policies in a contolled way without testing the effects in the actual economy."

They presented their work at two European conferences in 2007—SAET and the XVI European Workshop on General Equilibrium—and also at the Institute for Advanced Studies in Austria. Their work was published in *Economic Theory* in 2008.

The credit factor

The second part of the project involves expanding the first model to include the role of credit and banking institutions.

"It's tough to get credit in the first place," Krasa says. "But without credit, you can't run a business; it's like without oil you can't drive a car."

Because of the influence small firms have on the economy and job market, the professors wanted to know how access to credit impacts these businesses. Villamil used the current increase in U.S. default rates to demonstrate that if default rates on business loans rise because of poor economic conditions, a chain reaction could form. Banks would fail and workers would lose jobs, perhaps defaulting on their mortgages and other debt.

"So these things are not isolated to small firms," Villamil says. "They affect the economy as a whole."

New models

The project's new model illustrates supply and demand for firms and banks. It is more complex and will take more than 20 times the amount of hours used to complete the former model. The expanded model studies the interaction of many firms rather than focusing on the individual firm and permits the analysis of real time policy experiments.

The research involves three important steps. First, to understand how firms and banks operate and interact, the researchers had to create an economic model.

Next, Krasa, Villamil, and Shorish transform the model into computer code and develop algorithms to compute solutions. The 2005 model used MATLAB programming. The new model needed a much more complex environment because of the added parameters. The professors also wanted to make the computation easily accessible to others to use and test. Python programming seemed to be the best code language to do the job. They are currently in the process of testing this code.

The final stage in the project is to simulate the effects of alternative policy proposals in the model. Economists call this type of research a counterfactual experiment, Villamil says.

In this method, researchers ask a "what if" question and use the model to evaluate the effects. This approach allows one to compare alternative policies and better design regulations without testing the effects in the actual economy.

"That's a real virtue of having a computable model that you can go through and look at different policies in a controlled way," Villamil says.

She used banking crises as an example. While the U.S. has recently experienced its own banking crisis, such problems happen around the world each year. The team hopes their model can help governments and organizations develop better policies to use in times of crisis and create better regulations to prevent them.

The current state of the U.S. economy has raised the stakes of this research. "It certainly made it a much more interesting topic for us," says Krasa. The current economic downturn is an example of what the researchers say they hope their model would prevent.

Other researchers have used supercomputers to study economic policies, but few have used the systematic analyses of this project. Villamil says the opportunity is unique to NCSA and Illinois researchers.

"We're very lucky at the University of Illinois to have access to both the supercomputer itself and also the people at NCSA to discuss these things with," she says.

The supercomputing power at NCSA speeds the entire process and allows the researchers to develop more complex computations. With the stakes set high from the current economic crisis, this is important, she emphasizes.

The two professors say the ultimate goal of the project is to help economies around the world develop policies that could possibly avoid future crises. In order for this to happen, they need the speed of supercomputers to handle complex model computations.

"Before you do a new policy you'd really like to understand how it works in the context of a model rather than trying it out on an entire macro economy," Villamil says. "That's really the exciting part of this; that the computational environment provides a laboratory in which we can do these controlled experiments." □

Project at a glance

Team members

Stefan Krasa
Anne Villamil
Jamsheed Shorish

Funding

National Science Foundation

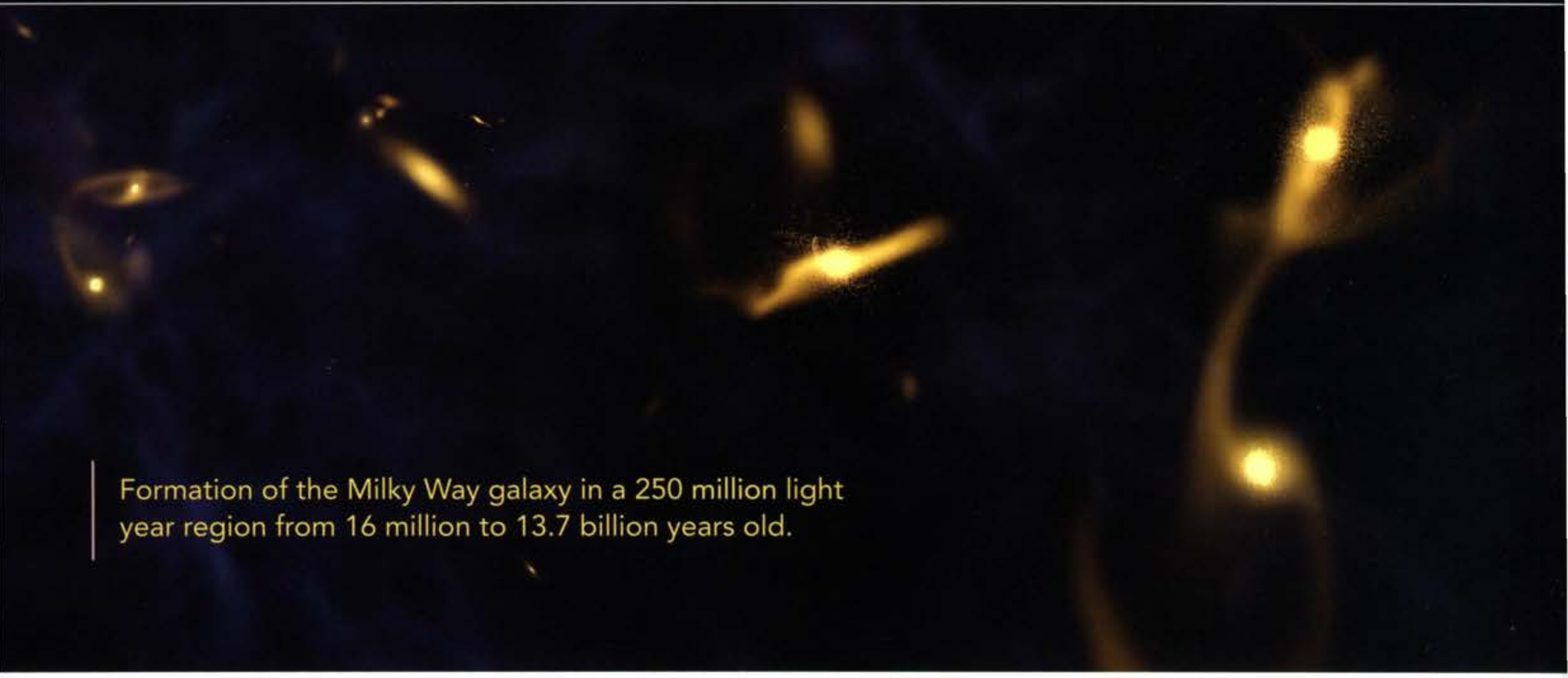
Access online

www.ncsa.illinois.edu/News/Stories/risky_business

Leaving the dark days

by J. William Bell

As part of the Petascale Computing Resource Allocations program, a longtime NCSA collaborator and his team will make the improvements needed to run a popular cosmology simulation code on Blue Waters. ▶



Formation of the Milky Way galaxy in a 250 million light year region from 16 million to 13.7 billion years old.

BRIAN O'SHEA started as an assistant professor at Michigan State University just last year, but he's already been at this a long time. For more than a decade, he's been using NCSA supercomputing resources to simulate how galaxies form in the early universe. He began as undergrad at the University of Illinois working at NCSA with Mike Norman, who is now interim director of the San Diego Supercomputer Center.

"Those were dark days," he says with a chuckle. "We could run a simulation on 128 processors, and I believe I shepherded a single simulation through the machine for an entire year. There were maybe 1,000 galaxies in the entire simulation."

The NCSA relationship continues as O'Shea is one of the first researchers to win a National Science Foundation Petascale Computing Resource Allocations award. These research teams will work closely with the Blue Waters project team at NCSA and the University of Illinois in preparing their codes to run on the sustained-petascale supercomputer.

With Blue Waters, O'Shea expects to see more than 1,000 times the mass resolution and 32 times the spatial resolution when compared to those simulations from the late 1990s. In other words, he expects to probe the universe to much smaller physical scales.

That will translate into simulations of hundreds of thousands of galaxies instead of a thousand galaxies.

Simulations on Blue Waters should allow the team to get a much better look at the first billion years after the Big Bang, a time in the development of the universe that is only murkily understood. "A whole lot of stuff went on in that first billion years...A lot of galaxy formation took place. The universe was dense. Everything was close together. The rate at which things happened was really, really fast," he says.

Keeping up with the Webb

Star gazing is also gazing back in time. Objects are so distant that the light from them takes millions or billions of years to reach us. We're observing things as they appeared way back then. What's happening today won't be visible for eons.

In 2013, NASA will launch the James Webb Space Telescope. Its primary function will be to look back on these most distant—and thus oldest from our perspective—galaxies. Other telescopes with similar capabilities will follow suit.

O'Shea, Norman, and their collaborators will use Blue Waters and other petascale systems to make predictions about what the Webb telescope is going to see and how galaxies formed in the first billion years after the Big Bang. They'll also explore what's known as reionization, the process by which galaxy formation caused cold, neutral gas in the early universe to heat up and eject electrons and significantly change its properties.

"We've been more worried about matching observations at later times. The universe started out with tiny galaxies, and they merged together to make bigger and bigger galaxies over time. So nowadays, we mostly worry about really big galaxies like the Milky Way," O'Shea says.

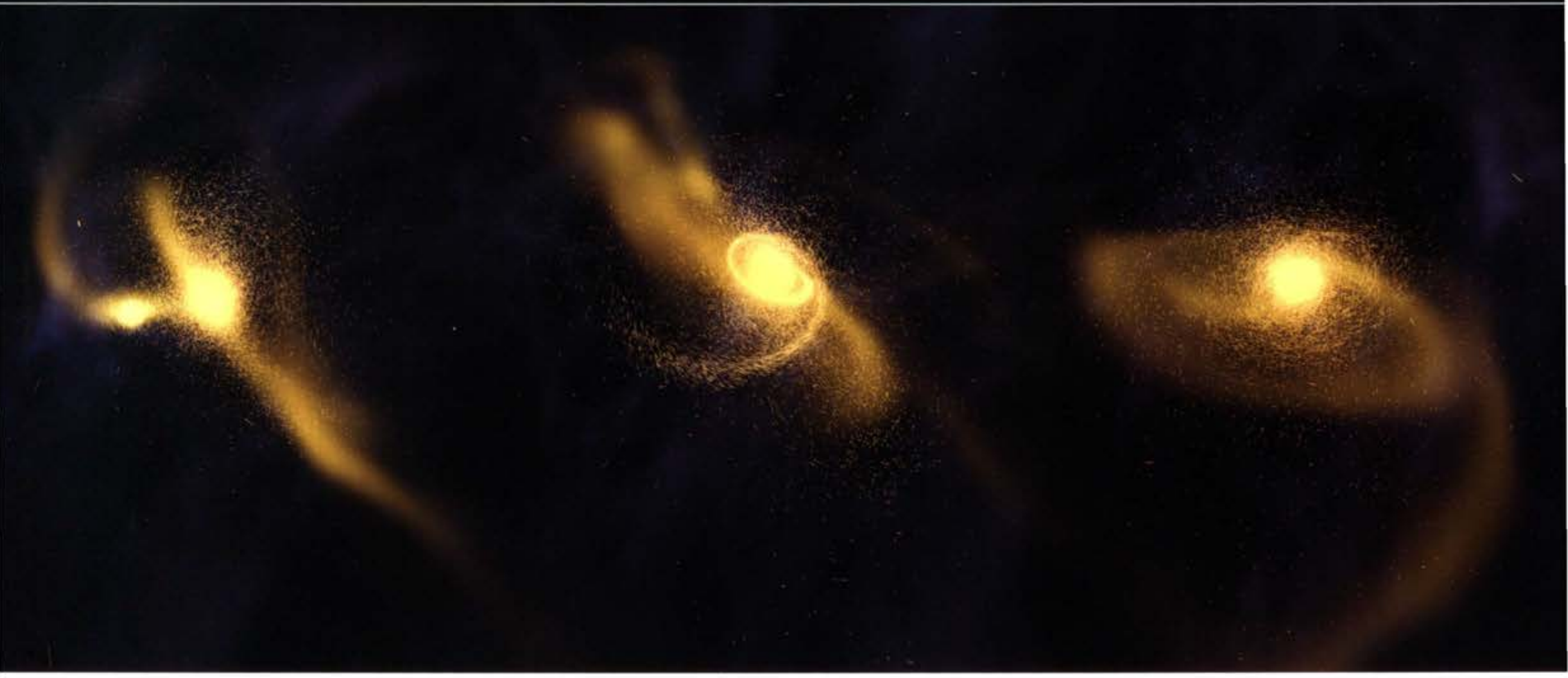
But in the coming era of instruments like the Webb telescope and Blue Waters, the focus will change. "What we're interested in at times early on is maybe one ten-thousandth the size of the Milky Way. And lots and lots of them."

"These are questions that we never would have dreamed of being able to attack on a computer 10 years ago. It's just such a comically large amount of computing time... With Blue Waters, we can attack these huge problems that we never would have been able to before."

Diving into Blue Waters

O'Shea and his colleagues do their work on large supercomputers, day in and day out. Still, running on Blue Waters will require several significant improvements to the simulation code they use.

Called Enzo, the code was conceived in the 1990s by Greg Bryan, who was part of Norman's team at NCSA. The code now has



more than a dozen developers across the country working on it and has users at more than a dozen universities.

O'Shea's work with the Blue Waters team will focus on issues of scaling—unsurprising, given that the code was first developed to run on systems with hundreds of processors and Blue Waters will have hundreds of thousands. Enzo is an adaptive mesh refinement code. It automatically zeros in on the more interesting parts of the model and simulates those sections in greater resolution. This approach makes the overall simulation less expensive computationally at the cost of greater simulation complexity.

"A given point in space is covered by overlapping boxes, grids of cells at different resolutions. You have to keep all of that synced up. The grids need to know if there are finer grids below them, coarser grids above them and so on and so forth," O'Shea says. "That is a bookkeeping nightmare."

Currently, each processor that the simulation is running on keeps a copy of the entire grid hierarchy, tracking where all the cells are and how they are all related to one another. On older simulations, with fewer grids and lower resolution, this wasn't an issue. Each processor might be keeping a few megabytes of such data. On today's simulations, that number has jumped to two gigabytes of data—a thousand times more.

"There's a tremendous amount of redundant information and bookkeeping to do, and that's what gets in the way of scaling to a gigantic extent," O'Shea says.

With this in mind, the team will work on streamlining the way the bookkeeping is done. Instead of each processor keeping all of the grid hierarchy, the code will be rewritten such that each processor will only know the details of the immediate neighbors of the grids it is working on. They also plan to introduce a chaining mesh into the code, which allows the processors to call for additional information from more distant grids if it is needed.

The team will also shift Enzo over to a hybrid parallelism model, using MPI to communicate between nodes on supercomputers and OpenMP within a node. Nodes on supercomputers refer to collections of processors that, in this case, share memory. Nodes are then connected to one another by ultrafast networks. By combining different means of swapping information among processors depending upon how fast the connection between the processors is, researchers using the code will get the best of both worlds.

"Those changes are going to give us huge improvements in performance," O'Shea says. "It'll help performance on any system, but it's what will actually allow us to do computation on Blue Waters at all." □

Project at a glance

Team members

Brian O'Shea
Michael Norman
Robert Harkness
James Bordner
Matthew Turk

Funding

National Science Foundation

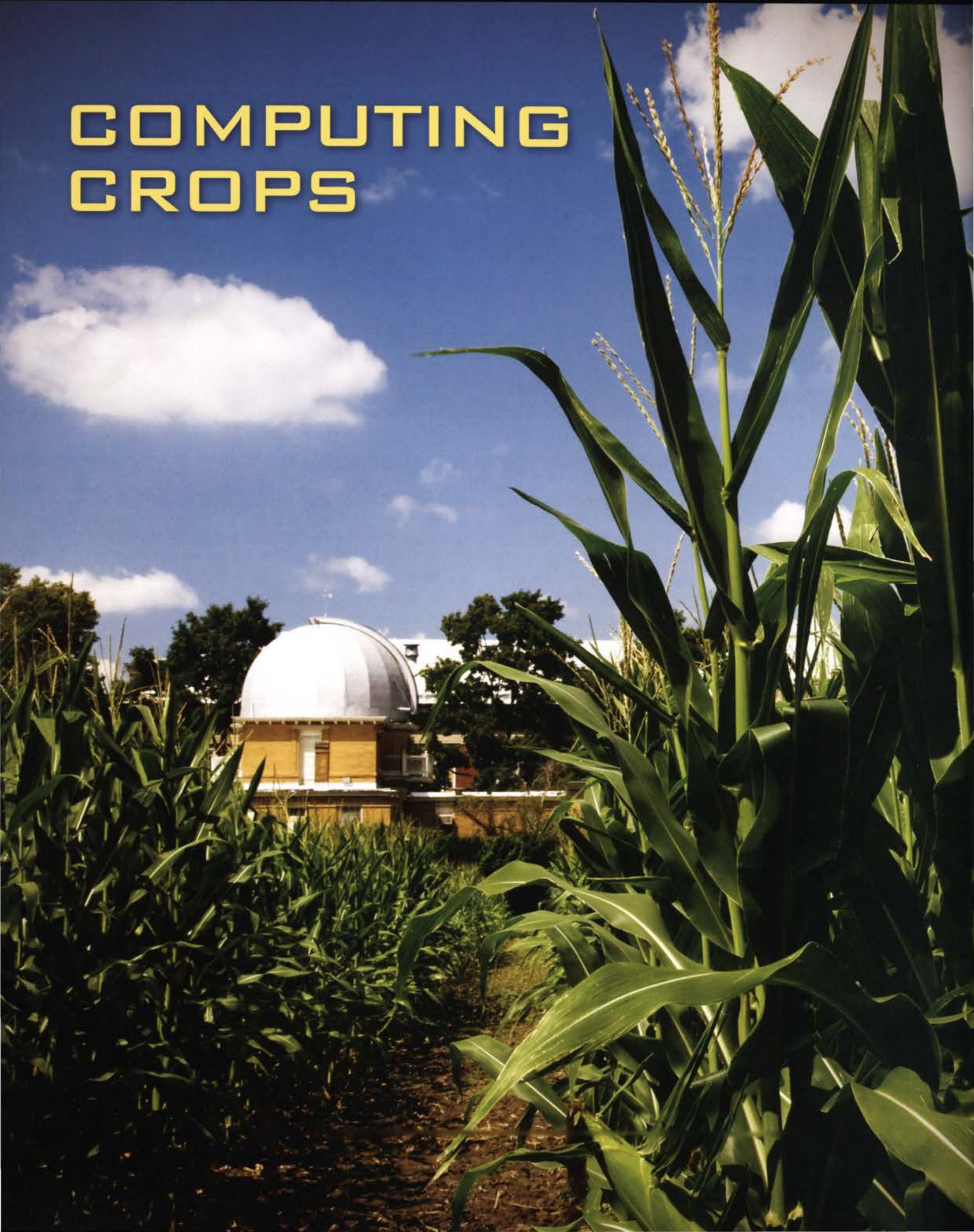
For more information

www.pa.msu.edu/~osheabr/index.html
lca.ucsd.edu/projects/enzo

Access online

www.ncsa.illinois.edu/News/Stories/dark_days

COMPUTING CROPS



By Trish Barker

A collaboration between University of Illinois Extension and NCSA is putting tools for scientific inquiry and learning at 4-H'ers fingertips.

NCSA AND UNIVERSITY of Illinois Extension worked together to produce an online learning environment that incorporates scientific modeling. The site will be used by Illinois youth participating in 4-H, a land-grant university outreach program that serves more than 6 million youths across the United States.

4-H has made science, engineering, and technology one of its core focus areas, so Extension specialist Lisa Bouillion-Diaz was interested in ways to update long-standing programs, such as the 4-H curriculum on crop and soil science, with opportunities for young people to get hands-on experience with the latest research and tools used by scientists.

A mathematical model developed by Stephen Long and other researchers at Illinois' Institute for Genomic Biology was a natural fit. The Windows Intuitive Model of Vegetation response to Atmospheric and Climate Change (WIMOVAC) is a tool to model plant growth and investigate the impact of changes in atmospheric carbon content on vegetation.

NCSA provided the final necessary ingredient—cutting-edge tools for the analysis and visualization of data. NCSA staff developed a Digital Synthesis Framework that integrates data from multiple sources, enables on-demand execution of scientific workflows, and provides multiple visualization and analysis widgets through dynamically generated web pages. To enable multiple users to run models simultaneously, NCSA also provides a scalable virtual machine environment that distributes modeling runs over a cluster of computers.

The final result is iGrow, an interactive website (http://igrow.ncsa.illinois.edu/) where 4-H participants (and eventually a wider public audience) can learn, ask questions, and carry out scientific experiments, receiving real-time results. So far, the site includes three modules, enabling users to:

- Select locations on a map and compare corn and soybean yields in those regions.
- Input CO_2 concentrations and see how the WIMOVAC model predicts this will impact corn and soybean yields.
- Alter seed spacing and see how this affects crop yields.

"This isn't like any other website where you get canned answers to questions. This is actual real-time data analysis being conducted with the same technological tools that scientists and practitioners

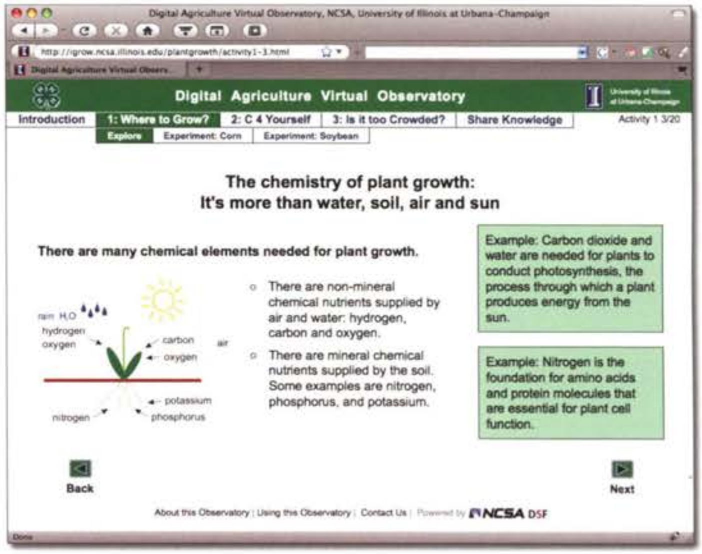
Agriculture researchers at the University of Illinois grow crops at the Morrow Plots. 4-Hers using iGrow can choose a virtual version of Morrow Plots to grow their virtual crops.

have available to them," says Bouillion-Diaz. "To know as a young person that you have access to the same tools as scientists do, and to appreciate the role of those tools in addressing today's problems, is part of the career awareness and science excitement we hope to build."

Sixth- and seventh-graders at a Chicago-area middle school tested the iGrow website in the spring, providing valuable feedback. After some final adjustments and testing, Bouillion-Diaz expects to roll out the site to several Illinois 4-H clubs this fall. As 4-H'ers work on the crop and soil curriculum, the iGrow website will be an additional resource and tool for them to extend and apply their learning.

Both Bouillion-Diaz and Jim Myers, leader of NCSA's Cyberenvironments and Technologies Directorate, see potential for the site to be expanded with modules to address other topics, such as fertilization and crop rotation, and for the same concept and underlying technologies to be applied to other areas of inquiry.

"I see this collaboration as having created a prototype of a learning space that we could apply to many other topic areas," says Bouillion-Diaz. □



A module on the iGrow website that helps teach students about the the best locations for growing crops.

Project at a glance

Team members

Raouf Berrabah
Lisa Bouillion-Diaz
Dennis Bowman
Dairui Chen
Rob Kooper
Stephen P. Long
Luigi Marini
Terry McLaren
Bill Million
Jim Myers
Michal Ondrejcek
Anand Padmanabhan
Andrew Wadsworth
Wen Wu Tang
Xinguang Zhu

Funding

Office of Naval Research

For more information

igrow.ncsa.illinois.edu
cet.ncsa.uiuc.edu/projects.html
www.life.illinois.edu/plantbio/wimovac

Access online

www.ncsa.illinois.edu/News/Stories/computing_crops

Framework for digital scholarship

According to Jim Myers, leader of NCSA's Cyberenvironments and Technologies Directorate, the Digital Synthesis Framework underlying iGrow can be used to provide data analysis and visualization capabilities for virtually any topic. The same tools already are the underpinnings of an interactive interface to look at sensor data from Corpus Christi Bay and a system that generates real-time precipitation estimates from weather radar data, for example.

The Digital Synthesis Framework also keeps track of data provenance—the connection between model outputs and the model, parameters, and input data used to create them.

Myers sees this technology as helping science move into a new age of digital scholarship. While today a scientist could read a paper about a colleague's research results and then try to recreate or extend the work by tracking down the data, downloading the software, and trying to guess at the precise workflow used, in the era of digital scholarship all of these tools and services will be readily available and easy to use.

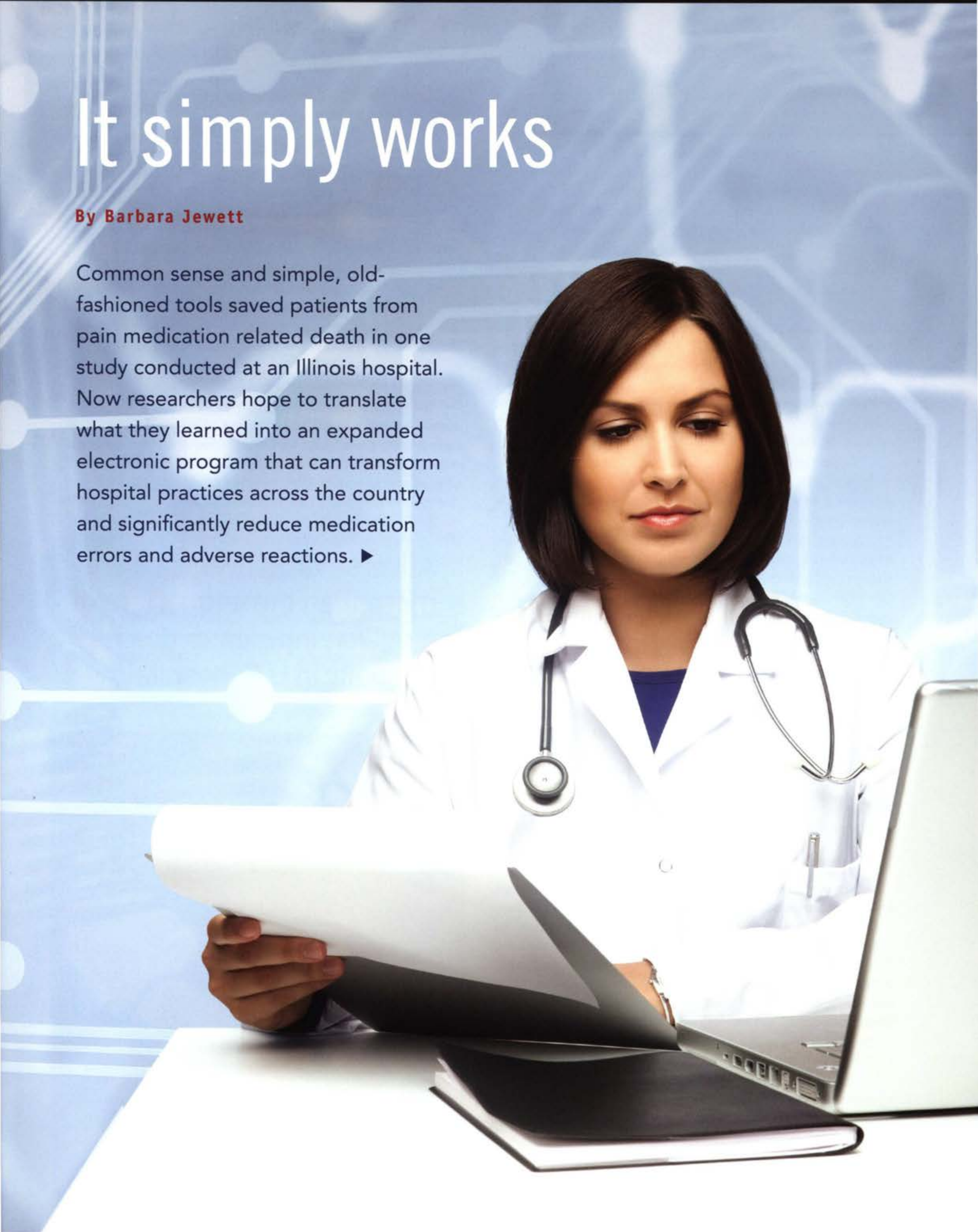
"We're increasing the richness of what we can give to people and getting more fidelity in the transfer of your research environment to the next person," Myers says. "Papers are already linking to data. Soon there will be links to the full procedure used in the research and to a live environment where the next person can quickly recreate and extend the work.

"Scientists 'stand on the shoulders of giants,' but it can take an awful long time to climb up on their shoulders, and we want to speed that up." □

It simply works

By Barbara Jewett

Common sense and simple, old-fashioned tools saved patients from pain medication related death in one study conducted at an Illinois hospital. Now researchers hope to translate what they learned into an expanded electronic program that can transform hospital practices across the country and significantly reduce medication errors and adverse reactions. ▶



IT'S ESTIMATED that adverse drug events (ADE) cause more than three-quarters of a million injuries or deaths annually in U.S. hospitals and that hospitalized patients are subjected to an average of one medication error per day.

But a team of researchers, including Ian Brooks, head of NCSA's health sciences group, made an intriguing observation: prescriptions are medical algorithms. What would happen, they wondered, if software design principles and debugging methods were applied to improving the quality of prescriptions used in a hospital?

ADEs and medication errors are disproportionately severe when they involve opioids used to treat pain. One in four of all fatal ADE among hospitalized patients are associated with the use of opioids, drugs such as Vicodin, OxyContin, morphine, and fentanyl. So the team—which, in addition to NCSA's Brooks, was composed of nurses, pharmacists, physicians, clinical pharmacologists, quality assurance specialists, and statisticians from the University of Illinois College of Medicine in Peoria, OSF Saint Francis Medical Center in Peoria, and Jesse Brown Veterans Affairs hospital in Chicago—set their sights on reducing the rate of opioid ADEs.

"A prescription is a treatment plan. And that treatment plan is, in its most general sense, an algorithm," says Brooks. "So you can apply the same processes to a prescription as you can to a computer science program."

To test this hypothesis, the team created and debugged a "Patient-Oriented Prescription for Analgesia" (POPA), a pain management protocol that was followed for adult patients at OSF Saint Francis Medical Center in Peoria, Illinois, over a five-year period. The results were astounding: while there were seven severe or fatal patient ADEs in one month during the study's first year, as the POPA protocols were introduced and consistently followed this number steadily declined, reaching zero for the study's final six months. These results were published in Clinical Pharmacology and Therapeutics in 2008.

The initial POPA study concluded in December 2002. In 2003, the POPA protocols were implemented hospital-wide. Amazingly, as of February 2009, the last month for which Brooks has information, the hospital's severe or fatal ADEs related to pain management has remained at zero. That's right, not a single severe or fatal opioid ADE in the hospital in more than six years.

Back to basics

The techniques employed were fairly simple. Once anesthesia and initial surgical pain medicines were out of the patient's system, non-opioid analgesics, such as acetaminophen, ibuprofen, or ketorolac, were administered on a fixed round-the-clock schedule. This cut patients opioid requirements in half. The highly potent opioid fentanyl was then given through a subcutaneous catheter—avoiding the interruptions that can occur with intravenous administration of drugs. The fentanyl was provided via a patient-controlled analgesia pump, thus allowing the patient to have more control over the amount of pain relief.

Patients' pain severity was assessed on a fixed schedule with a visual-analog pain scale—a device that looked like an old-fashioned slide rule. Patients slid the marker to indicate their pain level, from no pain at the left edge to intolerable pain at the right edge. The side of the pain gauge the patients saw was plain, while the underside had numerical markings from zero to 10.

After the patient noted their pain level, the nurse would flip the gauge to read the number, record it on a paper POPA prescription form, and then follow the specified protocol for that pain level. A fingertip pulse oximeter was also used to record the amount of oxygen in the patient's blood. A falling blood oxygen level is an early sign of opioid-associated respiratory depression.

In addition to including explicit instructions for pain medication dosing, pain severity monitoring, and pulse oximetry, POPA includes orders to handle common post-surgical complaints such as nausea and constipation, and most importantly, detailed instructions for recognizing and responding to severe opioid-associated ADEs.

Expanding POPA

The "prescriptions are programs" insight validated by the POPA study, combined with the increasing use of computers on hospital wards and the current push for the expansion of electronic medical records, means the time is right to pursue POPA's potential.

Adverse drug events cause more than three-quarters of a million injuries or deaths annually in U.S. hospitals...

By using POPA, the hospital has gone more than six years without a severe or fatal adverse drug event related to pain management.

Brooks says the POPA team has regrouped into a new one that includes computer science professors from the University of Illinois, pharmacists, clinicians, Veteran's Affairs hospitals, and the Institute for Safe Medical Practices. This team has three objectives, he says.

The first is to make an electronic POPA to interact with hospital medical record systems. Because there are various types of electronic medical records systems, developing an electronic POPA will be challenging, says Brooks. Widespread POPA adoption depends upon creating a tool that can be integrated into all, or nearly all, of the records systems currently on the market.

Another objective is to make the protocols adaptable to other diseases, such as treatments for diabetes or congestive heart failure. Many disease treatments rely on established best practices, making the protocol structure of explicit procedures and subroutines a good choice for standardizing care.

Lastly, the team wants to develop an electronic framework that can support multiple types of treatments. Since many hospital patients have more than one issue, medical staff and the patient would benefit from having all of their treatment plans and medications in the protocol format.

The team is just beginning their work on these new objectives, but they hope it won't be too many years before hospitals and the patients they serve will be benefiting from them.

Why POPA worked

POPA empowered the nurses to rapidly respond. The measurements were easy for the nurses to convert directly into action as the POPA procedures and subroutines were explicitly laid out: First you do a, then b, then c. If you observe x, you do y.

"The ward nurses loved it," says Brooks.

Another facet of POPA's success that was equally simple—yet not widely employed prior to the study—was around-the-clock use of common non-prescription painkillers that have a lower incidence of adverse effects. Maintaining a steady dose of those analgesics aided patients in managing their pain, often reducing a patient's need for stronger painkillers.

POPA is powerful but simple. When a prescription makes sense to a nurse and patient, it is more likely to be properly executed. Which bodes well for the future success of the expansion into electronic POPAs. □

Project at a glance

Team members

S.M. Belknap	A. Peterson
H. Moore	J. Akeson
S.A. Lanzotti	T. Maurer
P.R. Yarnold	R.C Soltysik
M. Getz	G.A. Storm
D.L. Deitrick	I. Brooks

Funding

U.S. Food and Drug Administration
Caterpillar
OSF Saint Francis Medical Center

Access online

www.ncsa.illinois.edu/News/Stories/Painmgt

American-Chinese Cyberinfrastructure and E-Science Workshop

September's American-Chinese Cyberinfrastructure and e-Science Workshop (ACCESS 2009) was the first of a series of workshops to bring together researchers, educators, users, and practitioners in the area of cyberinfrastructure and e-Science in China and the United States, and to foster international collaboration and cooperation in this area between the two countries. The workshops provide a forum for sharing cutting-edge research, education, and training experiences covering all aspects of cyberinfrastructure and e-Science, ranging from specific cyberinfrastructure components and capabilities to applications, industrial relations and partnerships, and user support. Participants explore and develop tangible strategies and action plans for collaborative projects and strategically important cooperative agreements.

Stephen Hawking narrates NCSA visualizations

Renowned physicist Stephen Hawking narrates the science behind the "greatest hits" of NCSA's Advanced Visualization Laboratory in a new outreach production. These artful high-definition 3D animations of black holes and other phenomena were a key component of Quantum to Cosmos: Ideas for the Future, a 10-day festival held in October to mark the 10th anniversary of Canada's Perimeter Institute for Theoretical Physics.

NCSA is a Perimeter Institute partner and sponsor of the Q2C 3D exhibit. Professor Hawking is a Distinguished Research Chair at Perimeter Institute and is Honorary Festival President. He last worked with AVL in preparation for iGrid 2002 in a collaboration demonstration at his Cambridge University lab.

The collection of educational visualizations is on view at NCSA and eDream (the Illinois Emerging Digital Research and Education in Arts Media Institute), which is dedicated to promoting arts that are conceived, created, and conveyed through digital technologies. edream and the Advanced Visualization Laboratory are led by Donna Cox.

The AVL team includes Robert Patterson, Matthew Hall, Stuart Levy, Jeff Carpenter, Alex Betts, and Deanna Spivey.

Students across the country participate in Virtual School

Dozens of graduate and doctoral students from a wide range of disciplines participated in two summer school courses offered by the Virtual School of Computational Science and Engineering, which was established to help today's students learn all they need to know to become tomorrow's innovators in high performance scientific computing.

Two weeklong courses were offered this summer: Scaling to Petascale and Many-Core Processors. Participation in the courses expanded dramatically; while fewer than 50 students could be seated for the inaugural course at NCSA in 2008, this year HD video capability enabled students to take the course from multiple locations. For Scaling to Petascale, students were assigned to either NCSA at the University of Illinois, the National Institute for Computational Sciences in Oak Ridge, Tennessee, Louisiana State University, or the University of Michigan. For the many-core course, students participated from NCSA, the University of Michigan, the Ohio Supercomputer Center at The Ohio State University, and the Electronic Visualization Laboratory at the University of Illinois at Chicago.

More than 100 students participated in the Scaling to Petascale course, and 130 attended the Many-Core Processors course.

Streaming video also was offered, so even un-registered students had the option to watch lectures from their home or office computers. Video lectures and other materials are archived on the course websites:

- **Scaling to Petascale:** www.greatlakesconsortium.org/events/scaling/agenda.html
- **Many-Core Processors:** www.greatlakesconsortium.org/events/manycore/agenda.html

For more information on 2010 summer courses, visit: www.greatlakesconsortium.org/education/VirtualSchool.

Connectivity provider Darkstrand partners with NCSA

Darkstrand Inc., which provides high-speed connectivity via a 12,000-mile continuous optical network that connects 28 U.S. cities and 187 leading labs and universities, will collaborate with NCSA's Private Sector Program to help corporations shorten the path from discovery to product development.

U.S. corporations connecting to Darkstrand will now gain access to NCSA's research and technological capabilities along with those of other Darkstrand Network partners.

Over the years, a third of FORTUNE 50 companies have partnered with NCSA.

For more information, go to industry.ncsa.illinois.edu, or contact Merle Giles, mgiles@ncsa.illinois.edu.

I-CHASS names new director

Marshall Scott Poole, an NCSA senior research scientist, has been appointed director of the University of Illinois' Institute for Computing in Humanities, Arts, and Social Science (I-CHASS). Poole is also the David and Margaret Romano Professorial Scholar and Professor in the Department of Communication.

At NCSA, Poole is working to build a relationship with the Costa Rican government in the area of emergency management systems and is the co-PI on the Virtual Worlds Exploratorium project, which studies behavior of individuals and teams in the massive multiplayer online game EverQuest II.

The mission of I-CHASS is to identify, create, and adapt computational tools that advance research and education, particularly in the application of high-performance computing to the humanities, arts, and social sciences. The institute is supported by NCSA and the Illinois Informatics Institute (I3), with funding from the Office of the Provost.

NCSA, I-CHASS, and NICS provide 3 million hours of computing time

The Institute for Computing in the Humanities, Arts, and Social Science (I-CHASS), NCSA, and the National Institute for Computational Sciences (NICS) at the University of Tennessee, Knoxville, recently announced that three million hours of supercomputing time will be provided to projects that are pushing the boundaries of humanities, arts, and social science discovery. Applications just closed for the two million hours available at NICS and will be announced in December. Five projects totaling one million hours of computing time at NCSA have been announced. The new projects are:

- **Census Without Boundaries**, led by the University of Illinois' Zorica Nedovic-Budic and City University New York's Jochen Albrecht.
- **The Credit Crunch:** An Evaluation of Alternative Policy Responses with High-Performance Computing, led by the University of Illinois' Stefan Krasa, Anne P. Villamil, and Jamsheed Shorish. (See story on page 12.)
- **Networked Environment for Music Analysis:** Structural Analysis of Large Amounts of Music Information, led by the University of Illinois' J. Stephen Downie, McGill University's Ich Fujinaga, and Southampton University's David De Roure.
- **The Tambora Project,** led by the University of Illinois' Gillen Wood and Don Wuebbles.
- **18thConnect:** From PDF Images to Clean Data Sets, led by the University of Illinois' Robert Markley.

For more information on I-CHASS and these projects, please visit: www.chass.illinois.edu.

NCSA receives almost $900,000 to build community of science education advocates

NCSA recently received almost $900,000 from the National Science Foundation's Robert Noyce Teacher Scholarship Program to create a community of science education advocates who are expert in 21st century science and pedagogy and who will be well prepared to teach in today's rural high school classroom.

This project builds on the success of the Institute for Chemistry Literacy through Computational Science (ICLCS) by deepening teachers' understanding of computational methods and their role in the chemistry classroom. Selected educators will become computational chemistry champions and have the support to earn national recognition. Teachers will participate in a research experience to better understand the nature of science and will work with University of Illinois chemistry faculty to better prepare students for college-level work. By the project's end, participants will gain National Board Certification and the Illinois Master Teacher designation. The participating teachers will become advocates of science education in their communities, school districts, and the state of Illinois.

The first group of 15 educators selected for the new program is from the first cadre of ICLCS fellows, who have completed all three years of the program.

Begun in 2006, ICLCS is a partnership among NCSA, the Department of Chemistry and the College of Medicine at the University of Illinois at Urbana-Champaign, and A-C Central Community Unit School District 262 in Chandlerville. ICLCS is strengthening rural high school teachers' knowledge of the application of chemistry by providing intensive hands-on training in the use of computational chemistry tools and technologies during successive summer institutes. Teachers and mentors also communicate and collaborate online throughout the school year.

For more information on the program, see www.iclcs.illinois.edu.

NCSA's Peter Bajcsy to guest-edit special issue of ACM journal

NCSA researcher Peter Bajcsy and colleagues Thomas Haenselmann (University of Mannheim, Germany) and Shao-Yi Chien (National Taiwan University) will guest edit a special issue of the journal ACM Transactions on Multimedia Computing, Communications and Applications to be published in fall 2010 that will focus on multimedia sensor fusion.

In this special issue, surveys and original work on the joint analysis of multiple sensors will be addressed. These may be (but are not limited to): movement, acceleration, vibration or the tilt of a device; data from force feedback devices, pulse clocks, etc.; temperature, humidity and brightness; the presence of other wireless mobile devices or base stations; information from ZigBee appliances; images from multiple or self-propelled cameras; and images from camera arrays and infrared cameras.

NCSA researchers receive CI security software grant

Jim Basney, Von Welch, and Randy Butler of NCSA's Cybersecurity Directorate have received a two-year $400,000 grant from the National Science Foundation to maintain and provide critical enhancements for cyberinfrastructure (CI) security technologies developed at NCSA and to foster science and engineering by helping additional communities build secure CI on these technologies.

The new project, called "CILogon," will support the continued community-driven development of the MyProxy, GridShib, and GSI-OpenSSH software. MyProxy is a globally used grid credential management service. GridShib bridges campus to grid identity management systems, facilitating seamless access from campuses to the NSF computational centers, observatories, and other major projects. GSI-OpenSSH provides a single sign-on remote login and file transfer capability using grid security.

For more information about NCSA's cybersecurity research and development, see: security.ncsa.uiuc.edu.

NCSA researchers receive patent

NCSA research programmer Alan Craig and a colleague have received a patent for their method of determining the completeness of a knowledge base by mapping the corpus and locating weak links and gaps between important concepts.

Craig, who is also the associate director of human-computer interaction for I-CHASS, and Kalev Leetaru, a former NCSA staffer who is now coordinator of information technology and research for the University of Illinois' Cline Center for Democracy, were building databases using automatic Web crawling and needed a way of knowing when to stop adding to the collection. "Identifying Conceptual Gaps in a Knowledge Base" is the patented result.

Using any collection of information, Craig and Leetaru's method graphs the data, analyzes conceptual distances within the graph, and identifies parts of the corpus that are missing important documents. The system then suggests additional concepts that best fill the gaps, creating an otherwise non-existent link between two related concepts. Leetaru says it helps users to complete knowledge bases with information they are initially unaware of.

NCSA staffers author books

NCSA senior security engineer Adam Slagell has co-edited a book on computer security that will be available in a few weeks. *Collaborative Computer Security and Trust Management* combines perspectives of leading researchers in collaborative security, covering topics such as trust-based security, threat and risk analysis, and data sharing.

Slagell is the security architect and policy developer for the Blue Waters project, and will be developing the operational security program for GENI. His co-editor, Jean-Marc Seigneur, is assistant professor at the University of Geneva.

A book on virtual reality co-authored by NCSA staffer Alan B. Craig with William R. Sherman and Jeffrey D. Will is now available. *Developing Virtual Reality Applications* details several virtual reality applications and how they are used in a variety of fields. The authors examine what makes the applications workable and how principles and theories of virtual reality are applied.

Craig has worked for NCSA for more than 20 years. He is a research programmer and also the associate director of human-computer interaction for I-CHASS.

Hakan Gunaydin, Kendall Houk, and Vidvuds Ozolins
University of California at Los Angeles

A new solution to a decade-old chemical mystery could be the first step to making hydrogen-powered vehicles commercially practical.

Since 1997, hydrogen researchers have known that titanium allows hydrogen to be generated at lower temperatures and with higher efficiency, which means hydrogen can be stored onboard a vehicle at realistic pressures and temperatures. What they didn't understand was how it happened. Using the hydride sodium alanate as a starting point, UCLA researchers Hakan Gunaydin, Kendall Houk, and Vidvuds Ozolins finally figured out just how titanium acts as a catalyst, reacting with metal hydrides that can store hydrogen and release it in gas form when heated. The method can now be used to analyze other materials that would make for better storage systems than sodium alanate.

The team says that by figuring this out computationally using NCSA's Cobalt and clusters at the California Nanosystems Institute, engineers can use the results to create the lightweight, high-density on-board hydrogen storage system a vehicle requires. Their work was published in the Proceedings of the National Academy of Sciences in 2008. This project was funded by the Department of Energy.

Walter Wilcox and Ron Morgan
Baylor University

Lattice quantum chromodynamics (LQCD) provides a framework where theoretical physics and applied mathematics come together to provide insights into the behaviors of physical quantities such as quarks and gluons, and ultimately predict the outcome of experiments.

LQCD is formulated on a grid, or lattice, of points in space in time. Quarks and gluons may reside only on lattice points and can only travel along lines between them. The smaller the spacing between the vertices, the more computer power is needed.

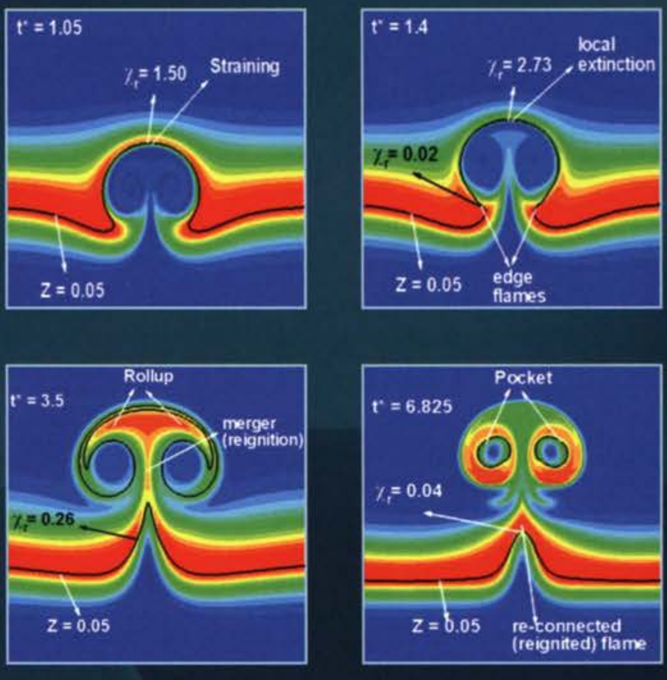
Walter Wilcox and Ronald Morgan of Baylor University are making major advances in the iterative solution of linear equations in QCD and other scientific areas. The team used NCSA supercomputers to propose and evaluate basic algorithmic improvements, and pioneered so-called matrix "deflation" techniques in the context of GMRES and BiCGStab to speed up lattice QCD calculations.

Their work was published in the Proceedings of Science, and presented at the 25th International Symposium on Lattice Field Theory. This work was partially supported by the National Science Foundation and Baylor University.

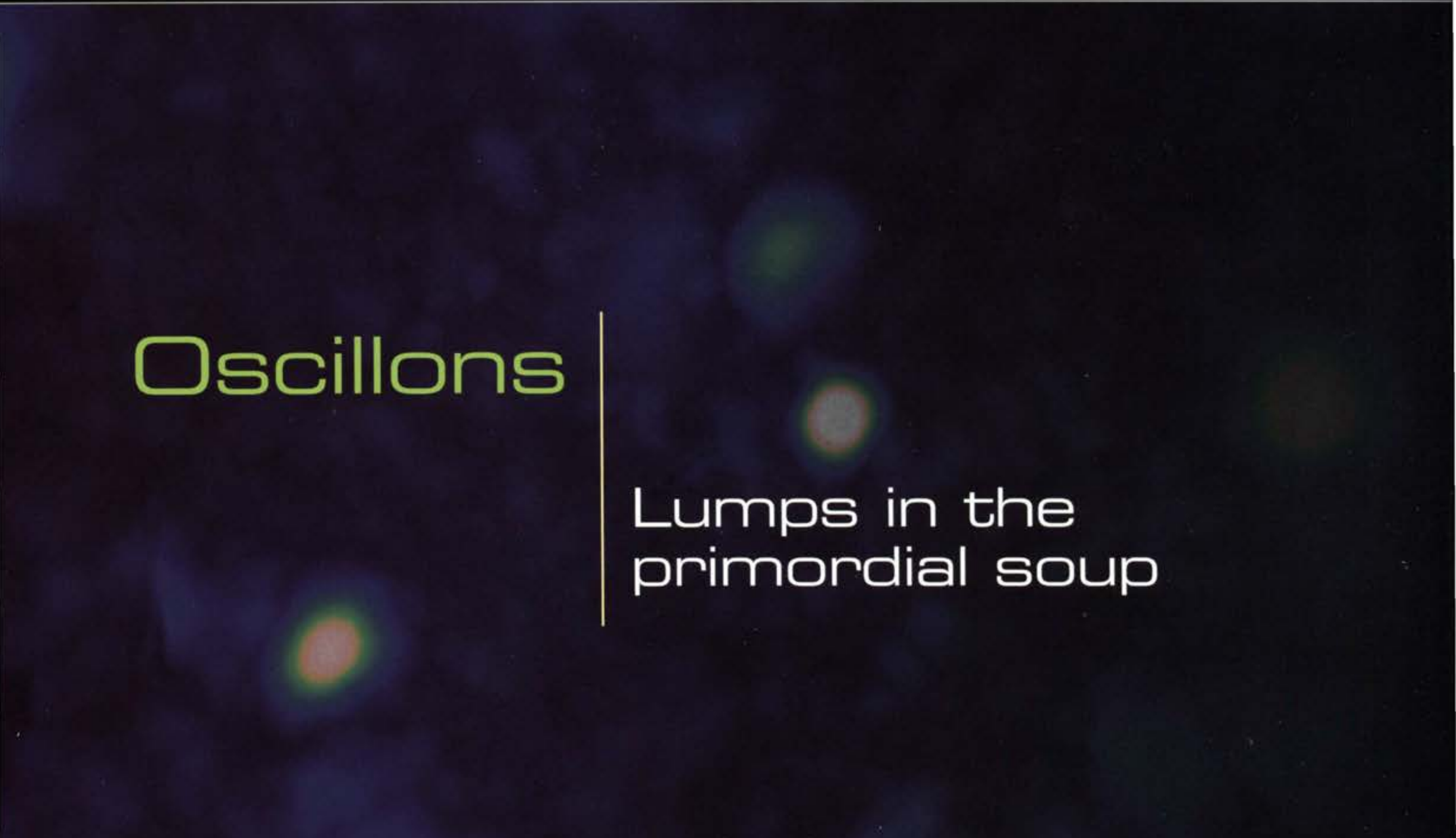
John Abraham
Purdue University

The objective of John Abraham's research is to extract the statistics in turbulent jets under internal combustion engine conditions, and then use the statistics in direct-numerical simulations (DNS) in simplified configurations to study turbulence-chemistry interactions. This work is of interest to engine manufacturers who are investing large amounts of resources in improving engine efficiency and reducing harmful emissions. The turbulent jets of interest are those encountered in direct-injected compression-ignition engines, for example, diesel engines, and in spark ignition engines, for example, natural gas and hydrogen engines. The team uses NCSA's Abe to conduct large-eddy simulations of non-reacting transient turbulent gaseous jets of three fuels hydrogen, methane (surrogate for natural gas), and heptane (surrogate for diesel), under conditions that are relevant to engine operation.

Their work has been published the Proceedings of the 2008 Technical Meeting of the Central States Section of the Combustion Institute, the AIAA Journal in 2008 and 2009, and in Physics of Fluids in 2009. Funding for this work is provided by Caterpillar Inc., EMCON Inc., Sandia National Laboratories, and the National Science Foundation and NDSEG.



Flame dynamics in the near-field of high-Reynolds number turbulent jets.



Oscillons

Lumps in the primordial soup

FOR MOST OF HIS CAREER, Middlebury College physicist Noah Graham has been focused on the physics of the very large and very small. He's recently been investigating oscillons, clumps of waves that are localized in space but oscillate in time and do not disperse. Because of the large amount of energy required to form oscillons, a natural place to study them is in the early universe.

Using compute clusters at Middlebury College, the California NanoSystems Institute High Performance Computing Facility at the University of California, Santa Barbara, and the Applied Mathematics Computational Lab at MIT, Graham proved oscillons exist in models of particle physics. That work was published in 2007 in *Physical Review Letters* and *Physical Review D*.

Now Graham's using supercomputing resources to scale up to more realistic situations to see if these oscillons form spontaneously from the hot, chaotic conditions of the early universe as it expands. He used NCSA's now-retired Tungsten to begin scaling up his simulations; currently he relies on NCSA's Abe and Pittsburgh Supercomputing Center's Big Ben.

"To see oscillons form in a simulation, you have to describe a large volume of universe compared to the fundamental scales in the system, meaning you need a large lattice, which then expands as the simulation proceeds," he says.

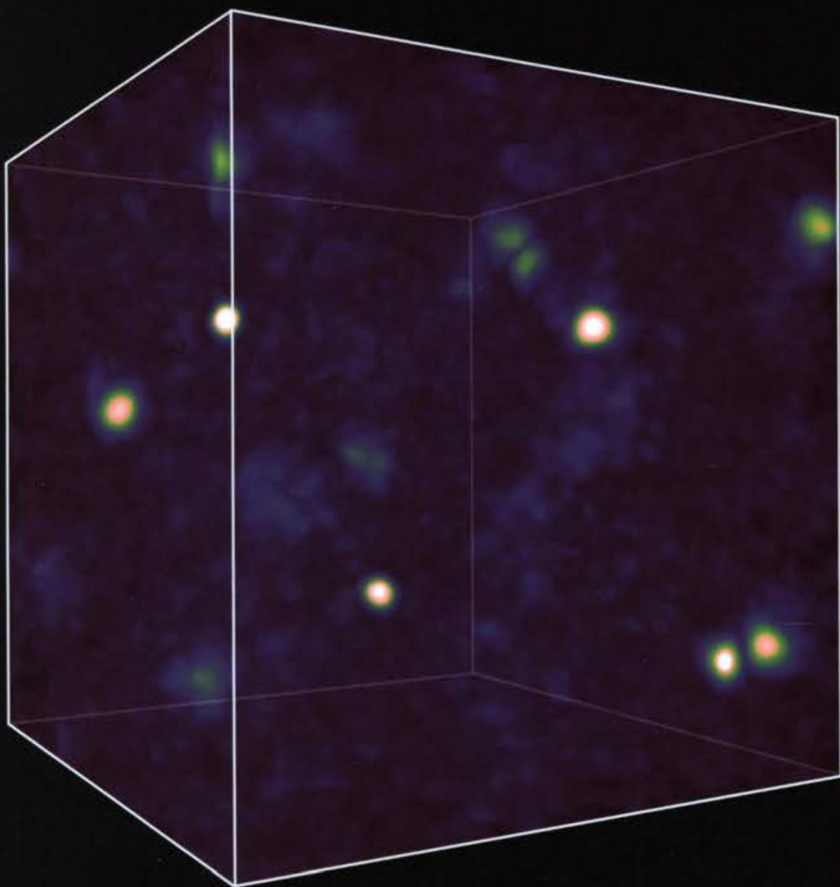
The importance of localized objects has been recognized for a long time, Graham says, but most of the attention has been focused on the case of static solutions, which are easier to analyze.

"This work, however, suggests that the more general case of oscillating solutions, while more difficult to calculate, might be of considerably broader applicability. Stable objects of this kind are particularly interesting in the early universe, because they are out of thermal equilibrium—at equilibrium they would disperse as the universe cools. Such a departure from thermal equilibrium is a necessary condition for baryogenesis, the process that formed the protons and neutrons we see today," he explains. "Finding the mechanism of baryogenesis remains a major unsolved problem in cosmology; while it's too early to say if oscillons played a role in this process, it's at least an intriguing possibility."

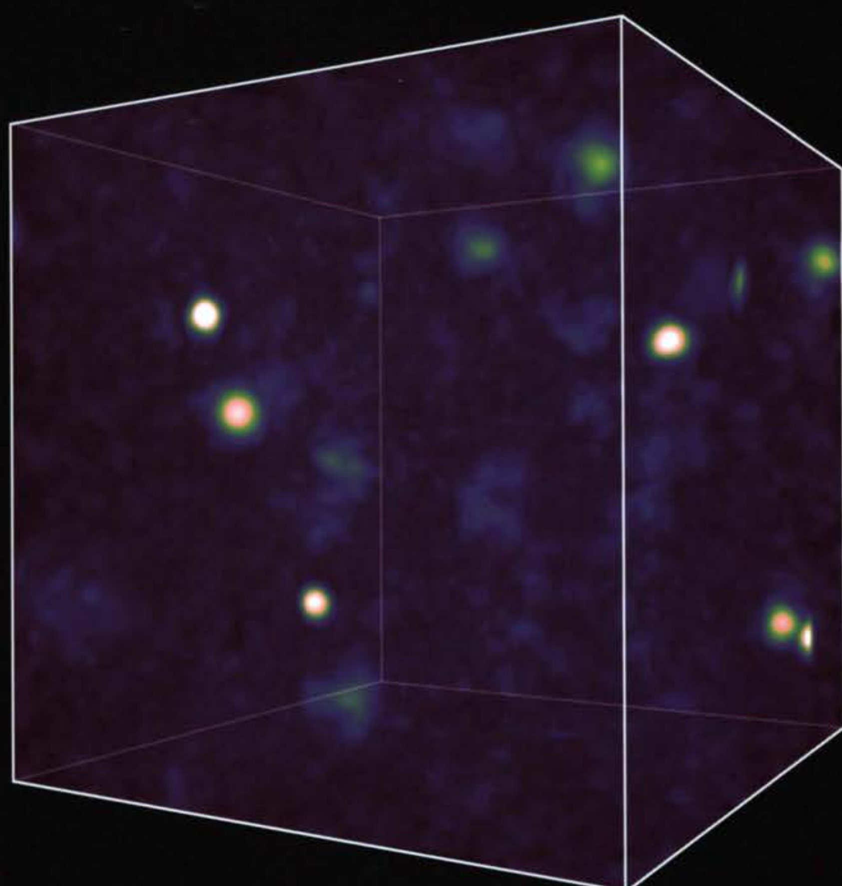
Large-scale computing is needed not only to run the simulations, but also to extract meaningful results from the correspondingly large output, says Graham. Due to the extremely vast quantity of the data, the team was unable to analyze relationships within the entire dataset using off-the-shelf visualization software. So they turned to NCSA's Advanced Applications Support Visualization Group. Visualization expert David Bock is using a custom renderer he developed to volume visualize the entire dataset.

"Using my custom renderer, we were able to analyze the entire oscillons dataset using a variety of volume visualization methods," says Bock. "Modifications were made to the simulation based on these representations, more data was generated, and new visualizations were produced. This analysis and discovery process has been iterated several times over the past year."

Graham says his work would not be possible without access to leadership-class supercomputing resources. "Because the phenomena I'm looking for appear only when the simulation is scaled up beyond what can be handled with ordinary computational resources, it's extremely valuable for me to be able to draw on NCSA expertise to help me optimize my code and process the output." □



The images here are frames from a visualization depicting a single oscillon dataset rotating about its axis. The data is rendered using a volume visualization method that maps color to the maximum data value along a ray cast through the volume at each pixel location. Dark, cold hues (purple, dark blue) represent lower values while bright, warm hues (yellow, bright white) represent higher values of data.



National Center for Supercomputing Applications
University of Illinois at Urbana-Champaign

1205 West Clark Street
Urbana, IL 61801

www.ncsa.illinois.edu