Who we are
The National Computational Science Alliance (Alliance) is a partnership among more than 50 academic, government, and industrial organizations from across the United States to prototype an advanced computational infrastructure for the 21st century. This model infrastructure, called the Grid, will link together advanced supercomputers, visualization environments, and mass storage devices into a powerful, flexible problem-solving environment. This computing environment will be accessed via high-speed networks from anywhere in the country—eventually, the world.

The Alliance is led by the National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign with major support from the National Science Foundation's Partnerships for Advanced Computational Infrastructure program. Additional funding for NCSA comes from the state of Illinois, the University of Illinois, industrial partners, and other federal agencies.

Cover
Supersonic turbulence in the outer envelope of a red giant star. Using NCSA's 64-processor prototype Itanium cluster, this 1-billion-cell turbulent flow simulation was created by Paul Woodward and his colleagues at the University of Minnesota's Laboratory for Computational Science and Engineering. The team will soon take advantage of Titan, the 1-teraflop Itanium Linux cluster under construction at NCSA, to develop a similar 8-billion-cell simulation.
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Every great advance in science has issued from a new audacity of imagination. —John Dewey
A new audacity of imagination," Coined by philosopher John Dewey in 1929, that phrase still shows us the heart of scientific research. At the turn of the century, we are still driven by our most daring dreams.

Our new TeraGrid efforts are both a dream and a tool for realizing even larger dreams. Supported by the National Science Foundation and developed in collaboration with Argonne National Laboratory, the San Diego Supercomputer Center, and the California Institute of Technology, the TeraGrid will soon be the largest, most comprehensive computational infrastructure ever deployed for open scientific research.

This sustainable national infrastructure will bring together new utilities, powerful computers, and some of the best minds in the country. Anchored by 8 teraflops of Linux clusters at NCSA, the TeraGrid will offer 13.6 teraflops of aggregate computing capability with partners at Argonne, SDSC, and Caltech. It will also support more than 400 terabytes of secondary storage, hosting large-scale scientific datasets. To operate as a single facility, the clusters will be linked via a dedicated optical network that will initially operate at 40 gigabits per second—16 times faster than today's fastest research networks.

Scientific discovery has always been motivated by such new instruments and technologies—Dewey's audacity of imagination manifest. The telescope revolutionized astronomy. The microscope revolutionized biology. The TeraGrid will revolutionize computational science, and with that, it will revolutionize all scientific disciplines. It will allow researchers to work together with capabilities orders of magnitude beyond what they have now. The world will dream in ways it's never been able to before and solve problems that it heretofore thought intractable.

With the TeraGrid, we offer a tool. A compass by which tomorrow's healers, explorers, and inventors will guide human achievement in the 21st century. But we also issue a challenge. A challenge to imagine the future, investigate the world around us, and probe each new frontier.

This issue of Access represents Alliance researchers' ongoing response to that challenge. One of the largest calculations on terascale clusters to date, a new framework for scientific collaboration, and decisive work in biology, chemistry, and atmospheric science—you'll find them all here. This issue also contains a look at the teams that constitute the Alliance and the people who guide the Alliance. Together we are changing the world and dreaming tomorrow's dreams.

Excelsior!

Dan Reed, Director
National Computational Science Alliance
National Center for Supercomputing Applications
With the TeraGrid, we offer a tool. A compass by which tomorrow's healers, explorers, and inventors will guide human achievement in the 21st century.

But we also issue a challenge. A challenge to imagine the future, investigate the world around us, and probe each new frontier.

—Dan Reed
The Next Big Thing

With $53 million from the National Science Foundation, NCSA, SDSC, Argonne, and Caltech will create the largest, most comprehensive computational infrastructure ever deployed for open scientific research.

by

Karen Green
In the near future, scientists will have access from their desktop workstations to some of the world’s fastest computers, data archives from around the world, and sophisticated software and visualization tools. Without leaving the office or lab, researchers will be able to collaborate in real time with colleagues thousands of miles away, manipulating computer simulations and mining insights from the petabytes of data collected daily by scientific instruments.

That’s the vision of the TeraGrid, a project that will include the fastest unclassified supercomputers, a wealth of scientific applications and visualization environments, and toolkits for grid computing linked through the world’s fastest network into an integrated information infrastructure.

“The TeraGrid is about a vision of the future that will radically transform the way we interact and the way we work,” predicts Dan Reed, director of NCSA and the Alliance and co-principal investigator of the TeraGrid project. “Unprecedented amounts of data are being generated by new observatories and sensors, and groups of scientists are conducting new simulations of increasingly complex phenomena. This new age of science requires a sustainable national infrastructure that can bring together new tools, powerful computers, and the best minds in the country. This is the infrastructure that will allow us to solve the most pressing scientific problems of our time.”

In August NSF awarded funds to build and deploy the TeraGrid to a partnership of four sites: NCSA, the San Diego Supercomputer Center (SDSC) at the University of California at San Diego, Argonne National Laboratory (Argonne), and the California Institute of Technology (Caltech). To build the facility the partnership expects to work primarily with IBM, Intel Corporation, and Qwest Communications along with Myricom, Sun Microsystems, and Oracle Corporation.

Linux cluster power

A majority of the TeraGrid’s computational power—an 8-teraflop IBM Linux cluster powered by the next generation of Intel® Itanium™ processors, code named McKinley—will be based at NCSA. This TeraGrid system, which will incorporate some existing PACI hardware, will build upon the two existing clusters of more than 1,300 Itanium and IA-32 processors already deployed at the center and will include 240 terabytes of secondary storage.

NCSA’s 8-teraflop system will be part of a 13.6-teraflop Linux cluster system distributed across the four sites—the fastest Linux cluster ever deployed and the fastest supercomputer in a nonclassified setting. The distributed system will consist primarily of clustered IBM servers based on the Intel Itanium family of processors interconnected with Myricom’s Myrinet. The system will be capable of managing and storing more than 450 terabytes of data.
The network that will connect the four TeraGrid sites will be 16 times faster than the fastest high-speed research network available today.

To operate as a single distributed facility, the clusters will be linked via a dedicated optical network that will initially operate at 40 gigabits per second and later be upgraded to between 50 and 80 gigabits per second. This TeraGrid network, developed in partnership with Qwest, will transport data 16 times faster than the fastest research networks now in operation. It will connect to Abilene, the high-performance network that links more than 180 research institutions across the country, STAR TAP, an interconnect point in Chicago that provides access to and from international research networks; and CENIC's CalREN-2, an advanced high-speed network that connects institutions in California. Illinois' I-WIRE optical network will provide the TeraGrid with network capacity and will give Argonne and NCSA additional bandwidth for related network-research initiatives.

The TeraGrid network could revolutionize collaborative science, according to Argonne's Charlie Catlett, architect of the network, simply by giving researchers the bandwidth they need to do large-scale data analyses across geographic locations. "Many of the things scientists have wanted to do over the past several decades have been left untried simply because moving the data around can take days or weeks. This network will reduce that time to minutes or hours, opening up entirely new possibilities," says Catlett.

A needs-driven project

According to Fran Berman, co-principal investigator on the TeraGrid project and director of SDSC and NPACI, development of the TeraGrid will be driven by the needs of society. "We are in the decade of data, and analysis and synthesis of those data are an important part of enabling scientific advances." She said use of the TeraGrid and its terascale computing system will help scientists develop better drugs for cancer treatment, allow further in-depth study of the human genome and brain, and enable scientists to analyze weather data so quickly they will be able to create real-time forecasts that can predict down to the kilometer where a tornado or severe storm is likely to strike.

The Globus toolkit, a set of services and software libraries that supports grid computing and grid applications, will be an integral part of the TeraGrid. Developed by Argonne and the Information Sciences Institute at the University of Southern California, Globus includes software for security, information infrastructure, resource management, data management, communication, fault detection, and portability. More than 100 institutions will contribute additional applications to the TeraGrid.

"Recent breakthroughs in chemistry and the life sciences have presented us with an even greater demand for advanced computation," says Argonne's Rick Stevens, the Alliance's chief computational architect. "If we are to achieve the performance necessary to support these new applications, we must develop capabilities to harness the collective power of not only dozens of supercomputers but thousands of individual PCs. The TeraGrid will provide critical insight into building such systems, while immediately enabling new classes of science."
Complementing NCSA’s 8-teraflop cluster will be a data-intensive IBM Linux cluster based on Intel Itanium family processors. This cluster will be located at SDSC and have a peak performance of just over 4 teraflops as well as 225 terabytes of network disk storage. In addition, SDSC will deploy a next-generation Sun Microsystems high-end server, which will provide a gateway to grid-distributed data for data-oriented applications.

Argonne will lead the effort to deploy high-resolution rendering and remote visualization capabilities and networks. This effort will require a 1-teraflop IBM Linux cluster with parallel visualization hardware.

Caltech will focus on providing online access to very large scientific data collections and will facilitate access to those data by connecting data-intensive applications to components of the TeraGrid. Caltech will deploy a 0.4-teraflop cluster and an IA-32 cluster that will manage 86 terabytes of online storage.

But beyond the teraflops of computing power, the data storage facilities, and the ultrafast network, the TeraGrid represents a leap forward in creating a comprehensive computational, data management, and networking infrastructure of unprecedented scale and capability. It connects scientists and engineers as a cybercommunity with distributed scientific instruments, terascale and petascale computing facilities, multiple-petabyte data archives, and gigabit (and soon terabit) networks.

“The TeraGrid is a transforming idea in which reference to ‘place’ becomes obsolete,” says Reed. “It will be a far more powerful, more flexible, and more inclusive scientific tool than any single supercomputing system could ever be, and it will give us the power and the resources we need to head into a new age of scientific discovery.”

Access Online http://www.ncsa.uiuc.edu/News/Access/Stories/DTF/

For further information:
http://www.ncsa.uiuc.edu/UserInfo/Resources/Hardware/IA32LinuxCluster/
http://www.ncsa.uiuc.edu/TechFocus/Deployment/

In-a-Box seeds the TeraGrid

For the TeraGrid to develop as a sustainable national infrastructure for computing and communications, it must be built on a pool of shared resources, standard hardware, and standard software packages. Reliable, scalable, interoperable, and well-maintained hardware and software are essential if the latest technologies are to be deployed beyond the four TeraGrid anchor sites and if the TeraGrid is to truly function as a national infrastructure for scientific research.

For these reasons, the Alliance has created a set of four interrelated software packages known collectively as the In-a-Box initiatives. These initiatives promise to lower the cost and expertise needed to utilize new technologies and to create a new level of interoperability to support the needs of the national research community.

At the heart of the Alliance In-a-Box strategy is the Cluster-in-a-Box (CiB), an effort that builds on the growing interest in commodity-based cluster computing and open source software. The first goal of the CiB effort is to develop and package software that greatly simplifies the task of installing and running a parallel Linux cluster that is compatible with large-scale production clusters. The second goal of the CiB effort is to provide a software foundation on which other software packages—including grid toolkits and scalable display wall software—can be built. CiB itself builds on the work of the Open Cluster Group, which developed the Open Source Cluster Applications Resources (OSCAR). OSCAR targets clusters up to about 64 nodes that support Ethernet-based messaging. By supporting Myricom’s Myrinet as the interconnect among cluster processors and by integrating Alliance software into the overall package, the larger CiB effort lets users create clusters of more than 64 nodes.

The Grid-in-a-Box (GiB) deployment initiative is a natural extension of years of work prototyping the national technology grid. GiB is a set of tools, designed for maximum compatibility and ease of use, that make it easier to access computational grids, use grid resources, and offer resources to others. It includes middleware for tasks such as authentication, job management, and information discovery, as well as Globus, a distributed computing toolkit, and Condor, a high-throughput computing environment that utilizes unused compute cycles on desktop workstations.

The Display Wall-in-a-Box (Dbox) initiative builds upon the Cluster-in-a-Box software and makes it simpler and less expensive to offer high-end display capabilities on top of Linux clusters. Costs are controlled by using commodity projectors and infrastructure and by supplying well-documented open source utilities and applications. The Dbox package includes display wall construction information, guidelines for choosing projectors and graphics cards, a software toolkit of utilities and applications, and descriptions of existing Alliance display walls. Sophisticated visualization applications and utilities for optimized movie playback and display of precomputed geometry are also included.

The Access Grid-in-a-Box (AGiB) is the Alliance’s effort to package and deploy Access Grid software, thereby making it easier for users to join the Access Grid community. The Access Grid is an integrated environment that supports distributed meetings, remote visualizations, and distance education. AGiB allows users to join the Access Grid community with ease, adding new entry points to the collaborative environment. Five AGiB teams are developing AGiB-related codes, producing end-user documentation, identifying problems with new software, developing training materials, and contributing and integrating software from outside sources to the overall Access Grid project.
Going with the

Using the power of NCSA's new Itanium Linux cluster, a University of Minnesota research team will simulate turbulent flow in greater detail than ever before.

by
Karen Green
Anyone who has traveled on an airplane is aware of turbulence. This atmospheric phenomenon, which makes your tray table jiggle and leads the captain to turn on the “fasten seat belts” sign, is caused by instabilities of shear flow that result from atmospheric convection. This turbulence, although annoying and sometimes unnerving, pales in comparison to the supersonic turbulence found in the outer envelopes of red giant stars.

Simulations of convection in such stars by Paul Woodward's team at the University of Minnesota's Laboratory for Computational Science and Engineering (LCSE) show that heat rising from the interior of a star stirs up the outer envelope of the star and can result in gas motions that exceed the speed of sound near the stellar surface. These turbulent convective motions give rise to shocks—sudden compressions of the gas—of Mach 2 or more.

**Turbulent motions in detail**

To improve our understanding of such violent turbulent flows, Woodward's team is using the new Itanium Linux cluster at NCSA to simulate turbulent motions in detail. Violent turbulence that causes compression in gasses is less common than the turbulence airplanes encounter or the turbulence in the wake of a boat, which involve much slower relative velocities. But research so far suggests that the three are very similar and that understanding one will help in understanding the others. In the long run, a better understanding of turbulence will help in everything from analyzing weather patterns to designing airplanes and boats.

"Fluid turbulence is important in many areas of science and engineering," says Woodward. "It is a factor in the design of aircraft engines, boats, and even cars. It also influences the behavior of rivers, oceans, and the atmosphere, so this work should have an impact on a wide variety of disciplines."
Woodward’s team concentrates on a phenomenon that is still not fully understood: what happens between the point at which stirring causes motion on a large scale (the big eddies right behind a boat, for example, or the large convection cells that cause cumulus clouds) and the point at which the resulting small-scale turbulent motion dissipates as heat. Figuring out what happens on the middle scales of turbulent flow is important because these turbulent motions are believed to strongly influence large-scale fluid flow. The steadily increasing power of supercomputing systems is just beginning to make possible these simulations of turbulence on smaller scales. Woodward and his colleagues were quick to jump at the opportunity to develop high-resolution simulations that could follow a turbulent flow from the macro level—where energy causes motion—down to the levels that lead to dissipation as heat.

An experimental approach

Woodward and his colleagues are no strangers to large, computationally intensive simulations. For years this research team has studied fluid dynamics in red giant stars in an effort to better understand stellar convection as well as the pulsation and ultimate mass ejection of red giants. The team’s efforts to simulate the broad range of scales in turbulent flow date back a decade or more.

The largest of these earlier runs, a simulation of turbulence induced by a shock wave passing over an interface between two fluids of different density, won the 1999 Gordon Bell Award in the performance category. This simulation involved collaborators at Lawrence Livermore National Laboratory and IBM. Woodward’s LCEP team most recently ran a 1-billion-cell simulation on a prototype 64-node Itanium Linux cluster at NCSA. Because of the configuration of the Itanium cluster and the fast network connection to the team’s Minnesota lab, this newest run generated a rich dataset that documents the complete time history of the simulation. The team will use these data to validate much more conclusively ideas for turbulence modeling suggested by their earlier work, particularly the large simulation done at Livermore.

“Our approach to the study of turbulence is experimental,” says Woodward. “We are trying to use the Itanium cluster to generate an extremely detailed set of data describing a turbulent flow, with the density, pressure, and three components of velocity sampled on a sequence of hundreds of times at each of a billion mesh points.” Such mind-boggling kinds of data can be compared to existing turbulence theories or even used to develop new theories, he adds.

Three intervals of gas compression from a 1-billion-cell turbulent flow simulation by Paul Woodward and researchers at the University of Minnesota’s Laboratory for Computational Science and Engineering. Red to white streaks indicate strong compression of the gas, while green to blue streaks show weaker compression.
The key to using data from computer simulations as if they were experimental data is to be very certain of the data's accuracy. Just as experiments involve errors in measuring data values, computer simulations involve numerical errors—failures of the computational model to accurately follow the behavior of a real gas. To simulate turbulent flow, Woodward and LCSE scientist David Porter use a method called piecewise parabolic method (PPM). In interpreting their data, Woodward and Porter carefully filter out the smallest-scale motions, where viscosity is an influence and numerical errors are most likely to occur. Since they are interested in the larger-scale motions where viscosity is not a factor, this filtering process removes errors without sacrificing simulation detail. To achieve the level of detail they require, they need a very fine grid that will result in a high-resolution simulation. For this reason, they are planning an 8-billion-cell turbulence simulation that will run on Titan, NCSA's brand-new 1-teraflop Itanium Linux cluster. With the data from the 8-billion-cell simulation, the researchers will have the data they need to make comparisons to their 1998 Livermore run.

The new simulation will probably require all of the cluster's 320 processors. A full Navier-Stokes simulation—a process that would follow the flow from its start to its dissipation as heat—would require a grid of 340 billion cells and 150 teraflops of computing power. Overall the LCSE team expects to generate 40 terabytes of data on turbulent flow in the most complete detail possible on today's computing systems.

"We view this data as much more than a bunch of numbers saved to a disk, because high-quality data like this has many uses," he adds. "If you have high-quality data, you can test theories and be confident of the results, and we believe these simulations will give us this special kind of data."

This research is supported by the National Science Foundation, the Department of Energy Office of Science, and the University of Minnesota's Minnesota Supercomputing Institute.

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

For further information:
http://www.lcse.umn.edu

Team members
Benjamin Allen  David Porter
Sarah Anderson  Igor Sytine
Kevin Edgar  Paul Woodward
Michael Jacobs

Vorticity at three intervals in a turbulent flow. Blue and cyan indicate low vorticity, orange shows mid-level vorticity, and yellow indicates high vorticity. Over time the turbulent flow shows more vorticity.
Stuck in the middle

by J. William Bell

Where experiment and theory overlap, Stanford University researchers explore the behavior of organic and inorganic molecules on semiconductors' silicon surfaces.
They're researchers stuck in the middle—between theories of varying precision, between models of varying size, even between the worlds of theoretical and experimental chemistry. Like a farm cut into a mountain foothill, it's a challenging but fertile row to hoe.

The team, out of Stanford University and headed by Charles Musgrave, studies the chemical reactions that occur on the surface of microchips during their manufacture. By looking at the reactions at the atomic level, team members hope to illuminate the basic science that will improve production and perhaps lead to novel applications and devices.

"Attempts to computationally prototype the reactors used to manufacture computer chips have really only been around for about 10 years," says Musgrave, an assistant professor of chemical engineering and materials science. "In order to create these prototypes, you have to be able to model and change all the elements of the reactor used to build the chip, but you also need to fully understand the chemistry at the chip's surface. That's where we come in."

With the help of an Alliance SGI Origin2000 supercomputer at NCSA, two members of the team—PhD candidates Collin Mui and Yuniarto Widjaja—are becoming particularly "expert at predicting the energetics and behavior of the species that populate the surfaces," according to Musgrave.

**Chip chemistry**

A computer chip begins its life as simple quartz (SiO$_2$), that transparent rock underfoot every time you hit the beach. Quartz is easy to come by—it makes up about a quarter of the planet's crust—but tough to make useful to manufacturers. Only a handful of companies around the world process quartz into the pure silicon used as the chip's base. To conjure up the purification process, imagine the smelting heat of a foundry coupled with the precision of a surgical theater. Chip-quality silicon is heated to more than 2,500 F, and only defects less than 1/300$^{\text{th}}$ the width of a human hair are acceptable in the silicon ingots that are cut into wafers.

As a semiconductor, silicon can be manipulated into either a conductor or an insulator by selectively introducing different impurities. These intricate patterns of conducting and insulating silicon form the basis for the complex circuits of the chip, which are built on the silicon wafer by depositing and removing different materials. More than 20 layers of deposited films are used to complete the three-dimensional structure of the chip's circuitry. Metals such as copper and aluminum are introduced as conductors to wire the chip, and various reactants are used to create insulators.

The team starts their models—just like a chip—with a silicon surface, modeled as clusters of nine, 21, or 33 silicon atoms. Bonds that are broken when extracting this virtual chunk of the silicon surface are "terminated" with hydrogen atoms. Adding hydrogen atoms creates a slightly different chemical environment than the pure silicon of a chip. But not adding the hydrogen causes a modeling problem that's more difficult to address. Untermminated, hypothetical clusters of atoms would have different hybridizations than the pure, real-world silicon; attaching hydrogen in the right places allows researchers to avoid this issue. The goal is to simulate reactions on the small virtual surface of the cluster. If successful, the simulated reactions will mimic reactions on a wafer in a modern semiconductor fabrication plant.
Becoming expert

The Stanford team is currently focused on how and under what conditions reactants break down and how components incorporate themselves into the chip surface. Most of their models rely on density functional theory (DFT) calculations, which solve the Schrödinger equation that governs the behavior of subatomic particles in molecules.

Widjaja, for example, studies the behavior of ammonia during deposition. Ammonia (NH₃) is known to be adsorbed—retained on the cluster's surface without penetrating its bulk—on silicon and to dissociate into NH₂ and a hydrogen atom. Designers aren't much interested in that lonely hydrogen on the surface, however. In deposition of ammonia on silicon, they are really interested in the nitrogen that ammonia offers. Nitrogen reacts with the silicon to produce silicon nitride, which is commonly used as an insulator, oxidation mask, or diffusion barrier on chips. The unwanted hydrogen atom, on the other hand, pairs with a neighboring hydrogen atom and desorbs.

Chemical engineers know that if you raise the temperature in the reactor to between 700 and 1,000 K, the NH₂ will further decompose, hydrogen will desorb from the silicon surface, and silicon nitride will form. The details of how this happens aren't known. The nature of the chemical species formed, the mechanisms that cause the formation, and the precise energies required to trigger these mechanisms have gone largely unexplored. Widjaja's models give some of the first atomistic views of those features and events.

Mui, meanwhile, looks at methyamines, organic ammonia derivatives in which methyl groups (CH₃) replace ammonia's hydrogen. Though it is more thermodynamically favorable for the methyl groups to break from the nitrogen before the hydrogen does, the models show that the hydrogen-nitrogen bonds break first. The models also show that trimethylamines, which have only methyl groups and no lone hydrogens, do not dissociate at all because there are no hydrogen-nitrogen bonds.

By understanding the basics of this interaction—and lack of interaction—new applications that exploit previously ignored materials may be developed. "Organics like methyamines currently aren't used in industry, so we're looking at how they react. We want to build up a knowledge base. Find out what might be useful. What is even possible," Mui says. Ultimately, this knowledge might allow designers to use more complex reactants to build more complex structures, such as molecular switches and sensors and nanotechnology machinery. Quantum chemical techniques are essential to exploring these systems.

Farther than fingerprints

The nature of these highly specialized models makes it difficult, if not impossible, to confirm most of the findings through laboratory trial. "A big effort goes into the entire mechanism, showing all the fundamental steps involved, all the pathways," says Musgrave. "[Experimentalists] often get the first steps, but we get chemistry that's most often not attainable experimentally."
Adds Mui, "At this level, experiments give you fingerprints of the reactions' products, but they don't tell you why you get those products. Why the reaction takes place. Why the reaction stops or continues."

"Experimentation allows you to see. Theory explains what you saw and even lets you predict what you are going to see," he says. "It is the ultimate microscope in that it lets you study atomic-scale systems in great detail, even if they haven't yet been made."

The team bridges the gap between modeling and experimentation in at least two ways. First, there's constant interaction and collaboration with chemists who specialize in more traditional research methods. Mui, in fact, splits his time between Musgrave's team and the lab of another member of Stanford's faculty, Stacey Bent, an assistant professor of chemical engineering. As with Musgrave's team, her research team focuses on fundamental chemistry—including the mechanisms, kinetics, and reaction pathways of product growth—under the extreme heat and pressure that mark chip production. But Bent's research does keep its feet firmly planted in situ and uses a variety of spectroscopic techniques.

Second, the team spends a portion of their NCSA computing time modeling with a method, known as quadratic configuration interaction (QCI), that is generally accepted as more accurate than DFT. This accuracy is often needed to predict properties like chemical kinetics that require more precision. Unfortunately, QCI is too computationally expensive for general use. "The smallest model takes about 20 to 30 hours with DFT on a single workstation. With QCI it could take 3,000 hours. The largest models we look at would take years with QCI," Widjaja says.

Using QCI sparingly on the Origin2000 gives the team the freedom to run some of these otherwise intractable models. The results allow team members to substantiate the accuracy of the DFT models. "With just DFT, you're done. But you don't know if you're right, especially when you're working in an area that doesn't have an experimental base. With the Origin2000 runs, we've gained a lot of confidence in our results," Musgrave says.

Perhaps it's not the same level of confidence that an experimental confirmation would afford. But for researchers who revel in being stuck in the middle, it's a great start. It's just a matter of waiting for the experimentalists to catch up.

**Access Online** [http://access.ncsa.uiuc.edu/CoverStories/chipchem/](http://access.ncsa.uiuc.edu/CoverStories/chipchem/)

**For further information:** [http://chemeng.stanford.edu/html/musgrave.html](http://chemeng.stanford.edu/html/musgrave.html)

**Team members**
- Collin Mui
- Charles Musgrave
- Yuniarto Widjaja
Alliance scientists have their eyes on cholesterol, all right, but not just for their health. They're set to make discoveries about how cells communicate and take some of the first steps toward nanodevices based on living cells.
Cholesterol. The word itself evokes images of arteries narrowed by atherosclerotic plaque, the gunk that sticks to vessels and impedes the passage of blood the way a kink in a garden hose slows the flow of water. Or perhaps we think of cholesterol as something our favorite foods—ice cream, two-crust pies, steaks, French fries—are rich in, a culinary spoiler that makes us choose the fish yet again. (Hold the Béarnaise, please.)

But the drumbeat of public health messages about the hazards of too much dietary cholesterol obscures a more complex reality, namely that cholesterol is essential to animal life. In fact, much of the cholesterol in us is manufactured by our own bodies, not obtained from our foods. It serves as a precursor to the sex hormones estradiol and testosterone and to vitamin D, which is necessary for the formation of bone. Cholesterol is also needed to produce the bile acids that digest fats. Cholesterol is only dangerous when the body's regulation of it goes away, owing to genetic or environmental causes.

For a group of scientists using Alliance resources, the most fascinating aspect of cholesterol is its role in regulating membrane fluidity in animal cells. This group—Eric Jakobsson of the Beckman Institute for Advanced Science and Technology, Urbana, Illinois; H. Larry Scott, chair of biological, chemical, and physical science at the Illinois Institute of Technology in Chicago; and R. Jay Mashl and See-Wing Chiu, also of Beckman, the University of Illinois at Urbana-Champaign, and NCSA—use the prototype 64-processor Itanium-based Linux cluster at NCSA to perform computational studies that could lead to a deeper understanding of how cells communicate with each other. What's more, their work may contribute to the development of nanodevices based on living cells.

Liquid crystal membranes

Far from being simple walls, cell membranes are instead complicated liquid crystals. About 50 percent of a cell membrane is composed of lipids (oily organic compounds like fats) and most of the rest is made of proteins. The whole lot is characterized by randomness, chaos, and subtlety. "It is amazing," Scott says. "Membranes are not rigid little sheets. They fluctuate a lot, they're dynamical systems, and it really is remarkable."

The normal fluidity of cell membranes is now thought essential to life functions, and disruptions can have dire consequences. Just this year scientists reported that cholesterol's regulation of membrane fluidity may be involved in the destruction of brain cells that leads to Alzheimer's disease; that reduced fluidity in the membranes of red blood cells may be related to psoriasis outbreaks; that abnormalities in membrane lipid content may cause resistance to leptin, the hormone that regulates appetite to maintain normal body weight; and that chromium, a carcinogen, causes tumors by reducing membrane fluidity. "Membrane fluidity is probably involved in all cell processes associated with communication of cells with each other and with the outside world," Jakobsson says.
Until recently, researchers studying cell membranes had to make do with “toy” systems, little patches of assemblies that everyone hoped would faithfully represent the complete system, but whose chief virtues were that they were simple enough for computation. “It’s really just now that [supercomputing] is kicking in,” Jakobsson notes.

Similarly, while many experimental studies suggest that membrane fluidity and cellular communication are related, up until now they have been handled separately in computational studies owing to limited computing power. “With the new NCSA Linux superclusters Platinum (now up and running) and Titan (coming on line later in the year), we have the exciting prospect of finally having enough computer power to consider these two aspects of membrane biology together,” Jakobsson notes.

Big calculations, bright discoveries

Over the past year, the group’s pace of discovery has quickened. Jakobsson attributes this not only to the use of the Linux cluster, but also to Gromacs, the open-source molecular dynamics software. “Gromacs is exceptionally efficient on Linux clusters, as well as being highly flexible for adaptation to particular biomolecular calculations,” Jakobsson explains.

Scott has also used Monte Carlo techniques, which help ensure the efficient sampling of a system’s important configurations, to write additional computer code. This code homes in on states that are important to the study and will eventually occur in nature. These configurations would probably not be accessible to the simulated system over the nanosecond timescale of the molecular dynamics simulations.

These tools have enabled the group to sample enough different concentrations of cholesterol in cell membranes to characterize both the individual molecular interactions of cholesterol and lipid as well as the collective effects. For example, the group has shown that membranes consisting of the lipid diphenoylposphatidylcholine and cholesterol undergo a clear phase transition between a gel and a fluid state at a lipid/cholesterol ratio of about eight. At this and higher concentrations of cholesterol, the lipid is held in a gel-like state by the cholesterol. At lower concentrations of cholesterol, the lipid melts into a fluid state.

This observation is significant, because phase change is associated with a significant change in the character of the cell membrane. The high-cholesterol gel phase is much less fluid than the low-cholesterol phase. The cholesterol-induced phase change observed in a membrane patch in the computer shows the mechanism for the experimentally observed cholesterol-induced fluidity changes, presumably those associated with the normal processes of cell fusion and perhaps even the pathology of Alzheimer’s disease. “We also think the observed phase change is cool computational surface chemistry,” Jakobsson adds.
Little living batteries

The group also looks at the ion channel proteins embedded in cell membranes. These little living batteries convert the chemical potential of ions into electrical currents. They are essential to intercellular signaling and to transporting material between the inside and the outside of a cell. Jay Mashl notes that if scientists can understand these biomolecules on the atomic level—understand exactly how a given protein structure results in an observed current—then it should be possible to engineer ion channels into the workhorses of nanodevices built partly of biological materials.

Jakobsson predicts that, in time, the role of computer simulation will expand from understanding natural cell membranes to designing artificial membrane complexes for nanodevices. In the relatively new field of nanobiotechnology, scientists attempt to integrate life forms with nonliving materials on a nanometer (one billionth of a meter) scale.

These living machines might accomplish, in a precisely controlled way, the functions, such as signaling and energy transduction, of biological membranes. This possibility brought the Scott-Jakobsson group into collaboration with a group from another scientific discipline altogether, the Beckman Institute Computational Electronics Group that includes Alliance users Karl Hess, Umberto Ravaioli, and Narayan Aluru.

Eventually the components of highly sophisticated nanodevices might be embedded into engineered cell membranes. Such nanodevices would live in the body much like any other cell, taking over functions lost to disease or injury. Although scientists have already demonstrated the feasibility of building such hybrid nanodevices, much more work is needed before such devices can be successfully installed and function in a living organism.

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

For further information:
http://glycine.ncsa.uiuc.edu
http://www.beckman.uiuc.edu/research/compe.html

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Simulated rafts becoming a reality

In addition to cholesterol's general role in membrane fluidity, cholesterol may have some role in the formation of "rafts." Rafts in cell membranes are regions enriched in cholesterol and protein. They appear to bring into close physical proximity networks of membrane proteins that need to function together, making interaction with each other rapid, intense, and reliable. Scientists suspect that rafts serve as communication hubs for cells, so naturally they provoke keen interest. Their complexity, however, makes them difficult to study.

Recently Jakobsson's group gained access to Platinum, one of the Alliance's Linux clusters. Platinum is based on 1,024 Intel Pentium III processors. Together with the Titan cluster currently being installed at NCSA, Platinum will provide more than two teraflops of computing power to Alliance users. Now that the group has begun to benchmark the Gromacs code on Platinum, they realize that, even with the speed of the 64-processor prototype cluster, Platinum and Titan promise to enable computations on a whole new scale.

"It has just hit us that it is now feasible to simulate something like a full raft, containing a gel-like mix of ion channels, cholesterol, and lipids, surrounded by a sea of fluid lipid," Jakobsson says. "Different members of our research group can analyze different aspects of the behavior of the entire system, where each component is functioning not in isolation, but in the full complex environment characteristic of real membranes. This starts to have a flavor of simulated natural history, which is a totally different way of doing biomolecular simulations that was never possible before. It marks a transition from doing computational chemistry on biological molecules, to really doing the biology."
Every scientist a maestro

Alliance partners build and integrate high-performance computing tools to create science portals.

by J. William Bell
High-performance computing offers an array of instruments to be played: Supercomputers and scientific code to simulate real-world phenomena that are impossible to study at the lab bench or under the microscope. Scalable display systems to explore data in new ways and at high resolution. Knowledge discovery techniques to gather insight from otherwise impregnable datasets. And high-speed networking to connect all of these tools in a single grid.

Not every music lover is a great composer, though. Steep learning curves, the distributed nature of the tools, and a broad range of required expertise keep many scientists toiling away as Salieri, even as they long to be Mozart.

“The scientific method depends on comparing observations with hypotheses. Now that sophisticated numerical simulations are used to express hypotheses, the divergence between the observational skills researchers have and the computational skills they need is so great that it threatens the scientific method,” says Richard Alkire, a chemical engineering professor at the University of Illinois and a member of the Alliance science portal team.

Collaboration is one way of overcoming this divergence, and it’s critical among the coders and the experimentalists, the visualization experts and the environmental hydrologists, the networking gurus and the geophysicists. But, according to Dan Reed, director of the Alliance and NCSA, “Our goals have to be bigger than ad hoc solutions to individual challenges. Scientists must be able toexploit hardware, simulation codes, and data without deep knowledge of the underlying computational infrastructure. This capability brings the leading-edge tools to life and allows them to perform most effectively in the advancing world of distributed terascale computing.”

Alkire adds, “Experimenters should be able to change their hypotheses and work with their data. They shouldn’t have to worry about the details of the computer science going on behind the screen. A small number of experts should do much of that for them.”

Members working in the Alliance’s science portal program are those experts.

Taming the grid

Running an application on the grid is a complicated undertaking. Multiple codes might reside on different computers, and the data that those codes are supposed to chew on may live still elsewhere. In most current cases, none of these codes, data, computing systems, and tools is aware of the others.

Researchers fight a constant battle in this environment. They have to manage each step of the process. Starting computational runs, passing data among the computations, authenticating and reauthenticating on each platform—the list of small tasks incumbent in the larger task goes on and on.

Science portals clean up this messy world. Portals are conceptually based on the computational workbenches pioneered at NCSA with the development of the Biology Workbench in the mid-1990s. A Web-based interface for using biological sequence tools and databases, the Biology Workbench—which is now maintained and developed at the San Diego Supercomputer Center—makes interoperable databases that once had to be searched manually one at a time and eliminates file-compatibility problems.

Expanding this concept, portals are more than a clearinghouse for popular tools and databases. They offer a grid-based framework that simplifies accessing, configuring, combining, and executing applications on the grid. By linking the various components required to solve a problem, portals create distributed, multidisciplinary applications.

“The job of any science portal, regardless of the field of research or the systems, is to tame the grid,” says Dennis Gannon, a computer science professor at Indiana University and a member of the Alliance science portal team. “Once you get a grid application right, you don’t want to start from scratch the next time. You want to do it again easily.”

Personal server and control scripts

But the bird’s-eye view of portals—their goals and all that those goals suggest—doesn’t necessarily bring the portals into focus. What does a portal look like? How do you build grid applications? And how do users do as their name implies and use them?

Let’s attack these questions by beginning at the computer screen. When users fire up a science portal, they’re actually starting what developers call a “personal server.” Written in Java and supporting connections from a Web browser or desktop applications, it’s a piece of software that can be installed on a desktop, laptop, or even palm computer. The personal server is the window to the portal. It allows users to find and execute grid applications. Technologies pioneered as part of the Globus toolkit and the Java CoG kit, developed by Argonne National Laboratory, allow users to integrate necessary grid services such as authentication and file management.

Users can view pages that explain what a particular application does, running a series of different environmental hydrology codes on the same dataset to model a river basin at a variety of scales, for example. Users can also tailor the parameters of the application through a series of simple Web forms within a portal notebook on the personal server. Unlike most Web tools, however, there is no central server brokering operations in the portal scheme; connections are made directly to the code, tools, and data to be used in the calculation.

These connections and commands are established via control scripts. Scripts form a grid application by defining a sequence of operations. A script might be built to activate the appropriate software on both local and distant machines to: search for and select the computational resources to be used, search a database for data to work with, supply that data to a simulation code, launch other codes as necessary, and interact with the personal server to notify the user of events or problems and to allow the user to modify the job as it runs.

The script is like a sheet of music. The instruments in the pit during a given computational run follow the script’s lead, entering on cue and playing off one another. Scripts can be stored on and retrieved from the personal server. They can also be treated individually and passed along like any simple executable file—dashed off in an email attachment, for example. All that interested researchers need in order to use a script is the personal server.

“Ultimately we want to build a work environment that’s also a development vehicle,” says Jay Alameda, part of the Alliance’s science portal efforts.
Becoming grid aware

Scripts may serve as sheets music, guides that the grid computation can follow. But the instruments also have to be prepared to follow the conductor to play in an coordinated manner. Specialized codes known as application managers serve as conductors in the Alliance's science portals.

Following a standard established by the Department of Energy's Common Component Architecture group (of which the Alliance science portal team is a part), the application managers are small pieces of code that make other, larger pieces of code "grid aware." By building in application managers, codes designed to perform a specific task—such as solving a system of linear equations, modeling the fluid dynamics of a system, or managing a database—become part of a problem-solving orchestra. Without user intervention, the codes can pass data and take cues from one another.

The scientific portal team hopes that application managers will catch on in new code development, and they're not averse to ripping into old codes to, well, bring them up to code. But because of the time and intellectual property constraints inherent in rebuilding legacy code, team members have built a generic application manager "wrapper" that makes applications grid aware with minimal effort and without altering the existing code.

"There are two types of grid users," says Gannon. "Probably 90 percent of users just want a canned thing. They just want their problems solved and don't even want to know they're using the grid. The others want to get into the nitty-gritty. They want to change the way the thing works. Every aspect of the portal effort keeps both of those users in mind."

Some users want to compose while others simply want to call the tune.

This research is supported by the National Science Foundation and the National Computational Science Alliance.

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

For further information:
http://www.extreme.indiana.edu/an/index.html
http://sharan.ncsa.uiuc.edu/chemengathome/home.page/docs/chemeng.html
http://www.globus.org/cog/

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"The key benefit of the science portals is the intellectual freedom that they allow," according to Richard Alkire of the Alliance and the University of Illinois. No area of study has proven this statement more true and more quickly than Alkire's own field of chemical engineering. Alkire and his colleagues are already using the fledgling portal to study the electrodeposition of copper, a critical step in making interconnections on silicon computer chips. They are also using the portal to model the onset of pitting corrosion on stainless steel.

The portal's application managers recently allowed the team to link two codes—a finite difference continuum code and a Monte Carlo noncontinuum code—to one another to conduct coupled, multiscale computations. This ability is critical for chemical engineering processing, in which the multiple phenomena studied in concert can vary in length scales by a factor of $10^{12}$.

The application managers have also been successfully adapted to the popular multipurpose Cactus code by Karen Camarda and Ken Bishop at the University of Kansas. Bob Wilhelmson's environmental hydrology team at NCSA is also reworking a pair of codes to exploit the portal's application managers.

The wide range of scales studied by chemical engineers is not the only characteristic that makes the field an interesting case study. Intellectual property issues—a concern in most fields—are rife within chemical engineering. They are also well addressed by the portals.

Proprietary codes can become just another tool available to researchers. An application manager can be wrapped around the code without potential competitors digging into or even seeing the code itself. Authorization extensions and basic grid security tools from Argonne's Globus and Java CoG toolkits, meanwhile, will allow stakeholders to establish whatever protections they feel are necessary. Licenses and access rules are upheld, even in the most freewheeling computations.

And, in a familiar portal refrain, these machinations are all transparent to the day-to-day user.

"Chemical engineering really represents a convergence of the truth seekers, the problem solvers, and the moneymakers," says Alkire. "The portal offers a way to suture together all of those groups' knowledge while protecting their investments. In chemical engineering, we have to innovate rapidly. The portal provides a way to manage intellectual property concerns while speeding the pace of innovation."

**The big CoG**

**Many** useful grid services—like authentication, resource management and discovery, and remote access to computers—are and will be integral to users of the Alliance science portal thanks to the Java Commodity Grid (CoG) kit. It represents the clockwork gears that translate commands made through the personal server into the complex machinations that grid computing requires. It was developed as part of the Globus project, which is creating the fundamental technologies needed to build computational grids.

The Java CoG kit allows the rapid prototyping of new applications, components, and interfaces for the grid. The kit can be run through the Alliance science portal's personal server or any Java-enabled browser, representing the first opportunity for client interfaces to the grid on workstations running Microsoft Windows. CoG kits are also available for Python and Perl.

"How can commodity technologies that emphasize ease-of-use and code reuse in local environments and grid technologies that emphasize effective operation in large-scale, multi-institutional environments integrate and interoperate? And how, ideally, can we enhance the capabilities of both?" asks Gregor von Laszewski, an assistant computer scientist at Argonne National Laboratory. "Those are the questions that motivate the development of the Java CoG kit."

The kit currently provides most of the client-side functionality of Globus. Some of these capabilities include: the Grid Security Infrastructure, which enables secure authentication and communication over an open network; the Resource Specification Language, a method for exchanging information about resource requirements among all of the components in a resource management architecture; the Globus Access to Secondary Storage module, which allows applications to access data stored in any remote file system; and the Metacomputing Directory Service, which provides the tools to build information infrastructures for computational grids.
GLOBAL OZONE ODYSSEY

Researchers look into the lives of molecules and the future of the Earth.

by Oliver Baker
As high-school chemistry may have taught you, it's easy to calculate the odds that a molecule you've just inhaled came from the dying breath of Julius Caesar. But imagine you need to account for the molecule's experiences in the meantime. Say you have to weigh the chances of each chemical transformation it might have undergone as it ascended from ancient Rome, drifted through the dirt and droplets of clouds, and endured temperatures, solar rays, and collisions with gaseous chemicals in changing combinations. Now for extra credit, explain how the global distribution of gases shifts and evolves. Include all life, pollution, inanimate matter, and climate change.

You might raise your hand and ask to use a supercomputer. In fact, Don Wuebbles and Ken Patten of the University of Illinois at Urbana-Champaign and collaborator Rao Kotamarthi of Argonne National Laboratory did just that. Through simulations on an NCSA SGI Origin2000 supercomputer, they are examining the lives of molecules in Earth's atmosphere and contemplating the planet's fate.

Most closely they are watching ozone. At stratospheric heights, ozone shields Earth from solar radiation. But lower down it is a toxin, produced when benign gases react with car and factory pollution or with lightning. In collaboration with the U.S. Environmental Protection Agency (EPA), the researchers are evaluating alternatives to such notorious ozone-destroying compounds as chlorofluorocarbons (CFCs). With other simulations, they are pinpointing the sources of plumes of pollution above the supposedly pristine south Pacific. Ultimately, they want to predict the pace at which the protective ozone layer will recover under different international emission control agreements.

The researchers comprise one of a few teams charged with testing new software that simulates the chemistry and migration of gases around the globe. This software—a revamping of the Model for Ozone And Related chemical Tracers, or MOZART-2 for short—feeds on output from a global climate simulation and takes twice as much computer power as the climate simulation. The chemical transport model is a project of the National Center for Atmospheric Research (NCAR), which intends to release MOZART-2 by the end of this year.

Along for the ride

Testing how well the model works and using it to answer questions are intertwined activities, says Kotamarthi. Because the complexity of global processes involves so many variables and uncertainties, a "validated model" is rarely an option. "The preferred word around here now is 'evaluated model,'" he says.

Wuebbles, Kotamarthi, and their collaborators recently finished "probably one of the harshest tests MOZART was ever subjected to," says Kotamarthi. It took him aboard a NASA jet on missions across the south Pacific as an "onsite modeler." A modified DC-8 passenger plane with air inlets and instrument stations for 30 to 40 scientists, the plane flew up to 40,000 feet and made spiral-staircase descents to 1,000 feet above the ocean at sites along its route. "The idea is you are trying to sample the vertical profile of trace gases at various altitudes," Kotamarthi says.

The air of the remote south Pacific is supposed to be squeaky clean, and it generally was. But the scientists were surprised by fingers of polluted air—"dirtier than maybe in the LA city area on a bad day," says Kotamarthi. These fingers seemed to extend thousands of miles in strips only a few thousand feet thick. On the ground, Kotamarthi and fellow modelers compared the flight measurements to MOZART-2 predictions for the same region and time of year. The concentrations of ozone differed by about 30 percent, Kotamarthi says. But the model tracked seasonal changes.

To see the simulated plumes, the modelers had to double the burning emissions they had first assumed. But scientists' best estimates of the dirtiness and extent of such fires are just rough averages, says Kotamarthi, and they relate to 1991. The fires that produced the plumes NASA detected on its 1996 and 1999 south Pacific flights may have generated more pollution, he says. The model was further handicapped by having to work from generic seasonal winds created by a computer.

While MOZART-2 can't compute global chemistry from weather measurements alone, the modelers have begun using artificial weather steered by real data for specific years. A precise assessment of how MOZART-2 and the Pacific measurements disagree awaits the results of these runs, Kotamarthi says. But he says the team has already acquired confidence in using the model to answer basic questions.

Safe...or not

Some of these questions have immediate practical importance. For example, Wuebbles worries that many proposed alternatives to CFCs are not so benign as scientists have supposed. Using MOZART-2, he has set his team to examining them more rigorously before an international timetable requires countries to choose which ones to allow. Many of the new compounds that chemists have engineered are like CFCs, yet flimsier, so the molecules degrade before they reach the stratospheric ozone layer almost 100 percent of the time. Nevertheless some kinds of degradation reactions stall, Wuebbles warns, generating not-yet-neutralized compounds that are heartier than their progenitors. Wuebbles says such scenarios need to be considered. To make his case, he points to results his team reported in the July 16 Journal of Geophysical Research.

MOZART-2 simulates how atmospheric gases interact chemically and redistribute over time. The above snapshot depicts ozone in green and nitrogen oxides in blue. Image courtesy of the Visualization Lab and Brasseur et al. at NCAR.
From manuals and chemistry reports, the researchers culled constants for calculating how fast and in what way n-propyl-bromide (a CFC substitute) and its breakdown products react with different molecules in the atmosphere. Feeding the numbers to MOZART-2, team members then simulated the release of this compound from the equator and points north and south. The high and low latitude launches took n-propyl-bromide on a slow journey to the stratosphere that few molecules survived in any form. But trips from the tropics were fast and delivered many molecules in a merely maimed state in which they were as dangerous as CFCs.

The results are surprising, says Jeff Cohen, chief of the EPA branch formulating U.S. recommendations on CFC alternatives for the United Nations. He says the inventors of n-propyl-bromide are already manufacturing and selling it in anticipation of a multinational thumbs up. "I think some countries will be inclined not to allow its use," he says.

What lies ahead

Wuebbles next wants to simulate how the ozone layer will recover under alternate schedules for the phase-out of CFCs and their successors. "It's important for us to know just what it's going to take for ozone to recover," he says. Because the repair is liable to last decades, the simulations will need to account for climate change—both how warming impacts ozone and how ozone impacts warming.

No doubt exists that ozone and the climate interact powerfully, says Wuebbles. Antarctica would have no hole were its winters slightly balmier, he says, citing the comparative health of Earth's opposite pole as illustration. Meanwhile, as the planet's ultraviolet shield, ozone controls how much sunlight penetrates the atmosphere; and as the third most influential greenhouse gas after water and carbon dioxide, it regulates how much of that energy the Earth retains for warmth. Finally, the climate and ozone are connected through their interdependence on the ecology carpeting Earth's surface.

The time is ripe for learning how such interactions play out, Wuebbles says. Already NCAR scientists are fitting a stratosphere around MOZART-2's naked troposphere (the layer that holds the clouds and weather) so that the ozone layer and hole may be part of future simulations. Patten is preparing to extend the study of CFC substitutes into the unique chemical environment high above the south pole, which he will do on NCSA computers next year. And NCAR, Wuebbles' team, and other collaborators are arranging a duet between MOZART and BACH—a Biosphere-Atmosphere-Chemistry model—that will include ecology. Harnessed to a computer, this fused application would be the most gargantuan ever to draw the Earth—and not every student of the atmosphere will be able to run it.

Wuebbles predicts that he and his collaborators will soon be raising their hands again for supercomputing time from NCSA.

This research is supported by the Environmental Protection Agency and NASA. The development of MOZART-2 is supported by the National Center for Atmospheric Research. Guy Brasseur leads the MOZART team at NCAR, which includes Louisa Emmons, Claire Granier, Didier Hauglustaine, Larry Horowitz, Doug Kinnison, Denise Mauzerall, Martin Schultz, and Xue-Xi Tie.

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

For further information:
http://acd.ucar.edu/models/MOZART/

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Femi Ogunsola, Vaishali Naik, Don Wuebbles, Chu-Feng Wei, Rong Li, Ken Patten, Long Cao, and Atul Jain.
NCSA

The National Center for Supercomputing Applications, one of the five original centers in the National Science Foundation's Supercomputer Centers Program and a unit of the University of Illinois at Urbana-Champaign, opened its doors in January 1986. NCSA earned and maintains an international reputation in high-performance computing and networking and in developing innovative software applications. NCSA greatly broadened the user base of remote supercomputing and the Internet with NCSA Telnet in 1987. In 1992 the center introduced NCSA Mosaic, the first readily-available graphical Web browser.

Since 1997 NCSA has been the leading-edge site for the National Computational Science Alliance, one of two partnerships of the NSF's Partnerships for Advanced Computational Infrastructure program. The center anchors all Alliance teams and oversees the administration of all Alliance programs. It has the largest production high-performance computing facility in the Alliance, and it works with government agencies, communities, and schools to discover how high-performance computing and communication can benefit them. Through its Private Sector Program, top researchers from Fortune 500 companies 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.

In August 2001 NCSA—as part of a team of institutions that also includes the San Diego Supercomputer Center, Argonne National Laboratory, and the California Institute of Technology—was tapped by the National Science Foundation to build the most comprehensive computational infrastructure ever deployed for open scientific research. Besides offering the world's fastest unclassified supercomputers with 13.6 teraflops of aggregate computing power, this "TeraGrid" hardware and software will include ultra high-speed networks, high-resolution visualization environments, and toolkits for grid computing. Building and deploying the TeraGrid will take three years.

2001 Strategic industrial partners
Allstate Insurance Company
The Boeing Company
Caterpillar, Inc.
Eastman Kodak Company
J. P. Morgan Chase and Co.
Kellogg Company
Motorola, Inc.
Sears, Roebuck and Co.
Shell Oil Company

Government partners
Defense Advanced Research Projects Agency
Department of Defense High Performance Computing Modernization Program's Programming Environment and Training Initiative
Department of Energy Accelerated Strategic Computing Initiative
Illinois Auditor General
Illinois Municipal League
Illinois State Board of Education
NASA
National Imagery and Mapping Agency
National Response Center
NSF Digital Government Consortium
NSF Partnerships for Advanced Computational Infrastructure

Strategic technology partners
IBM Corporation
Intel Corporation
Myricom, Inc.
Oracle Corporation
Qwest Communications
SGI
The Alliance

The National Computational Science Alliance is a nationwide partnership of more than 50 academic, government, and business organizations working together to prototype an advanced computational infrastructure for the new century. This infrastructure, called the grid, is rapidly developing into a ubiquitous, pervasive, national-scale information infrastructure that links supercomputers, virtual environments, scientific instruments, large databases, and research teams.

The Alliance includes an Enabling Technologies team, which builds the infrastructure of the grid, and five Application Technologies teams, which drive the development of applications and tools to meet the needs of specific scientific disciplines. The Partners for Advance Computational Services provide computing resources and training to the national high-performance computing community. The Education, Outreach, and Training Partnership for Advanced Computational Infrastructure spans the Alliance and the National Partnership for Advanced Computational Infrastructure. It brings innovations to new audiences, including schools, local, state, and federal government, and underserved populations.

Application Technologies

The Alliance’s five Application Technologies (AT) teams develop new technology and software and demonstrate their potential. They collaborate with the Enabling Technologies team to prototype new elements of the grid, while actively using grid applications in a broad range of scientific research. NCSA researchers anchor each AT team and act as a liaison to their discipline communities.

Chemical engineering
Massachusetts Institute of Technology
University of Illinois, Urbana-Champaign
University of Kansas

Computational biology
University of Illinois, Urbana-Champaign

Cosmology
American Museum of Natural History
Harvard University
Massachusetts Institute of Technology
Princeton University
Space Telescope Science Institute
University of California, San Diego

Environmental hydrology
Rutgers University
University of Iowa
University of Maryland, College Park
University of Oklahoma
University of Wisconsin, Madison
Virginia Tech

Nanomaterials and nanodevices
Arizona State University
North Carolina State University
Northwestern University
Ohio State University
Stanford University
University of Pittsburgh
University of Texas, Austin

Scientific instrumentation
National Radio Astronomy Observatory
University of Illinois, Urbana-Champaign

Enabling Technologies

The Alliance Enabling Technologies (ET) team, partnering with NCSA, is the core development engine of the Alliance. With the ultimate goal of improving scientific productivity, members at partner sites prototype new pieces of the Alliance computational infrastructure, including new grid technologies, cluster computing tools and system software, collaborative environments, and user portals.

Partner sites
Argonne National Laboratory
Clemson University
Indiana University
Northwestern University
Princeton University
Rice University
University of Houston, University Park
University of Illinois, Chicago
University of Illinois, Urbana-Champaign
University of Minnesota, Minneapolis
University of Tennessee, Knoxville
University of Utah
University of Wisconsin, Madison
Partners for Advanced Computational Services

The Alliance Partners for Advanced Computational Services (PACS) help disseminate and support technologies developed by the Alliance. They also coordinate the allocation of the Alliance’s high-performance computing resources and provide user support for these resources. Many PACS sites also serve as training grounds by hosting workshops, offering consulting services, and introducing researchers to high-performance computing.

Partner sites

- Albuquerque High Performance Computing Center at the University of New Mexico
- Argonne National Laboratory
- Boston University Experimental Program to Stimulate Competitive Research (EPSCoR)
- National Center for Supercomputing Applications
- Ohio Supercomputer Center
- Southeastern Universities Research Association (SURA)
- University of Kansas
- University of Kentucky
- University of Wisconsin, Madison

PACS resources

Albuquerque High Performance Computing Center at the University of New Mexico
- LosLobos Linux cluster—512 Pentium III processors
- RoadRunner Linux cluster—128 Pentium II processors

Boston University
- IBM Power3 SP—64 processors
- IBM Power4 SP—32 processors
- SGI Origin2000—192 processors
- SGI Power ChallengeArray—38 processors

National Center for Supercomputing Applications
- Titan Linux cluster—320 Itanium processors
- Platinum Linux cluster—1,024 Pentium III processors
- SGI Origin2000—1,520 processors
- HP-Convex Exemplar SPP-2000—64 processors

University of Kentucky
- Hewlett-Packard N-4000 cluster—96 processors
- Hewlett-Packard SuperDome cluster—224 processors

University of Wisconsin
- Condor computing environment—more than 1,000 processors

Education, Outreach, and Training

The Alliance’s education, outreach, and training efforts are part of NSF’s Education, Outreach, and Training Partnership for Advanced Computational Infrastructure (EOT-PACI) program. EOT-PACI is a joint undertaking with the Alliance’s sister program, the National Partnership for Advanced Computational Infrastructure. It is dedicated to making emerging technologies accessible to learners and educators at all levels, forging an inclusive computing community.

Partner sites

- Albuquerque High Performance Computing Center at the University of New Mexico
- American Indian Higher Education Consortium
- BioQuest Curriculum Consortium
- Boston University Coalition to Diversify Computing
- Committee on the Status of Women in Computer Science and Engineering Research
- Indiana University
- Maryland Virtual High School of Science and Mathematics
- National Center for Supercomputing Applications
- Ohio Supercomputer Center
- Rice University
- SRI International
- The Shodor Education Foundation
- University of Alabama, Huntsville
- University at Albany, SUNY
- University of Houston, Downtown
- University of Illinois, Urbana-Champaign
- University of Wisconsin, Madison
External Advisory Council and Executive Committee
The External Advisory Council’s members, who have decades of experience in computing and communications or in science and technology, advise the Alliance on issues in government, academia, and education. They also review the performance of the Alliance’s management.

Chair of the External Advisory Council, Philip M. Smith is a partner in McGeary and Smith, science policy consultants and authors. He has been involved in national and international science and technology policy and program development for more than four decades. Smith has held senior positions at the National Academy of Sciences and the National Research Council, the White House Office of Science and Technology Policy, and the National Science Foundation.

John Perry Barlow is a fellow at Harvard Law School’s Berkman Center for Internet and Society and co-founder of the Electronic Frontier Foundation, an organization that promotes freedom of expression in digital media. A former lyricist for the Grateful Dead, Barlow is a contributing writer for Wired and a contributing editor for numerous publications.

C. Gordon Bell served as the first assistant director for computing at the National Science Foundation and was an author of the NSF High Performance Computing and Communications Initiative during his tenure there. In 1991 he received the National Medal of Technology for work as head of research and development at Digital Equipment Corp. A senior researcher at Microsoft Corp., Bell works on telepresence and parallel processing.

Paul Bohn is interim vice chancellor for research and a professor of chemistry at the University of Illinois at Urbana-Champaign. Bohn received the Coblenz Award in 1990 and the ACS Spectrochemical Analysis Award in 1997. His research interests are in materials and analytical chemistry.

A former director of the National Science Foundation, Erich Bloch is a principal and president of the Washington Advisory Group, a consulting firm that provides strategic council and management consulting to companies, universities, governments, and not-for-profit organizations. He is also a distinguished fellow of the Council on Competitiveness, a private organization that represents a broad cross section of American businesses and universities to advance the country’s competitiveness. Before joining NSF, Bloch was corporate vice president for technical personnel development at IBM.

Chair of American Association for the Advancement of Science’s Board of Directors, Mary L. Good is the Donaghey University professor and dean of the Donaghey College of Information Science and Systems Engineering at the University of Arkansas at Little Rock. Good is also a managing member of Venture Capital Investors, LLC. A chemist, materials scientist, and engineer, she began her career at Louisiana State University, where she held increasingly significant positions, including the Boyd Professorship, from the mid-1950s through the 1970s. After 13 years as an industrial research manager, culminating in the position of senior vice president for technology for Allied Signal, she served as the undersecretary for technology in the U.S. Department of Commerce from 1993 to 1997.

Robert W. Lucky is corporate vice president of Applied Research at Telcordia Technologies, formerly Bellcore. He began his telecommunications career at AT&T Bell Laboratories in Holmdel, NJ, where he invented the adaptive equalizer, a technique for correcting distortion in telephone signals that is used in all high-speed data transmission today. Lucky is the author of Silicon Dreams: a discussion of the ways humans and computers deal with information.

Since becoming a professor of physics at the University of Michigan in 1987, Homer A. Neal has also served as chair of the physics department, vice president for research, and interim president of the university. Neal is director of the UM-ATLAS Collaboratory project, a regent of the Smithsonian Institution, and a fellow of the American Physical Society, the American Association for the Advancement of Science, and the American Academy of Arts and Sciences.

As a senior member of the W. K. Kellogg Foundation’s executive staff, Anne C. Petersen provides overall leadership for programming. Before joining the Kellogg Foundation, she was the deputy director of the National Science Foundation. In addition to a long career in academic and research administration, Petersen has had a productive research career, with more than a dozen books and more than 200 articles and chapters.

John Reynolds is the vice president of information systems at Celera Genomics. Prior to joining Celera, Reynolds worked at Sun Microsystems in their high performance computing area and at Los Alamos National Laboratory where he managed multiple high performance computing projects and developed strategic simulation capabilities. Reynolds obtained his undergraduate degree in mathematics from Rensselaer Polytechnic Institute and his PhD in applied and computational mathematics from Princeton University.
The Executive Committee (EC) focuses on long-range strategic and technical issues of interest to the Alliance. Its members are all leaders in computational science and engineering. It acts in an advisory role to the Alliance Steering Committee and the Alliance director. The Steering Committee's members represent the Alliance's major teams.

Dan Reed is director of the Alliance and NCSA and the Edward William Gutgsell and Jane Marr Gutgsell Professor at the University of Illinois at Urbana-Champaign. He is one of two principal investigators for the DTF TeraGrid and serves as the TeraGrid's chief architect. Reed is a member of several national collaborations, including the Center for Grid Application Development Software, the Department of Energy Accelerated Strategic Computing Initiative and the Scientific Discovery through Scientific Computing (SciDAC) program, and the Los Alamos Computer Science Institute. He also serves on the board of directors of the Computing Research Association.

Jerry Bernholc—Drexel professor of physics at North Carolina State University—uses high-performance computations to study problems in solid state and material physics. Bernholc is one of the leaders of the Alliance's nanomaterials team. In 1997 he was a finalist for a Computer World/Smithsonian Award for Science.

John W. D. Connolly plays many roles at the University of Kentucky, serving as a professor of physics and astronomy, director of Kentucky EPSCoR, and director of the Center for Computational Sciences. Before joining the faculty of the University of Kentucky, Connolly was the director of NSF’s Division of Advanced Scientific Computing, which initiated the NSF supercomputer centers program and NSFNET.

The Alliance’s chief applications scientist, Richard Crutcher is a member of the Alliance Steering Committee and head of the astronomy department at the University of Illinois at Urbana-Champaign. Crutcher is the team leader of the Alliance’s Radio Astronomy Imaging group and a member of the AIPS++ consortium and the BIMA radio telescope executive committees. His research interests include star formation, magnetic fields, and radio synthesis imaging.

Thomas Defanti is a distinguished professor of computer science, director of the Electronic Visualization Laboratory, and director of the Software Technologies Research Center, all at the University of Illinois at Chicago. He is also the principal investigator of the NSF STAR TAP and Euro-Link international networking projects. In 1991 Defanti and EVL codirector Daniel J. Sandin conceived the idea for the CAVE virtual reality theater.

Dennis Gannon is a professor in the department of computer science, which he also chairs, at Indiana University. He is a member of the Alliance EE team and the Alliance Steering Committee. He was involved in the design of the NASA Information Power Grid Project, and he is currently involved in the DoE 2000 Common Component Architecture software effort. He also cochaired the Concurrency and Parallelism subgroup of the Java Grande Forum and is currently the science director for the Indiana Pervasive Computing Research (IPEAR) center.

Fred Geinowski joined Allstate Insurance Co. as a systems programmer in 1967 and is now senior systems planning consultant in the company's Advanced Technology Research department. He has been the onsite coordinator of Allstate's relationship with NCSA since February 1996, when Allstate became a member of the Private Sector Program. He holds a bachelor's degree in finance from DePaul University and an MBA in quantitative methods and computers from Loyola University in Chicago.

As a co-founder and the deputy director of Boston University’s Center for Computational Science, Roscoe C. Giles promotes and develops applications of high-performance computing. Giles is a professor of electrical and computer engineering at Boston University and team leader for Alliance Education, Outreach, and Training. Giles is also the executive director of the Institute for African-American Eculture and serves on the Alliance Steering Committee.

Miron Livny is a computer science professor at the University of Wisconsin, a member of the Alliance Steering Committee, and leader of the Alliance Partners for Advanced Computational Services’ efforts. Livny has led the development of the Condor high-throughput computing system since 1986.

Gregory McRae is a Bayer professor of chemical engineering at the Massachusetts Institute of Technology. He studies the scientific aspects of pollutant transport, transformations in multimedia environments, and the design of products and processes that avoid environmental problems.

Prior to accepting the Plumian Professorship of Astronomy and Experimental Philosophy at the University of Cambridge, Jeremiah Ostriker served as provost of Princeton University, where he is still the Charles A. Young Professor of Astronomy. He is the principal investigator of the NSF Computational Grand Challenge Cosmology Project and is currently serving on the NSF Advisory Committee for Cyberinfrastructure.
Executive Committee
Continued

Larry Smarr is one of the pioneers in creating a national information infrastructure to support academic research, government functions, and industrial competitiveness. In 1983 he initiated the first proposal to the National Science Foundation to establish a national supercomputer center. He worked with Congress in 1984 to ensure passage of legislation that authorized the original NSF supercomputer centers and the NSFNET national network. Smarr became the founding director of NCSA in 1985 and of the Alliance in 1997. He is now Alliance strategic advisor, director of the California Institute for Telecommunications and Information Technology, and a computer science and engineering professor at the University of California at San Diego.

Valerie Taylor is an associate professor in the electrical engineering and computer science department at Northwestern University and holds a guest appointment with Argonne National Laboratory. Her research focuses on computer architecture and high-performance computing, with particular emphasis on mesh partitioning for distributed systems and the performance of parallel and distributed applications. In 1993 she received a National Science Foundation Young Investigator award.

Chair of the External Advisory Council, Philip M. Smith is a partner in McGeary and Smith, science policy consultants and authors. He has been involved in national and international science and technology policy and program development for more than four decades. Smith has held senior positions at the National Academy of Sciences and the National Research Council, the White House Office of Science and Technology Policy, and the National Science Foundation.

Mary Vernon has been a faculty member at the University of Wisconsin at Madison since 1983. Vernon received the NSF Presidential Young Investigator award in 1985, the NSF Faculty Award for Women in Science and Engineering in 1991, the ACM Fellow Award in 1996, and the University of Wisconsin Vilas Associate Award in 2000. She served on the Board of Directors of the Computing Research Association from 1994 to 1999 and was chair of ACM SIGMETRICS from 1999 to 2001.

Alliance chief computational architect and member of the Alliance Steering Committee, Rick Stevens is director of the Mathematics and Computer Science (MCS) division at Argonne National Laboratory. He also leads the MCS Futures Laboratory, an effort to develop multimedia collaborative environments, virtual reality, and advanced networking. His major research interests are collaborative and virtual environments, advanced scientific visualization technology, supercomputer performance modeling, and molecular nanotechnology simulation.

Paul Woodward's research explores nonlinear phenomena in fluid dynamics through large-scale computer simulations. He has concentrated on turbulent flows, especially in astrophysical contexts where the effects of compressibility are important. Woodward is a professor of astronomy and director of the Laboratory for Computational Science and Engineering at the University of Minnesota.
Whether in airplane engines or power plants, turbine blades are often subjected to extremely high temperatures. The blades are cooled internally with cold air flowing through serpentine channels. To enhance the rate of cooling, roughness elements or ribs are placed in the channels to generate turbulence.

The first image shows a section of a channel wall near a rib. Isosurfaces of instantaneous coherent vorticity created by shear layer instabilities on the rib enhance mixing and heat transfer. The regions of coherent vorticity are correlated to regions of high heat transfer (blue) on channel walls. Hot spots (red) are found at corners and immediately behind the rib.

The second image plots instantaneous velocity streamtubes and temperature on channel walls. The intertwined nature of streamtubes is a result of strong mixing in the flow.

A small section of a multi-louvered fin and the three-dimensional flow features around it are shown in the third image. Fins increase the surface area and rate of heat transfer in a system, and multi-louvered fins, which are often used in compact heat exchangers, enhance mixing and heat transfer. Instantaneous streamtubes illustrate a coherent vortex jet and its vorticity signature on a x-plane passing through the louver.

These simulations were created by Danesh Tafti and Randy Heiland of NCSA, using GenIDLES computational fluid dynamics software and NCSA VisBench, a visualization system. Research represented in the visualization of the multi-louvered fin is supported by the Air-Conditioning Refrigeration Center at the University of Illinois at Urbana-Champaign. For more information, see http://www.ncsa.uiuc.edu/Apps/CFD/ and http://visbench.ncsa.uiuc.edu/.