2008 Annual Research Report

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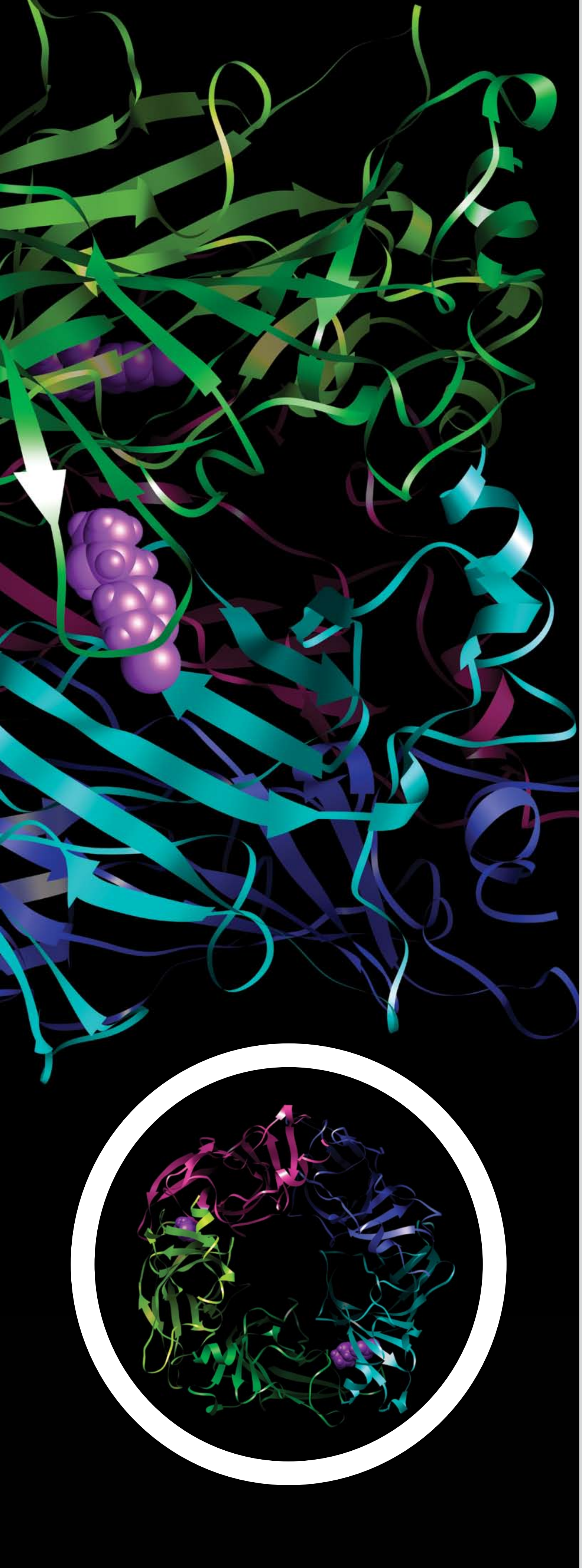
Ohio Supercomputer Center



features

cover & left: In an effort to find a treatment for neurodegenerative disorders, Ohio State University biochemists are studying the activities of chemicals that thwart messages sent to the brain by modeling a specific class of proteins called nicotinic acetylcholine receptors (nAChRs). These figures show a portion of an nAChR, its activating compound and the dynamics that occur when the two bind to each other **(see story, page 15)**.

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Ohio Supercomputer Center 2008 Annual Research Report
Published by OSC to present noteworthy research activities and grant funding during the 2007–08 fiscal period.

introduction

Ohio always has been a state renowned for its legacy of discovery and innovation. With a vision toward nurturing such lofty pursuits, the Ohio Board of Regents in 1987 created the Ohio Supercomputer Center to help position Ohio's research universities and private industry at the forefront of computational research. More than 20 years later, this enlightened vision still empowers the Center and its dedicated staff.

"The historic strengths and traditions of our individual universities will be drawn upon to create distinctive missions for each, leading to the establishment of nationally and internationally recognized Centers of Excellence that will be drivers of both the regional and state economies," Chancellor Eric Fingerhut said in his recent strategic plan for Ohio's colleges and universities.

"The plan recognizes that a measure of the success of the University System of Ohio will be increases in the amount of federal research funding received by Ohio researchers. Supercomputing is essential to this goal," he said.

The current and future competitiveness of innovators working at The Ohio State University, within the University System of Ohio, at private colleges, at federal labs, in private industry and throughout the State of Ohio rely upon the development and operation of a powerful, science-enabling cyberinfrastructure.

A physicist must have access to cutting-edge supercomputers. A pediatrician needs a fiber-optic network connection to a neonatal specialist. A medical student requires real-time, interactive computer simulations. And, a manufacturer wants new employees skilled in computational science.

These are just a handful of the current demands for robust cyberinfrastructure resources here in Ohio that you will see described on the following pages. The staff of Ohio Supercomputer Center and the Ohio Academic Resources Network partner diligently and collaboratively to provide effective responses to these demands … to further extend Ohio's legacy of discovery and innovation. ■

above: Stanley C. Ahalt, Ph.D., serves as executive director of the Ohio Supercomputer Center.

right: OSC offers an effective combination of power, including the IBM Cluster 1350, and people, represented by (from left to right) Jim Giuliani, client and technology support manager; Ashok Krishnamurthy, Ph.D., senior director of research; and Kevin Wohlever, director of supercomputing operations.

overview

above: Higher education Chancellor Eric Fingerhut utilizes high-definition videoconferencing technology of the Ohio Supercomputer Center and OARnet to coordinate the campus safety and security efforts of more than 100 colleges and universities across Ohio.

Ohio: Truly a State of Innovation. The names of Ohioans famous for their discoveries and inventions are known across this nation and around the globe. The register of names is endless, because the inventory of Ohio innovations continues to expand in the national annals.

Emerging as a significant player in the modern global, information-age economy, Ohio possesses one of the most potent combinations of statewide cyberinfrastructure elements in the world: high-end supercomputers, high-speed networking, research leadership and inspirational education.

"I believe that modeling, simulation and large-scale analysis with high performance computing is vital to maintaining an edge in American innovation," said Richard H. Herman, co-chair of the Council on Competitiveness HPC Initiative and chancellor of the University of Illinois at Urbana-Champaign. "High performance computing simply is transforming business processes worldwide."

Supercomputers, however, are only as powerful as the software they can effectively run. In order to expand that base of software, it must be easier to develop code for massively parallel systems.

"The cyberinfrastructure and software development program at the Ohio Supercomputer Center addresses this pressing need through a combination of software development, a robust production services environment and in-house research and consulting," said Ashok Krishnamurthy, Ph.D., senior director of research at OSC.

A rising national issue sponsored by OSC, Blue Collar Computing™ seeks to help industry gain easy and affordable access to advanced computing technologies **(see sidebar, page 6)**. Under this program, advanced computational technologies provide companies with innovative tools that allow for the virtual development of new and improved products.

OSC also has partnered with Ohio's higher education and business communities to develop the innovative, virtual Ralph Regula School of Computational Science to help ensure Ohio fields a highly skilled workforce in computational science **(see sidebar, page 8)**.

To energize these initiatives, OSC installed an IBM Cluster 1350 supercomputer earlier this year. OSC's array of equipment also includes a visualization cluster, a network research cluster and a large mass storage environment.

For Ohio, with widely distributed educational and research centers, OSCnet, managed by OARnet, provides the connectivity to enable widespread collaboration. OSCnet features more than 1,850 miles of fiber-optic backbone, and OARnet provides an array

(continued on page 7)

above: A recently established Center for Excellence in Advanced Materials Analyses will utilize Ohio Supercomputer Resources for research, analyses, modeling and commercialization of new refractory materials.

above: The Ohio Supercomputer Center has developed the ePolymer portal to make the state's plastics, rubbers and advanced materials industry more productive and more profitable through high performance computing.

Blue Collar Computing™

The Ohio Supercomputer Center's award-winning Blue Collar Computing™ program focuses on providing the power of supercomputing to companies that cannot afford to acquire the hardware, software and staff necessary to successfully compete in the global economy. Larger companies already possess the scale of operations to invest in this technology and the expertise to leverage advanced modeling techniques.

Supercomputing, known as high performance computing in the industry, can reduce the time required to design new products, lead to the discovery of new processes and products, reduce a product's time-to-market and improve production quality and efficiency. Leading companies are using sophisticated computer models to create and improve a diverse array of products, ranging from containers and pharmaceuticals to automobiles and airplanes, testing different product designs before physical products are manufactured.

This competitive edge is vital to keeping Ohio and America at the forefront of the global economy. The Center's BCC program has developed a strong foundation of technology infrastructure and staff expertise to infuse high performance computing into the industrial marketplace. Recent accomplishments include:

- Working with the Edison Welding Institute, OSC introduced the E-Weld Predictor portal, an easy-to-use, web-based interface that allows welding engineers to simulate "virtual" welds. Since its launch in 2007, more than 115 EWI members have tested pipe and sheet welds via the portal.
- Collaborating with PolymerOhio, OSC is developing the ePolymer portal for the state's plastics, rubber and advanced materials industry. PolymerOhio promotes dialogue between technology developers and technology implementers, and OSC partnered with the group to present the forum "Productivity—The Key to Profitability" in 2007.
- Partnering with the Ohio Supercomputer Center and Fireline TCON Inc., Youngstown State University will establish a Center for Excellence in Advanced Materials Analyses. The project will focus on research, analyses, modeling and commercialization of products with increased resistance to thermal shock and lower thermal conductivity.
- In conjunction with the University of Southern California's Information Sciences Institute and the Council on Competitiveness, OSC was awarded a Defense Advanced Research Projects Agency grant to study the migration of defense-critical modeling and simulation applications to high performance computing environments to speed the Defense supply chain procurement process.
- OSC is hosting supercomputing jobs for AP Solutions Inc., a minority-owned small business that provides designs and analysis of gas turbine engine components in support of the propulsion and power generation industries. ■

Blue Collar Computing™
an initiative of the Ohio Supercomputer Center

IBM Global Services, OSC's partner for BCC service development and business planning, recognized the program as a "unique concept" that "presents OSC with the opportunity to be the national leader in the development of applications for specific industries." The Center's current BCC efforts focus on three industry sectors – biosciences, advanced materials and data exploitation.

above: OSC created a web portal, E-Weld Predictor, that allows welding engineers to access high performance computing to evaluate various welded joints to reduce the extent of costly experimental trials during their design.

of networking services, such as videoconferencing, Internet2 connectivity, engineering consulting and satellite trailer systems for remote Internet connectivity. OSCnet has merged over the last year with a new state and local government networking initiative to create the Broadband Ohio Network.

With these statewide cyberinfrastructure elements largely in place, state policymakers in recent years moved to strategically align Ohio's research and technology portfolio to position the state for maximum and sustained economic growth.

Battelle, the Columbus-based international science and technology enterprise, compared the state's institutional and industrial technology platforms to identify those areas most promising for statewide economic impact. Seven specific technology platforms were identified, and the biosciences were organized into four additional technology platforms. Information technology was recognized as an important crosscutting technology platform on which numerous other fields rely and in which interdisciplinary research and development can occur.

OSC studied these dozen platforms and determined that three areas would be the most productive "areas of excellence" on which the Center could focus investments, collaborations, research and market solutions: biosciences, advanced materials and, within the IT platform, data exploitation.

The Center already had established close ties with the state's bioscience research community, especially within bioinformatics and biomedical sciences. OSC and OARnet have developed high-definition videoconferencing technologies to assist pediatricians in rural communities, created a virtual environment in which medical students can practice delicate surgical techniques and is helping to expand the highly skilled bioinformatics workforce.

A rising national issue sponsored by OSC, Blue Collar Computing™ seeks to help industry gain easy and affordable access to advanced computing technologies.

OSC staff members are improving research in advanced materials and multi-scale computational modeling and design. For example, physicists are developing new algorithms on OSC systems that could unlock the mysteries of superconductivity, a scientist is working with OSC staff to exploit the spin of electrons to create smaller, more efficient semiconductors, and a professor taps into OSC supercomputers to research new and improved materials that may lessen the impact of crashes.

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The Ralph Regula School of Computational Science

To provide Ohio workers with crucial training in computer modeling and simulation, the Ralph Regula School of Computational Science (RRSCS) is developing a new training and certification program. This project represents an important workforce component for the Ralph Regula School, a statewide virtual school focused on the use of computer modeling and simulation to solve complex business, technical and academic research problems.

The National Science Foundation-funded grant[*] also will supply Ohio businesses with advanced Internet portals — easy-to-use web-based interfaces that allow users to run complex scientific codes — including a portal being developed for Ohio's polymer industries.

"Computational science and the use of modeling and simulation have been cited by prominent state and federal committees and panels as keys to continued competitiveness in science and engineering," said Steven Gordon, Ph.D., director of RRSCS. "We intend to create more advanced, industry-driven computational science certificate programs to serve major groups of industry collaborators."

The certificate courses will link to a computational science concentration area within an emerging professional master's degree program at The Ohio State University's College of Engineering.

"The courses and certifications will be invaluable in preparing the workforce in our industry to move quickly and surely into the computer age," said Wayne Earley, executive director of PolymerOhio, an association serving Ohio's plastics, rubber and advanced materials industry.

The workforce program complements a robust educational pipeline at RRSCS that begins with the Young Women's Summer Institute (YWSI), a summer program for middle-school girls. YWSI was created by the Ohio Supercomputer Center to facilitate their interest in math, science and engineering and women's low participation trends in STEM career fields.

Summer Institute is an OSC summer program in its 20th year that offers gifted high school freshmen and sophomores project-based, hands-on learning. Participants use advanced technologies to solve complex problems and learn about careers in computing, networking, science and engineering.

The STEM Summer Academy in Computational Science and Engineering, funded through the Ohio Board of Regents, teaches computer modeling and simulation skills to high school juniors and seniors, as well as high school teachers. Participants receive college credit as they learn how physical phenomena are represented in mathematical models and translated into computer simulations.

RRSCS, the Ohio Board of Regents and Project Lead The Way are developing a computational science elective to add to the four-year curriculum that introduces high school students to the scope, rigor and discipline of engineering and engineering technology prior to entering college.

RRSCS and three Ohio community colleges are developing an associate degree program in science with a computational science emphasis under another NSF grant[**]. The goal is to develop programs that constitute the middle two years of an articulation from the high schools to the community colleges and four-year colleges and universities.

Last year, RRSCS launched a baccalaureate minor program in computational science in partnership with nine Ohio charter colleges and universities. Two other colleges have since joined the program. The virtual nature of this NSF-funded program[***] allows students at participating institutions to combine classes from their home campus with online classes from any other participating institution.

This complete pipeline of educational offerings comprises a unique middle school-to-graduate school-to-workforce training continuum in computer modeling and simulation education in Ohio. ■

* NSF # 0753287 ** NSF # 0703087 *** NSF # 0537405

below: Through the Ralph Regula School of Computational Science, the Ohio Supercomputer Center and its partners offer a continuum of science, technology, engineering and mathematics (STEM) educational opportunities, from junior-high summer institutes to college-level programs to workforce certificates.

above: Policymakers have begun to recognize the widespread adoption of computational science as crucial to America's scientific leadership and economic competitiveness. A limiting factor, however, is the education of sufficient numbers of computational scientists — a situation the Ralph Regula School of Computational Science aims to remedy.

The amount of data generated in research, engineering and medicine has grown astronomically, and researchers often are at a loss to exploit its full potential. OSC provides Ohio researchers with a combination of innovative data storage, annotation systems, file systems, advanced I/O and management systems, as well as analytical software and the computational muscle to exploit the data. Using OSC resources, a polar scientist combines a decade of land, sea and atmospheric measurements to understand climate changes at the North Pole, and researchers use a hardware/software package developed at OSC to manipulate powerful electron microscopes and mass spectrometers over the Internet.

OSC also has partnered with Ohio's higher education and business communities to develop the innovative, virtual Ralph Regula School of Computational Science to help ensure Ohio fields a highly skilled workforce in computational science.

OSC also supports basic and applied research outside of its three targeted areas of excellence, supporting a wide array of research being conducted at Ohio's institutions of higher learning. A researcher creates visualizations at OSC to provide forestry officials with new insights on wildlife survival of forest fires and a scientist processes satellite data on OSC systems to predict flood patterns for the central Amazon floodplain.

The research and discoveries enabled by the Ohio Supercomputer Center are valuable because of their contribution to the expansion of human knowledge, the improvement and saving of lives and the attraction of talent and valuable jobs.

"By attracting and supporting talented researchers who are interested in pushing the boundaries of existing disciplines, higher education can become the source of new inventions and technologies that spur the creation of entire new industries, transforming the economy of the state in the same way that the invention of the automobile transformed Ohio a century ago," Chancellor Eric Fingerhut recently noted in his strategic plan for Ohio higher education.

Whether scientific inquiry in Ohio delves into the furthest reaches of the biosciences, advanced materials, data exploitation or other fields across the research landscape, OSC is prepared to provide the computational resources and professional talent to help maintain Ohio's legacy as the State of Innovation. ■

biological sciences

Bioscience investigators in Ohio are accessing vast amounts of genetic, clinical, imaging and environmental data to individualize the diagnosis and treatment of disease. For instance, researchers employ a tool in the fight against cancer in the form of a web portal that correlates tumor images with their corresponding genetic codes. Neonatal specialists in large cities use high-definition videoconferencing to examine critically ill newborns at rural hospitals. And, medical residents train in virtual environments, improving surgery techniques and saving money. In addition to health care, the application of bioscience to agriculture, energy and industrial products are growing in importance. The bioscience industry in Ohio employs more than 1.2 million workers and contributes an annual statewide economic impact of $146 billion, according to BioOhio, a nonprofit industry association. The following pages illustrate just a few examples of cutting-edge research in the biosciences supported by the computational resources of the Ohio Supercomputer Center. ■

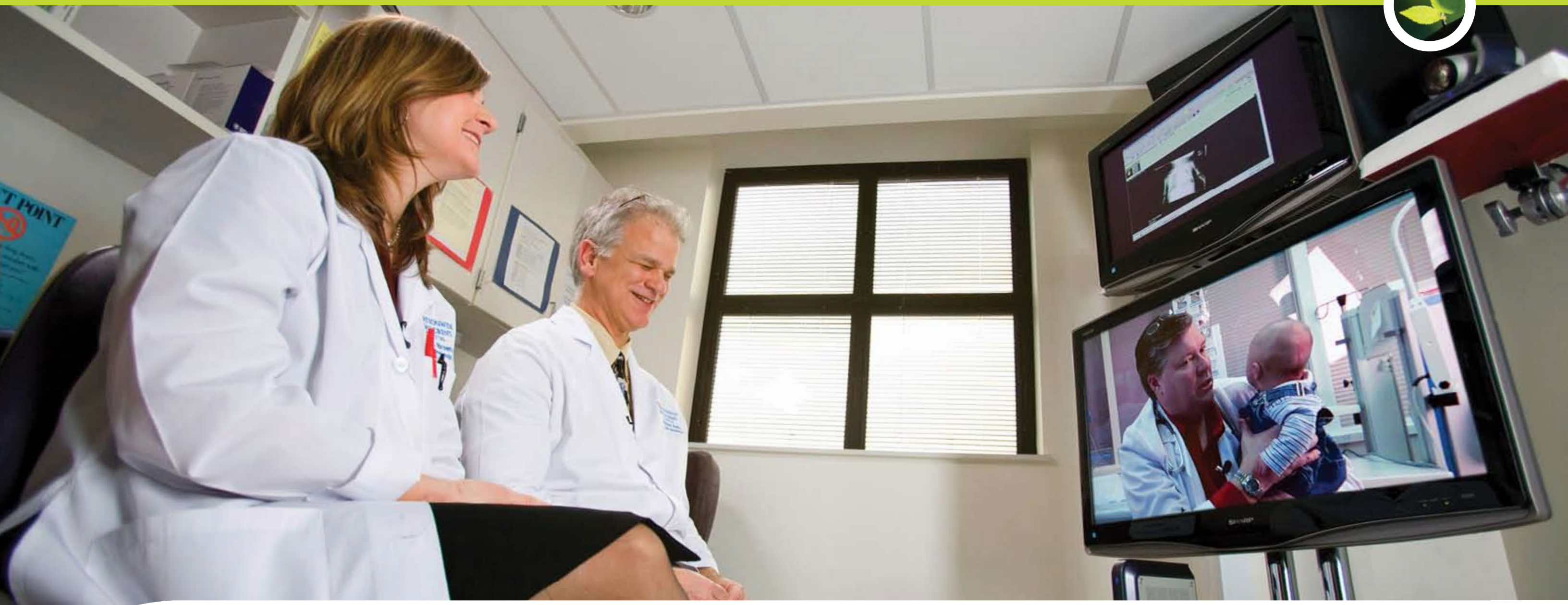


photo courtesy of Nationwide Children's Hospital

above: Neonatal specialist Rachel Brown, M.D., and Chief of Neonatology Stephen Welty, M.D., at Nationwide Children's Hospital consult with a pediatrician at Adena Regional Medical Center, via high-definition videoconferencing, to evaluate distressed newborns in the largely rural community.

Growing telemedicine trend impacts smallest of patients

Stacie Traylor delivered her tiny baby five weeks prematurely because of complications from gestational diabetes. Concerned doctors at Adena Regional Medical Center in Chillicothe, Ohio, informed Stacie that little Emilie had suffered a collapsed lung. They were considering moving Emilie 45 miles north to Nationwide Children's Hospital in Columbus, where top neonatal specialists could treat her.

The doctors reconsidered the move and chose a different, more innovative approach to caring for Emilie. Through a pilot project with the Ohio Supercomputer Center, both hospitals had positioned sophisticated cameras and monitors in their nursery facilities and established a high-definition video connection through the fiber-optic channels of the Broadband Ohio Network. With the equipment in place, the specialists observed sharp, colorful video of the baby and consulted with her Adena doctors, ultimately determining that Emilie could safely be treated in Chillicothe, near her loving, worried parents.

"Telemedicine dramatically increases the care of our youngest patients," said Dr. John Fortney, medical director for Adena Health System. "If we're looking for help with a diagnosis, someone from Children's — whether it's a neonatologist or a sub-specialist, such as a pediatric cardiologist — will see the patient and speak to the attending physician in real time.

"Before, information was relayed by telephone, which meant it was subject to interpretation," he said. "With high-definition videoconferencing, specialists can make a more thorough evaluation."

Adena Regional Medical Center was selected for the pilot project because the hospital sends more

above: Doctors at rural medical centers employ advanced videoconferencing technologies to access specialists who can help determine if a distressed newborn must be transported to a more advanced, but distant facility. Here, John Radford, M.D., a pediatrician at Adena Regional Medical Center, confers with Drs. Brown and Welty at Nationwide Children's Hospital in Columbus.

photo courtesy of Nationwide Children's Hospital

Nowhere is the need for broadband greater than in rural health care, where isolated clinics can save lives by using advanced communications technology to tap the expertise of modern urban medical centers.

photo courtesy of Nationwide Children's Hospital

left: High-definition videoconferencing equipment allows specialists — such as Nationwide Children's neonatologist Dr. Rachel Brown — to view distressed newborns with exceptional clarity, examine detailed x-rays, view lab results and consult with attending physicians in real-time.

far left: Often, in the case of distressed newborns, the mother and families often are unable to accompany the child to distant advanced medical centers. Because of high-definition videoconferencing consultations, newborn Emilie Traylor could receive in Chillicothe the care she needed, and stay close to her mom, Stacie.

pediatric patients to Nationwide Children's than any other outside of the Columbus metropolitan area. In their first year of operation with telemedicine, physicians were able to make quicker and more accurate clinical assessments via videoconferencing, especially regarding the need to transfer these critical-care newborns. The number of neonatal transports from Chillicothe, which cost thousands of dollars for each trip, has been reduced to half since the network consultations were introduced.

"If a baby needs to be moved to our facility, doctors have seen the child, reviewed their diagnostic images and can prepare for the infant's care as soon as he or she arrives," said Dr. Stephen Welty, chief of neonatology, Nationwide Children's Hospital. "Just as importantly, we also use this as a tool to determine if a baby doesn't need to be transferred. Then, the child can stay with family and avoid unnecessary stress."

In the successful wake of the Adena project, engineers at the Ohio Supercomputer Center are working with doctors at Nationwide Children's to expand the neonatal program to rural medical facilities in Portsmouth, Zanesville, Findlay and Marietta.

OSC engineers for several years have been playing a major role in the deployment of high-definition videoconferencing systems, in areas such as education, health care, judicial courts and entertainment. In addition to the neonatal project, OSC has conducted studies of HDVC usability and reliability at two university game research and design labs, an organ-transplant services facility and a renowned music school.

These advances coincide with a growing national trend toward universal access to telemedicine. Recently, the Federal Communications Commission's Rural Health Care Pilot Program awarded $417 million to 69 regional network projects around the nation to "significantly increase access to acute, primary and preventative health care in rural America." Three of those projects provide high-speed connections to health care facilities in nearly half of Ohio's 88 counties.

These regional networks will link to the Broadband Ohio Network backbone to transport intra-state data traffic and connect with Internet2, the primary national research and education network in the country.

"Broadband deployment is one of the Commission's top priorities — particularly in rural America," the FCC said in a release. "And nowhere is the need for broadband greater than in rural health care, where isolated clinics can save lives by using advanced communications technology to tap the expertise of modern urban medical centers."

Once these high-tech health care delivery systems are in operation, heart-warming success stories — such as little Emilie's — should be more commonplace. ■

Project leads: Nationwide Children's Hospital, Adena Regional Medical Center & OSC
Research title: Medical collaboration network demonstration project on OSCnet
Funding source: American Distance Education Consortium & Ohio Board of Regents

Virtual simulations prep future doctors for surgery

The next generation of surgeons — many who grew up playing video games — are using real-time, interactive computer simulations to learn delicate surgical techniques required for operations on the human skull.

Called the Virtual Temporal Bone Project, the system was developed as a collaborative project between physicians and researchers at Nationwide Children's Hospital, The Ohio State University Department of Otolaryngology and the Ohio Supercomputer Center.

Without virtual simulation, medical residents would learn surgery techniques by only working on a few cadaveric specimens and through apprenticeships in an operating room.

The complexity of the skull's temporal bone makes surgery exceptionally challenging to master. The bone forms a major portion of the skull base and encases some of the body's most minute and sophisticated sensory structures, including the cochlea and semicircular canals. Meanwhile, it sits intimately beside the carotid artery, jugular vein, cerebral cortex, brainstem and cranial nerves. Surgeons drill into the temporal bone to treat ailments such hearing loss, vertigo, chronic ear infections or tumors.

"The virtual bone simulation is a fantastic teaching tool," said Dr. Laura Matrka, a second-year resident at The Ohio State University Medical Center.

"I can use the tutorial mode to see the layers and structures under the bone. Then I can switch to a practice session and drill on the structure for a very life-like experience."

Co-investigators Dr. Gregory Wiet, a pediatric otolaryngologist, head and neck surgeon with Nationwide Children's Hospital and an associate professor of otolaryngology and biomedical informatics at The Ohio State University, and Don Stredney, director of the Interface Lab and a research scientist in biomedical applications at the Ohio Supercomputer Center, have begun a national multi-institutional validation study to determine how medical students trained with the simulator compare to those trained using traditional methodology.

"We want to know for certain that we've created a safer, more effective way to learn fundamental techniques," Dr. Wiet said.

For Dr. Matrka, the system has met its mark. "In terms of learning the anatomy and organizing in my mind the way I want to go about doing a temporal lobe dissection, it's excellent," she said. ■

above: For Ohio State medical student Dinah Wan, the force-feedback device creates the pressure and resistance experienced during surgery. Without a virtual simulation, medical residents would learn surgery techniques by working on cadaveric specimens and through apprenticeships in an operating room.

inset: The skull's temporal bone, as viewed here in simulation, encases some of the body's tiniest and most delicate sensory structures.

Project leads:
Gregory Wiet, M.D., Nationwide Children's Hospital & The Ohio State University, & Don Stredney, OSC
Research title:
Validation/dissemination of virtual temporal bone dissection
Funding source:
National Institute on Deafness & Other Communication Disorders, National Institutes of Health, 1-R01-DC06458-01A1

The Virtual Temporal Bone Project received the prestigious 'Dr. Frank H. Netter Award for Special Contributions to Medical Education' from the Vesalius Trust for Visual Communication in Health Sciences during the 2008 annual meeting of the Association of Medical Illustrators.

Finding treatments for neurological diseases

A treatment, or perhaps even cure, for neurodegenerative disorders such as Parkinson's, Alzheimer's or autism could lie in managing a specific family of proteins that control messages sent to the brain.

The proteins, called neuronal nicotinic acetylcholine receptors (abbreviated nAChRs), are often located at nerve endings. They selectively bind to certain chemicals and are responsible for sending multiple types of signals to the body.

To look for medications or substances that will bind with a specific member of the nAChR family of proteins and block the damaging signals, Ohio State University biochemists are modeling the activities of known nAChR antagonists — chemicals that thwart nAChRs' messages to the brain.

"Through this computationally intensive process, we are identifying — for the first time — which specific sites on the nAChR proteins will bind with a novel class of antagonistic compounds," said Chenglong Li, Ph.D., an assistant professor in OSU's College of Pharmacy. His collaborators are colleagues Ryan Pavlovicz and Dennis McKay, Ph.D.

Using the Ohio Supercomputer Center's IBM Cluster 1350, they are building and studying, through molecular dynamics simulations, the functions of various nAChRs. Then, they computationally let molecular partners "dock" to each other and predict how one molecule will bind to another to form a functional complex.

"We can then use virtual, high-throughput screenings [millions of compounds] and fragment-based designs [thousands of specific compounds] at these sites to optimize and design new, highly selective and potent compounds that will better inhibit the debilitating actions of nAChRs, with minimum side effects," Dr. Li added. ■

Project lead: Chenglong Li, Ph.D., The Ohio State University
Research title: Computational evaluation, design & discovery of nicotinic acetylcholine receptor noncompetitive antagonists

Visualization builds window to understanding

Ohio State's Graphics and Visualization Research Group embodies the proverb that "a picture is worth a thousand words." These researchers specialize in scientific visualizations — the science of translating data analysis into cutting-edge renderings.

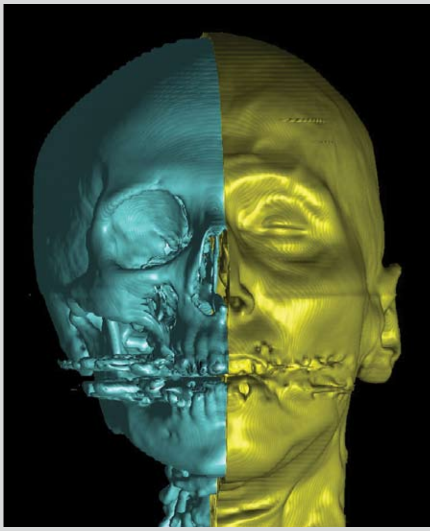
The graphics hardware market has advanced exponentially; commodity-based graphical processing units (GPUs) have become more programmable and easier to use for general applications. To empower research in this area, the Ohio Supercomputer Center's GPGPU/Visualization Cluster provides 36 graphical processing units capable of 11,800 peak gigaflops. The cluster's level of memory, speed and programmability is a necessity for realistic graphics.

"We have relied on the Ohio Supercomputer Center's GPGPU/Visualization Cluster to develop high performance, scalable parallel visualization algorithms targeted at very large data sets, as well as verify our research results," said Han-Wei Shen, Ph.D., an associate professor in computer science and engineering at The Ohio State University.

Parallel processing increasingly plays a more important role in the area of scientific visualization, especially as the size of data increases. Although many parallel visualization algorithms have been developed in the past, the complexity and scale of the data generated by terascale simulations demand even greater advancement in fundamental visualization algorithms and system designs.

Dr. Shen and his colleagues also tap OSC resources for flow visualization, time-varying data visualization and real-time applications, such as those used in medical surgical simulations. While each area uses different computational methods, all strive to create effective — and powerful — images to better illustrate the science behind the art. ■

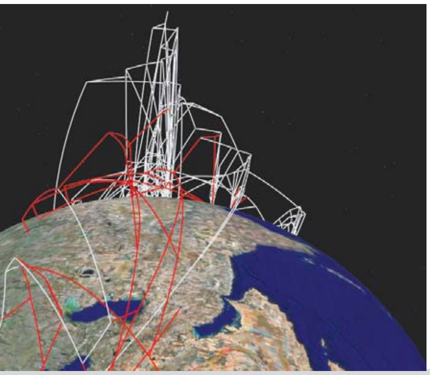
below: Using OSC computers, Dr. Han-Wei Shen detected a symmetry plan from the data of a skull's three-dimensional CT scan. He then applied different visualization techniques to the two halves of the skull.



Project lead: Han-Wei Shen, Ph.D., The Ohio State University
Funding source: Research supported in part by U.S. Department of Energy, Scientific Discovery through Advanced Computing, DE-FC02-06ER25779

Scholarship initiative to boost bioinformatics statewide

below: A prime example of bioinformatics research, this visualization depicts the westward spread of strains of the avian influenza virus (H5N 1) since its origins in Asia. (Janies et al. 2007)



Ohio ranks first in the Midwest and fourth-best nationally in the biosciences, according to a 2008 Business Facilities Magazine report. And, while Ohio annually produces more than 18,000 bioscience graduates, the labor needs of the industry remain unmet, especially in the growing specialty of bioinformatics. Bioinformatics merges biology, computer science and information technology into a single biosciences discipline that relies on supercomputing to analyze large amounts of data.

A new statewide scholarship initiative created the Ohio Consortium for Bioinformatics to attract and graduate 345 bioinformatics students over five years. The consortium is funded by the Ohio Board of Regents through the Choose Ohio First program, one component of the Ohio Innovation Partnership created by the Ohio General Assembly to attract and graduate more than 2,000 students in science, technology, engineering and mathematics.

To support the effort, the Ohio Supercomputer Center is developing cyberinfrastructure applications for bioinformatics and supplying software and other resources. The Ralph Regula School of Computational Science is developing a shared bioinformatics curriculum, and industries will provide internship, co-op and mentorship opportunities.

Ohio University's Lonnie Welch, Ph.D., and OSC's Terry Lewis lead the consortium's steering committee. In 2006, they co-founded the Ohio Collaborative Bioinformatics Conference (OCCBIO), an annual interdisciplinary forum they coordinate to promote discussion of methods, research findings and experiences.

These initiatives will make Ohio a national leader and position the state to better compete for federal research funding from sources such as the National Institutes of Health, National Science Foundation and Department of Defense. ■

Project lead: Lonnie Welch, Ph.D., Ohio University
Research title: Ohio Consortium for Bioinformatics, Choose Ohio First scholarship program
Funding source: Ohio Board of Regents

OSU scientists make BIG contributions to cancer research

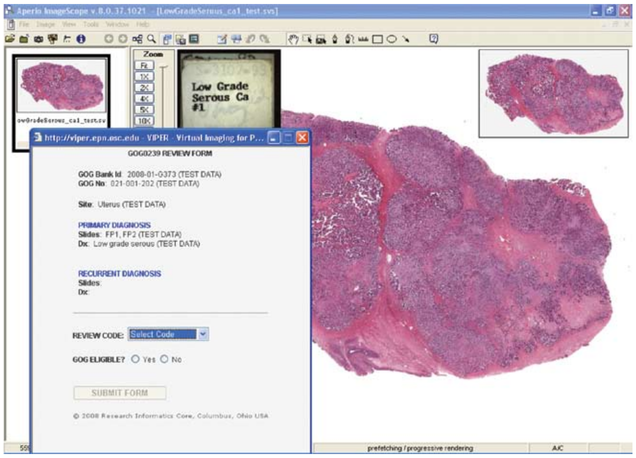
Project lead:
The Ohio State University Department of Biomedical Informatics
Research title:
High performance algorithms for scientific applications
Funding source:
National Cancer Institute

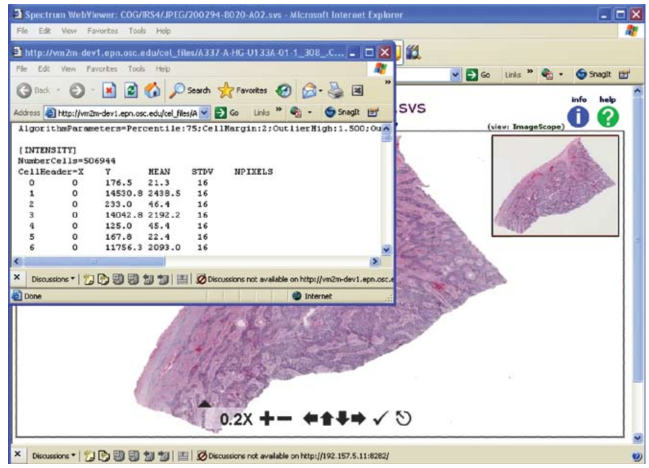
caGrid

As the Knowledge Center for caGrid, researchers at The Ohio State University's Comprehensive Cancer Center are using their expertise to develop software infrastructure and hardware resources that may speed cancer research discoveries. The Knowledge Centers are part of the National Cancer Institute's Cancer Biomedical Informatics Grid (caBIG™) program, an information network that provides cancer researchers, physicians and other participants with the ability to share basic-science, clinical-trials, imaging and other research data and analyses. The caGrid Knowledge Center provides expertise and serves as a resource on the network's infrastructure for the caBIG community, including assistance with community projects to ensure effective use of caGrid.

In close coordination with the caBIG leadership, OSU's Department of Biomedical Informatics team works as the lead developer for the caGrid infrastructure. In addition to providing development assistance, BMI provides technical oversight and guidance for caGrid architecture and implementation. The team has developed several core components of caGrid, including the GAARDS security infrastructure, the Introduce toolkit for caGrid service development and deployment, the caGrid data services infrastructure and the metadata management infrastructure.

OSC supports this effort by providing the caGrid infrastructure and key bioinformatics software on its IBM Cluster 1350, as well as dedicating significant supercomputer cycle allotments to bioscience users around Ohio and the nation. The availability of this resource at OSC, along with key bioinformatics applications/tools and the caGrid system, enables researchers to carry out analyses and information integration at scales that were previously impossible. ■





above: VM2M provides virtual microscopy data alongside microarray data. Once a desired sample has been found, the reviewer can inspect the corresponding digital image using a Web-based image viewer, which can zoom and pan across the image. At the same time, the reviewer will be able to access the microarray data corresponding to the same tissue sample.

Bridging the worlds of pathology, genetics and cancer treatment

The story unfolds all too frequently. Parents, worried about their baby's fever and severe abdominal pain, visit the emergency room — then learn their precious child has neuroblastoma, a debilitating pediatric cancer. As little as two years ago, all children with neuroblastoma received the exact same treatment: Chemotherapy, bone marrow transplant, surgery and radiation. But today, treatments can be tailored to the individual, delivering effective, targeted and less toxic treatments. This approach, one component of "personalized medicine," requires quick identification of the specific cancer type and access to genetic information about the tumor.

Virtual Microscopy to Microarray, or VM2M, will make this access a reality. An effort by the Research Institute at Nationwide Children's Hospital, Childrens Hospital Los Angeles and the Ohio Supercomputer Center, VM2M will give physicians and cancer researchers a comprehensive repository of tumor tissue samples and their corresponding genetic markers.

To empower quick and accurate access, the Center for Childhood Cancer at The Research Institute at Nationwide Children's Hospital developed custom computer software that allows multiple pathologists to simultaneously and securely review, via the Internet, digital, diagnostic-quality microscopy scans of diseased tissue with the corresponding molecular expression data. Virtual microscopy scans are paired with each sample's genetic code, or microarray, created by Childrens Hospital Los Angeles, while OSC provided a secure repository and hosted the development platform during the project's first phase.

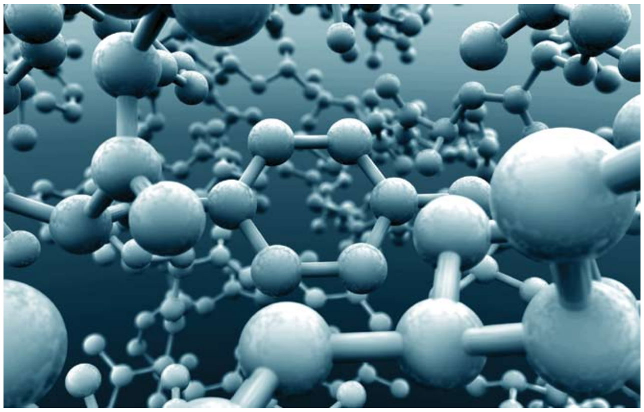
VM2M will provide two currently unavailable requirements for creating personalized treatment plans: 24/7 access to both the pathology of specific cancer tumors and the genetic information of the tumors.

"OSC's powerful, memory-intensive data management and networking resources enabled storing, organizing and retrieving this information," said David Billiter, director, research informatics core, Nationwide's Center for Childhood Cancer. "We are now poised to explore the next phase of development for VM2M by producing value-added functionality and moving into a production-supported environment."

That means the VM2M project, when fully implemented, will help children and adults fight all cancer with the best treatment option possible — one custom-made for the individual. ■

Project leads: The Research Institute at Nationwide Children's Hospital, Childrens Hospital Los Angeles, Children's Oncology Group & OSC
Research title: Integrated virtual microscopy & molecular analysis software for enhanced cancer diagnosis
Funding source: U.S. Department of Health & Human Services, through the Ohio Board of Regents

Proteomics: Calculating protein weight changes to detect cancer



above: Proteomics encompasses the large-scale study of proteins. With MassMatrix, scientists can more accurately identify differences in the protein structures of healthy cells and those with cancer.

below: Researchers at Ohio State University developed a unique search program, MassMatrix, to better evaluate protein-related measurements collected through liquid chromatography and tandem mass spectrometry.

Project lead:
Michael Freitas, Ph.D., The Ohio State University
Research title:
Assays for screening histone modification in cancer
Funding source:
National Institutes of Health, CA107106

As the expression goes, the devil is in the details. Fortunately, Ohio State University Professor Michael Freitas and his team have developed a way to leverage one of cancer's evil tell-tale signs: Changes in the weight of specific proteins, measured out to the third decimal place.

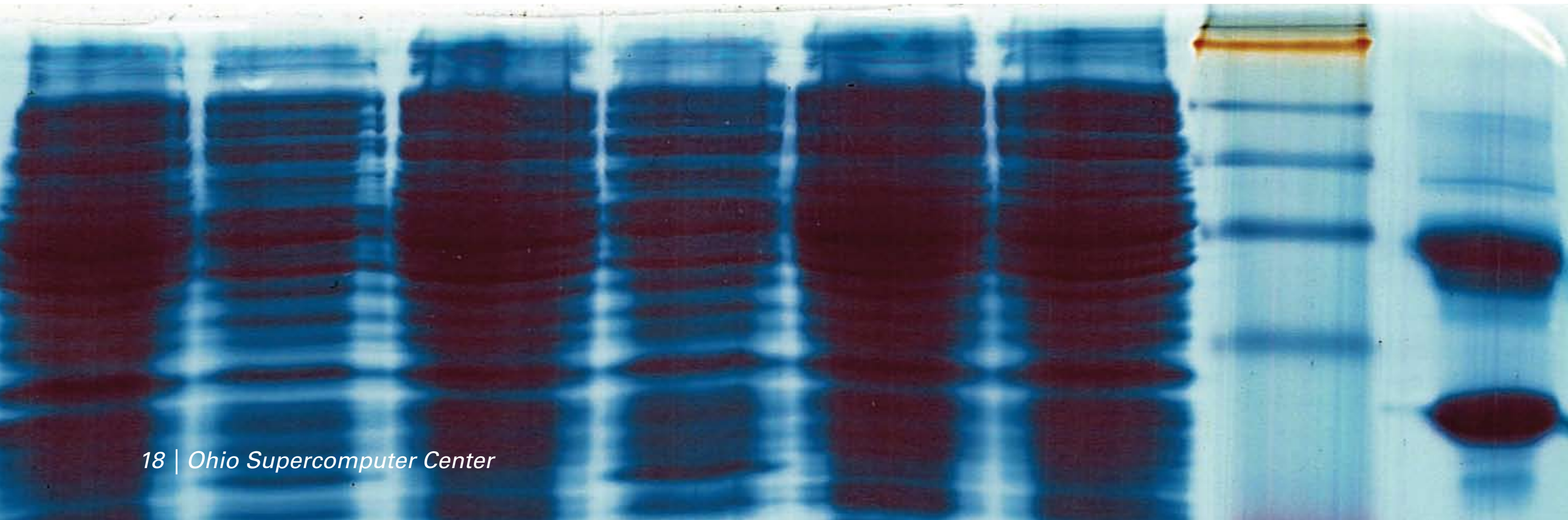
Dr. Freitas specializes in proteomics, the large-scale study of proteins, particularly their structures and functions. As part of his research, he uses liquid chromatography, coupled with tandem mass spectrometry (LC-MS/MS), to look for differences in protein structures between healthy cells and those from patients with chronic lymphocytic leukemia.

LC-MS/MS creates rich, data-heavy information — which requires extensive evaluation. Typically, various automated database search algorithms use an approach that averages the numbers. Because they don't take into account the precision of the data, the results frequently would falsely identify protein structures as ones with cancerous changes.

To reduce false positives and improve the scores of true positive matches, Freitas' team created MassMatrix, an automated database search program that relies on rigorously evaluating a variety of protein-related measurements, including the precise weight, to generate more accurate results.

"The Ohio Supercomputer Center provided resources to create a parallelized version of MassMatrix that ran efficiently on high performance clusters," said Dr. Freitas. "Now, we're using OSC to benchmark MassMatrix against similar types of software on the market. Our ultimate goal is to develop this as a resource for proteomics, to help all researchers.

"Because," Dr. Freitas said, "any difference we find between healthy and diseased cells may help us understand what influences the progression of chronic lymphocytic leukemia, and perhaps other cancers." ■



Using computational chemistry to understand oxygen-related diseases of the heart and lungs

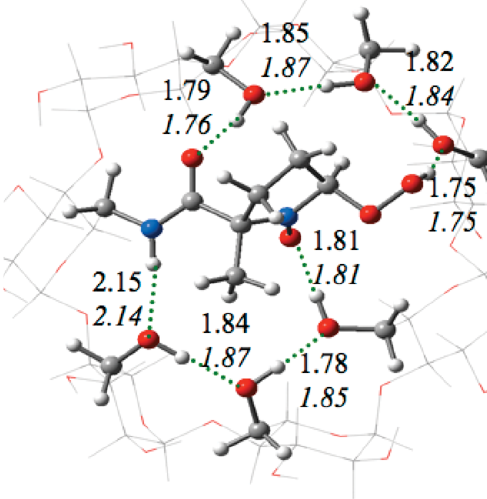
The average person rarely considers the antithesis of life-sustaining oxygen. The molecule can, in certain situations, become an aggressive, toxic chemical. At the center of this about-face are oxygen-based radicals – generally called reactive oxygen species (ROS) – that have an unpaired electron. Collectively called "oxidative stress," changes in ROS concentration accompany many ailments, including heart disease, lung damage, tumor growth and aging.

Because ROS are unstable and short-lived, detection through traditional means has been challenging. However, an Ohio State University team of multidisciplinary researchers is developing more effective means for monitoring them, in part by using the supercomputers at the Ohio Supercomputer Center.

"We're using computational chemistry models to develop new classes of spin traps," said Christopher Hadad, Ph.D, a professor of chemistry at Ohio State. Spin traps are chemical scavengers that react with the oxygen-based radicals to create stable compounds; these can then be examined using electron paramagnetic resonance (EPR) spectroscopy.

"Our project includes finding non-toxic spin traps that last long enough to use EPR spectroscopy, can be successfully administered, and uniquely mark each reactive oxygen species, " Dr. Hadad said.

These computational studies complement experimental efforts by other team members. "The computational chemistry models help narrow our decisions on which spin traps to make and test in vivo," said Frederick Villamena, Ph.D., an assistant professor at OSU's Heart and Lung Research Institute. "Eventually, we hope this work will enable the development of medications that prevent oxidative stress, instead of today's practice of treating the effects after an event." ■



Project lead:
Frederick Villamena, Ph.D., Ohio State University Heart & Lung Research Institute
Research title:
Development of spin traps for biological free radical detection
Funding source: National
Heart Lung & Blood Institute, National Institutes of Health

Plant pathologist analyzes disease resistance of world's most widely consumed staple food

Rice serves as the staple food for more than half the world's population, especially in tropical Latin America, and East, South and Southeast Asia. Additionally, rice is used in products such as straw and rope, paper, wine, crackers, beer, cosmetics, packing material – even toothpaste.

To safeguard such an essential global resource, scientists at The Ohio State University are using supercomputers to study rice's genetic information. In particular, they're looking for ways to combat diseases such as rice blast, a fungus that attacks rice and many other grasses and sedges that can reduce crop yields by up to 50 percent.

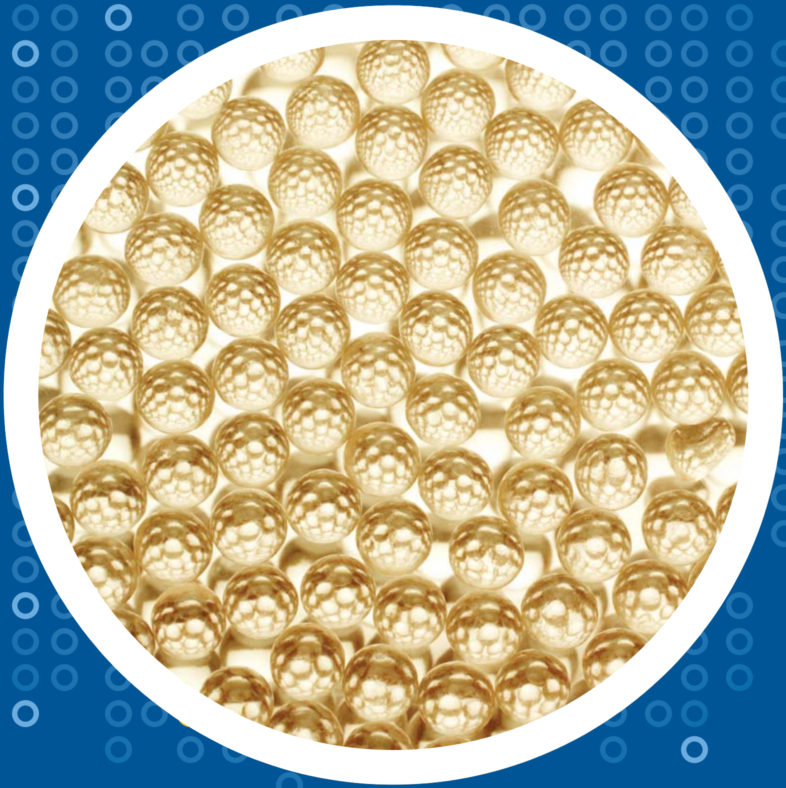
"Our research focuses on understanding how plants and their pathogens interact at the molecular level and how biochemical reactions control disease resistance," said Guo-Liang Wang, Ph.D., a professor in OSU's department of plant pathology. "Our long-term goal is to genetically engineer plants for disease resistance in such a way as to reduce reliance on environmentally damaging pesticides."

Dr. Wang and his research team also are developing new genomics tools and resources for functional analysis of the rice genome.

"Bioinformatic tools developed by OSC experts are essential in analyzing this huge set of sequence data," said Dr. Wang. "Six papers have been published from the collaboration with the OSC team in the last three years." ■

"We are currently using rice as the model plant because it is one of the most important food crops in the world." *–Dr. Guo-Liang Wang*

Project lead:
Guo-Liang Wang, Ph.D., The Ohio State University
Research title:
Rice functional genomics
Funding sources:
National Science Foundation, U.S. Department of Agriculture, United States Agency for International Development, International Rice Research Institute, & Ohio Agricultural Research & Development

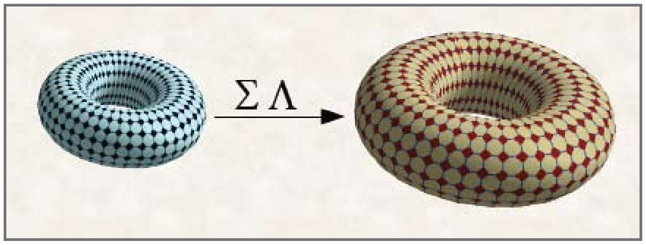


advanced materials

Researchers and scientists in Ohio are developing exciting new classes of materials with unusual properties. Their groundbreaking studies are based on the study of atomic and molecular physics and chemistry and involve the processing of polymers, metals, ceramics and composite materials. For example, a physicist delves into the interaction of electrons, superconductors and microchips. A chemist determines how NMR experiments can be used to learn about the bonds between hydrogen atoms. And, a "computational experimentalist" develops and uses high-performance software to study supersonic and hypersonic airflow phenomena of military jets. World-class materials manufacturing industries have long driven the state's economy, with just under 105,000 workers across 1,184 establishments, according to a recent report by Battelle. The creation and testing of computational models through the Ohio Supercomputer Center continues to set the bar high for materials science research in Ohio, as described on the next few pages. ■

above: By using OSC systems to develop a massively parallel, multi-scale method to study strongly correlated materials, researchers are working towards developing materials that will enable better, more efficient technology, such as the materials used in magnetic levitation trains.

Modeling at multi-scales, to better understand strongly correlated materials in massively parallel ways



above: Researchers are working to develop computational methods that separate a material's correlations by length scale, using a massively parallel, multi-scale method. Strongly correlated short length scales are calculated using Quantum Monte Carlo simulations, while intermediate length scales are evaluated using Feynman graphs.

"This project will advance researchers' understanding, simulation and design of magnetic materials and superconductors for energy and national security applications, as well as basic research applications."
–Dr. Mark Jarrell

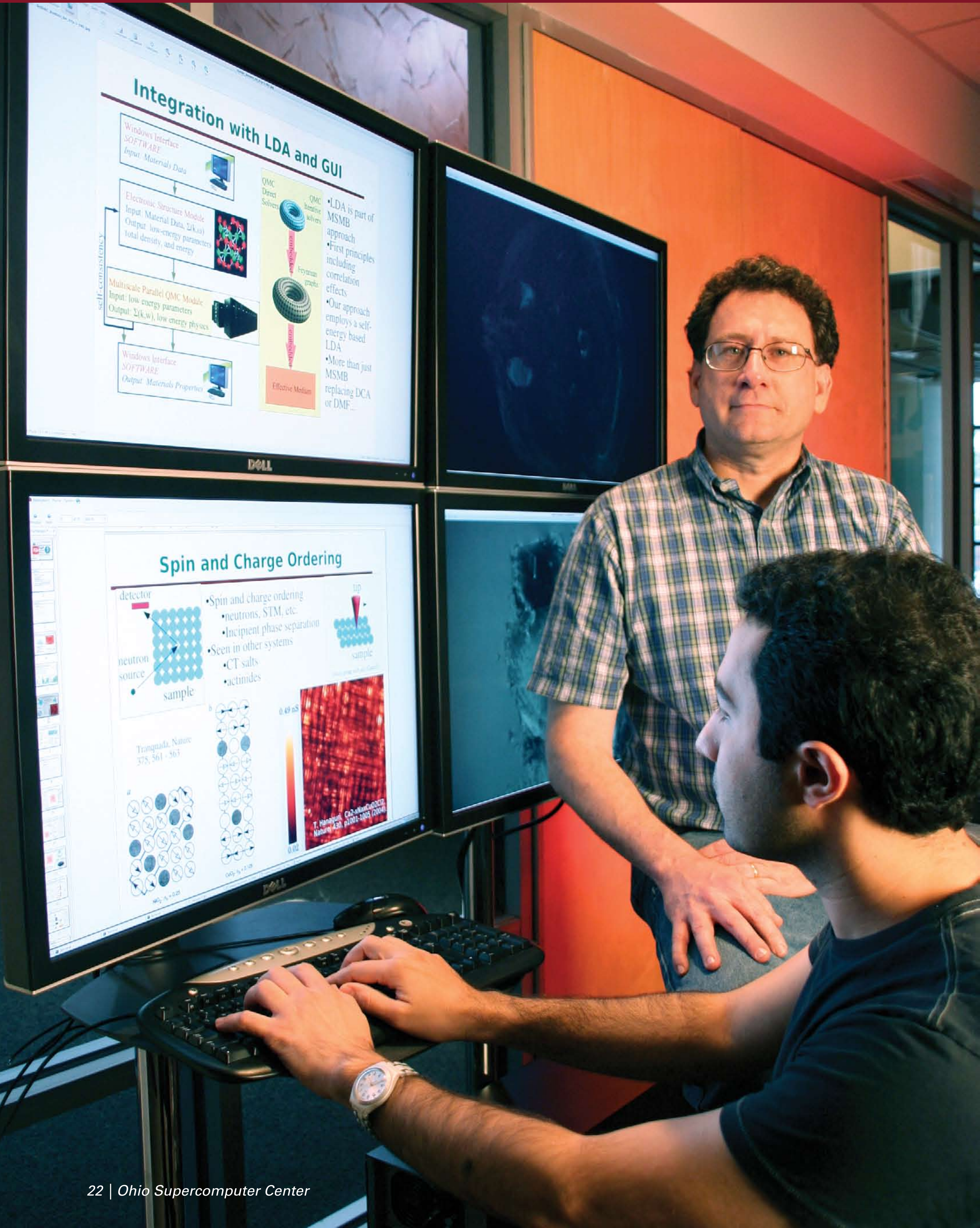
Materials are fundamental to all forms of technology; the examples are all around us. Magnetic Resonance Imaging machines, supercolliders and novel electronic computer circuits illustrate just a few ways that scientists and industries have leveraged the unique properties of strongly correlated materials, a wide class of materials with unusual electronic and magnetic properties.

However, while these materials hold great technological promise, they are poorly understood.

That should change, with the application of current research by an interdisciplinary team of investigators from the University of Cincinnati, Oak Ridge National Laboratory and the University of California-Davis. Led by Mark Jarrell, Ph.D., a physicist at the University of Cincinnati, the team of computational physicists, applied mathematicians and computer scientists is developing a massively parallel, multi-scale method to study strongly correlated materials.

"We are working towards developing better materials with greater functionality," said Dr. Jarrell, "whether it's for power transmission through superconductors or faster computer chips. We want this work to lead to materials that companies such as Goodyear, Battelle or Procter & Gamble can use to develop better technology for areas such as electronic devices, medical science — even magnetic levitation trains."

Strongly correlated materials include lanthanide and actinide heavy Fermion materials, transition metal oxides, high-temperature superconductors and high-density ferromagnets. These highly intricate materials display different characteristics at different levels, or length scales.


Integration with LDA and GUI
Windows Interface
SOFTWARE
Input: Materials Data
Electronic Structure Module
Multiscale Parallel QMC Module
Input: low energy parameters
Windows Interface
SOFTWARE
Output: Materials Properties
•LDA is part of MSMB approach
•First principles including correlation effects
•Our approach employs a self-energy based LDA
•More than just MSMB replacing DCA or DMF...
Effective Medium
DELL
Spin and Charge Ordering
detector
neutron source
sample
•Spin and charge ordering
•neutrons, STM, etc.
•Incipient phase separation
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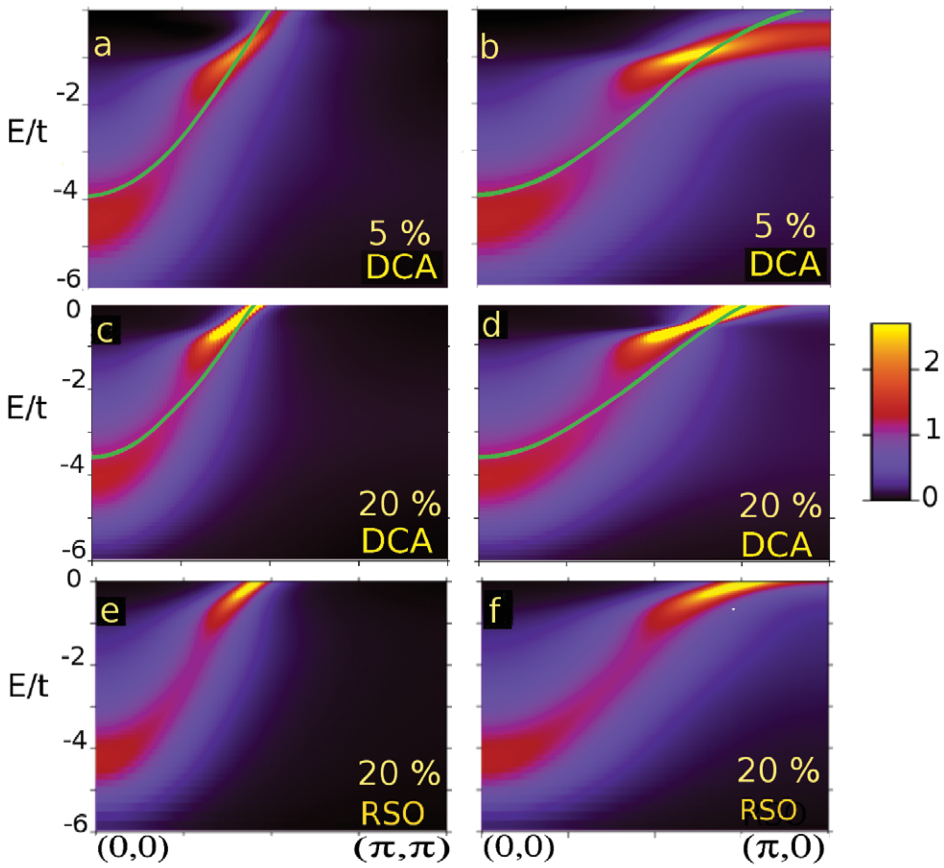


Project lead:
Mark Jarrell, Ph.D.,
University of Cincinnati
Research title:
Next generation multi-scale quantum simulations software for strongly correlated materials
Funding source:
U.S. Department of Energy, Scientific Discovery through Advanced Computing

left: These illustrations show computer-simulated spectral intensity of high-temperature superconductors. The green line in the top four quadrants represents the quasiparticle dispersion that occurs in normal metals. However, because of strong interaction present in the system, the spectral function shows broad features, similar to a waterfall, at higher binding energies.

"Our goal is to develop computational methods that separate a material's correlations by length scale," Dr. Jarrell said. "These algorithms will enable physicists, for the first time, to accurately study the complex interactions of strongly correlated materials."

At the smallest length scale, they are looking at atomic particles, such as electrons, where a change in the electrical or magnetic properties of one single electron, at one point in time, will affect a neighboring electron's electrical or magnetic behavior. These short length scales are considered "strongly correlated," and are calculated by numerically exact Quantum Monte Carlo simulations.

The second segment evaluates the material at the other end of the spectrum, where the interaction between particles is weak. Physicists have long used a mathematical approach called dynamic mean field approximation to evaluate these "long length" scales.

It's the space in the middle, the intermediate length scales, that could break open investigations of strongly correlated materials. Before, it was mathematically overwhelming to evaluate the collection of 10 or so atoms. Because of a variety of factors, the equations that looked at the interactions of this missing middle quickly scaled off the charts — it would have been impossible for even the most advanced supercomputers to crunch the numbers in a realistic timeframe.

However, today's trend toward petascale computing, combined with new mathematical equations and codes, holds the promise of fundamental discovery in the study of complex correlated materials. To evaluate the intermediate length scales, Dr. Jarrell and his team are tapping the power of massively parallel supercomputers by using a Feynman diagrammatic approach called the "parquet equations."

"Our approach, from the treatment of the correlations at intermediate length scales to the integration of the three length scales, is completely new," Dr. Jarrell said. "Resources at the Ohio Supercomputer Center have helped us both qualify and quantify the method. The codes we are developing will allow us to take advantage of the next generation of supercomputers, where the use of ten thousand processors — or more — will be common. ■

left: University of Cincinnati researcher Mark Jarrell (back) is leading a team of computational physicists, applied mathematicians and computer scientists, including UC doctoral candidate Ehsan Khatami (foreground), in the effort to develop new computational methods for studying the complex interactions of strongly correlated materials.

Understanding materials at the nanostructure level

Somnath Ghosh, Ph.D., a professor of mechanical engineering and materials science and engineering at The Ohio State University, believes that to develop new materials, it is paramount for researchers to understand material characteristics at the atomic level, especially when designing and fabricating nanostructures.

Recently, the Ohio Supercomputer Center awarded him 400,000 resource units to develop molecular dynamics based models that simulate polymer nanocomposites and polystyrene thin-films. Jim Giuliani, client and technology support manager at OSC, helped install and configure the project's required software.

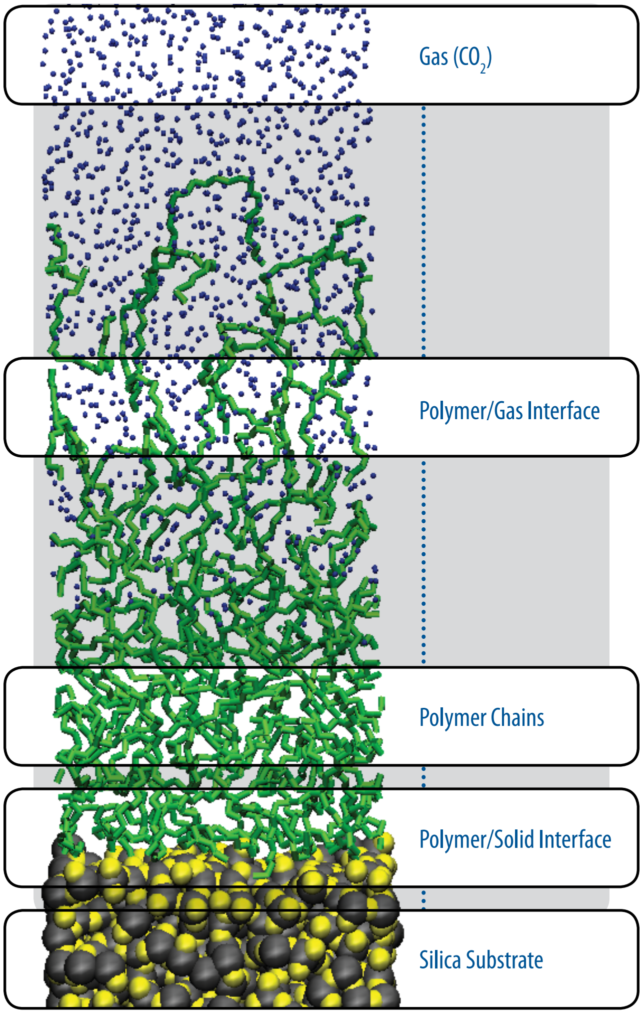
"Because of the extremely small size of nanostructures — often smaller than one millionth of a millimeter — we can't conduct ordinary experimental observations," Dr. Ghosh said. "So to study and understand how the material behaves at these infinitesimally small scales, we must rely on molecular modeling simulations. The key to material modeling and design is to understand the structure, dynamical characteristics and response of the material under different external stimulus."

In particular, Dr. Ghosh and his team will use the modeling simulations to estimate how material of different dimensions behaves at different pressures and temperatures. Of particular interest is the glass transition temperature, the temperature at which a polymer changes from a liquid to a solid state.

"There is strong experimental evidence that properties of polymer thin-films are remarkably different from their respective bulk properties. One of our objectives is to capture this difference," Dr. Ghosh said.

Additionally, they will be investigating liquid carbon dioxide's effect on the thin-film's mechanical behavior, as the amount of carbon dioxide added to the polymer's manufacturing process affects the final product. They are developing a molecular model of a three-phase material (substrate-polymer-gas), which will help to analyze future products and applications, especially in drug delivery systems. They also will be devising strategies for faster models that can depict larger, more realistic systems.

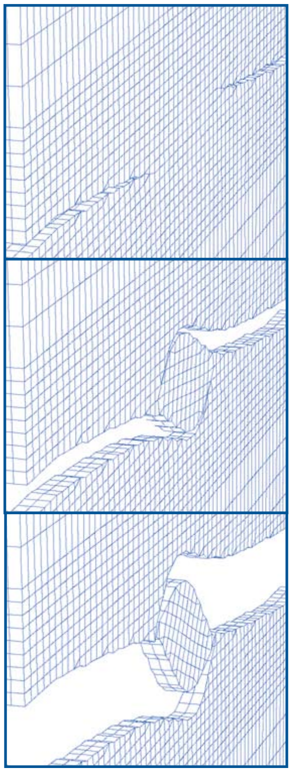
"These models can be used as specific design tools to achieve desired properties in thin-film polymer nano-composites for nanodevices," said Dr. Ghosh. "But, universally, they also will enable the development of new or improved materials for a variety of commercial applications." ■



above: Conducting research at the molecular level, OSU's Somnath Ghosh, Ph.D., uses the Ohio Supercomputer Center to create computer simulations such as this model of polystyrene-based polymer nanocomposite, with silica as a substrate. Carbon dioxide serves as a pressure-applying agent on polymer thin film. This modeling will help empower the design of nanosubstrates for use in biomedical devices.

Project lead:
Somnath Ghosh, Ph.D., The Ohio State University
Research title:
Multi-scale molecular simulation of polystyrene-based nanocomposite & thin-film for determination of thermo-mechanical properties at nano-scale
Funding source:
National Science Foundation Nanoscale Science & Engineering Center

Identifying the cracking point of laminates



Composite laminates — engineered materials made from two or more distinct properties — can be found everywhere, from asphalt-concrete roads to the shell of the space shuttle.

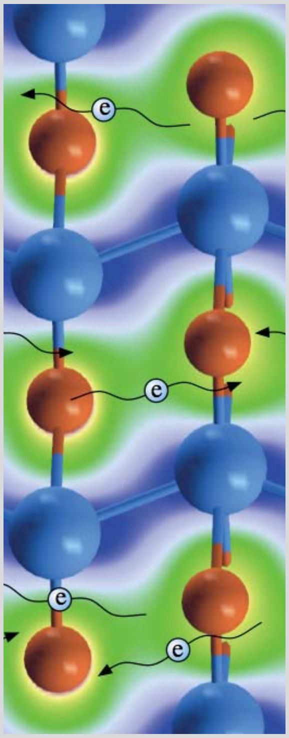
Normal stresses and impacts, as well as fabrication defects or misalignments of the composite fibers, can cause the laminate to separate at the junction point between the two layers. This condition, called delamination, is one of the predominant modes of damage to these materials.

University of Cincinnati aeronautical engineer Ala Tabiei, Ph.D., is using the resources at the Ohio Supercomputer Center to develop a better method for simulating how a laminate cracks and separates, within the non-linear, explicit finite element software DYNA3D. He is developing numerical methods to determine the dynamic energy released, measure stress factors on the crack under certain conditions and capture when a crack begins to expand. He's also implementing a method to recalculate the fracture model, which will allow researchers to simulate crack growth when the material is significantly stressed.

"Our goal is to develop an automated, dynamic fracture procedure that can be used to simulate delamination failure between adjacent layers of laminated composites," Dr. Tabiei said. "To effectively use laminate composites, researchers need to consider the characteristics that cause the material to fail. We think this new numerical model, when completed, will be a valuable tool for industries such as aerospace, automotive and construction." ■

Project lead: Ala Tabiei, Ph.D., University of Cincinnati
Research title: An automated dynamic facture procedure for finite element simulations of delamination failure in laminated composites

Bonding lithium and beryllium under pressure



The stalwart computing power of the Ohio Supercomputer Center recently played an integral role in a groundbreaking discovery by Cornell University scientists.

By combining theory and computational modeling, the researchers predicted that the lightest known metals in the universe, lithium (Li) and beryllium (Be), will bond under high levels of pressure and form stable — and possibly superconductive — alloys. Under normal conditions, Li and Be repel each other. Unexpectedly, they also found that the combination creates a quasi two-dimensional electron gas sandwiched between the Li layers of the LiBe alloy.

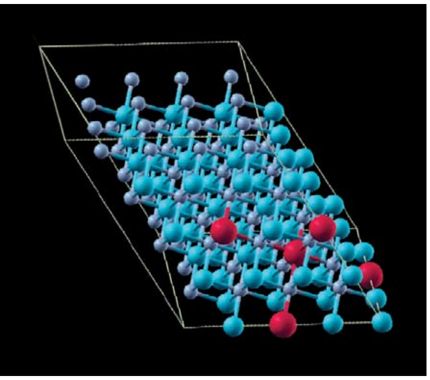
"While I searched for stable high-pressure structures using the random search method, my colleague used chemical information to determine likely stable bond arrangements for LiBe," said Richard Hennig, Ph.D., a Cornell University professor in materials science and engineering. "OSC's queuing system enabled us to simultaneously run large numbers of density functional calculations within a few weeks time. This is a great benefit over other supercomputing centers."

The research, supported by the National Science Foundation, appeared in the Jan. 24, 2008, issue of the journal *Nature*.

"The Ohio Supercomputer Center was my first choice for computing the structures at each composition and pressure," Dr. Hennig said. He previously used OSC extensively for ab-initio and quantum Monte Carlo calculations of defects in semiconductors and phase transformation in transition metal alloys as a post-doctorate researcher under Ohio State University Physics Professor John Wilkins. Their on-going collaborations grant Dr. Hennig access to OSC's supercomputers from Cornell. ■

Project leads: Roald Hoffmann, Ph.D., & Richard Hennig, Ph.D., Cornell University
Research title: Emergent reduction of electronic state dimensionality in dense ordered Li-Be alloys
Funding sources: National Science Foundation & the Petroleum Research Fund of the American Chemical Society

Spintronics adds new dimension to semiconductor development



above: The computer visualization depicts the atomic structure of the rock-salt structure semiconductor scandium nitride, doped with 8 percent manganese. The manganese is shown in red, scandium in light blue and nitrogen in silver.

Spintronics – short for spin-based electronics – may soon provide tinier, faster and more robust components for small electronic devices and computers. The spintronics approach stores electronic data through magnetic properties caused by the spinning of electrons, in addition to the fundamental electrical charge of electrons that is used by more conventional computers. The spin charge is assigned a value of "up" or "down" and, like the electrical charge, can be encoded with binary data.

"In semiconductors, one can possibly have far more detailed control over both the number of active electrons and their spin orientation in a device," said Walter Lambrecht, Ph.D., professor of physics at Case Western Reserve University. "The problem is to find magnetic semiconductors that retain these distinct magnetic properties above room temperature."

These specialized semiconductors are created through a process called doping: manufacturing into the semiconductor small amounts of transition metals or rare-earth elements, which possess distinctive electronic properties. While most work in this field requires a small percentage of the dopant, gadolinium-doped gallium nitride has been found during experiments to exhibit the desired magnetic properties even for part-per-million levels.

"We are accessing the computational resources of the Ohio Supercomputer Center to perform calculations of various possible irregularities in the atomic arrangement and studying their interaction with gadolinium in gallium-nitride to unravel the origin of this mysterious source of magnetism," said Dr. Lambrecht. ■

Project lead: Walter L. Lambrecht, Ph.D., Case Western Reserve University
Research title: Muffin-tin orbital based first-principles calculations
Funding sources: Office of Naval Research & the Army Research Office

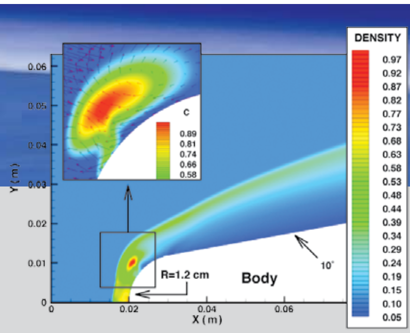


illustration courtesy of NASA

Ablation model measures hypersonic gas plumes

Scientists are developing hypersonic aircraft that can travel at speeds beyond Mach 5 (3,800 mph) and travel from New York to London in less than an hour. In military applications, flight above Mach 8 will be needed for effective homeland security.

Several technical obstacles remain, however. At hypersonic speeds, shock waves created by the compression of air in front of the aircraft increase in strength and number. The aircraft body experiences turbulence, and the air becomes a swarming jumble of hot gases, which transfers heat to the aircraft.

Engineers have addressed the problem by constructing thermal protective shields that slowly burn away — a process called ablation — creating gases that carry heat away from the aircraft and leaving behind a solid material that insulates the craft.

"Extensive research has been conducted that predicts the ablation rates of thermal protective shields due to hypersonic flow," said Alex Povitsky, Ph.D., an associate professor of mechanical engineering at The University of Akron.

"The interaction of small-scale, but high-intensity, plumes can significantly affect the heat transfer between hypersonic gas and the shield. However, the majority of studies based on heating tests or flight test data don't take into account the effects of gas plumes."

Through access to the IBM Cluster 1350 at the Ohio Supercomputer Center, Dr. Povitsky, Dr. Kedar Pathak and graduate assistant Nathan Mullenix are developing a computational methodology for simulating the ablation of carbon shields, complete with local and multiple ablation plumes and subsequent multiple plumes. ■

Project lead: Alex Povitsky, Ph.D., The University of Akron
Research title: Modeling of ablation in hypersonic flight
Funding sources: Dayton Area Graduate Studies Institute, Air Force Office of Scientific Research & Air Force Research Laboratory

Computational chemist computes to understand hydrogen bonds

Janet E. Del Bene, Ph.D., professor emeritus of chemistry at Youngstown State University, has relied on the Ohio Supercomputer Center since its inception in 1987 for her research in quantum theoretical chemistry.

"As a computational chemist, my laboratory is the computer," said Dr. Del Bene, an expert in hydrogen bonding. Hydrogen bonds are responsible for the properties of water. Because most chemical reactions occur in water, chemists need to understand how hydrogen bonds influence chemical reactions.

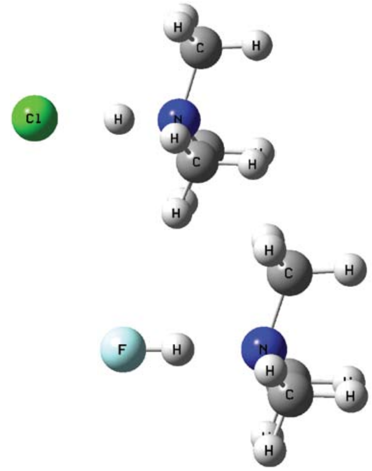
Dr. Del Bene has addressed questions concerning the stabilities of hydrogen-bonded complexes, the methodological dependence of their computed properties, and has connected their infrared (IR) spectrosopic properties to the type of hydrogen bond present. Her work resolved what appeared to be a contradiction between theory and experiment in the description of certain types of hydrogen bonds.

Most recently, she has focused on how nuclear magnetic resonance (NMR) spectroscopy can be used to extract structural information about hydrogen bonds. By computing magnetic properties that can be measured experimentally in an NMR spectrum, Dr. Del Bene developed a way to characterize hydrogen bonds from their spectra and to obtain structural data for hydrogen-bonded systems in solution. Through her work, Dr. Del Bene and her colleagues have developed the chemical equivalent of infrared and nuclear magnetic resonance spectroscopic fingerprints of hydrogen bonds.

So what is the ultimate purpose of this work? Computational chemistry leads to a better understanding of chemistry and chemical reactions, and that understanding is the key to progress. ■

Project lead: Janet E. Del Bene, Ph.D., Youngstown State University
Funding source: National Science Foundation, CHE-9873815

below: Hydrogen bonds are the 'chemical glue' that binds two molecules together and makes them act as one. They are crucial in applications such as enzyme kinetics, DNA replication and the binding of drugs to specific targets in the body.



New material could improve efficiency of solar power

Ohio State University chemists and their colleagues have created a new material that overcomes two of the major obstacles to solar power: it has an absorption spectrum that closely matches that of the solar spectrum, and it generates long-lived excited electrons that should allow solar cells to generate electricity more efficiently.

To design the hybrid material, which combines electrically conducive plastic with metals, including molybdenum and tungsten, the chemists first explored different molecular configurations using the high performance computing systems at the Ohio Supercomputer Center. Then, with colleagues at National Taiwan University, they synthesized molecules of the new material in a liquid solution, measured the frequencies of light the molecules absorbed, and also measured the length of time that excited electrons remained free in the molecules.

The chemists found that the new hybrid material emits photons in two different energy states — one called a singlet state, and the other a triplet state. While both energy states are useful for solar cell applications, the triplet state lasts much longer than the singlet state — which improves the ability to harness their power, explained Malcolm Chisholm, Ph.D., distinguished university professor and chair of the department of chemistry at Ohio State.

At this point, the material is years from commercial development, but Dr. Chisholm added that this experiment provides a proof of concept — that hybrid solar cell materials can offer unusual and beneficial properties. ■

Project lead: Malcolm Chisholm, Ph.D., The Ohio State University
Research title: The remarkable influence of MM delta orbitals with oligothiophenes
Funding sources: National Science Foundation & Ohio State's Institute for Materials Research, together with Wright Center funding for photovoltaic initiative for commercialization

data exploitation

With the growth of information technology, the levels of data generated for use in research, business and industry has risen astronomically. Scientists tap the power of supercomputers to collect, manage, process, interpret, present, deliver and protect these vast collections of information. Consider: a scientist combines polar climate data from the atmosphere, sea, ice pack and land to understand the impact of environmental changes there. A network engineer develops software to transmit large data files from powerful scientific instruments operated remotely over the Internet. And, a team of astronomers discovers new planets orbiting a star thousands of light years away by analyzing light patterns. Ohio jobs involving the exploitation, mining and administration of data are steadily increasing in number as companies look to the Midwest to establish immense data centers. The Ohio Supercomputer Center supplies the computational resources needed to power the vital, data-rich research projects explained on the following pages. ■

above: A reanalysis of the Arctic climate should help researchers better understand the melting of sea ice, which is drastically reducing the hunting grounds of the polar bear.

Climate models synthesis may clarify threats to 'world's last frontier'

photo courtesy of Woods Hole Oceanograhic Institute/NSF

above: In August 2008, melting sea ice opened both the Northwest Passage (Canada) and Northern Sea Route (Russia) simultaneously, the first time in 125,000 years.

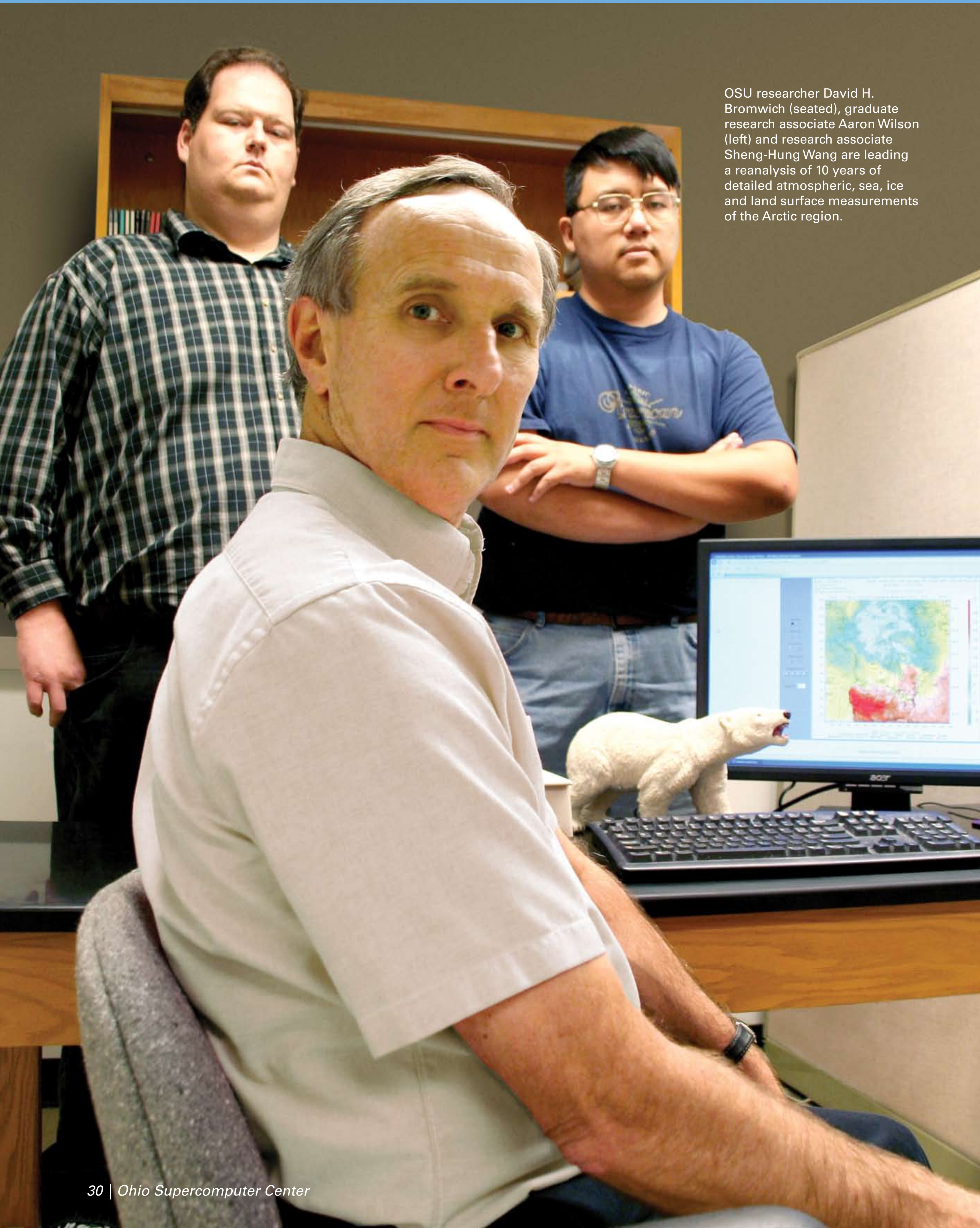
The sea-ice melt that last summer opened the Northwest Passage through the Canadian Arctic for the first time since satellite records began in 1978 may signal a significant climatic shift that has serious economic and ecological implications for wildlife, natural resources and world politics.

To better understand the evolving climate of the Arctic region, researchers have begun working to merge a decade of detailed atmospheric, sea, ice and land surface measurements into a single computer model-based synthesis. The coupling of these immense data sets will produce complex and instructive descriptions of the changes occurring across the normally frigid, remote region.

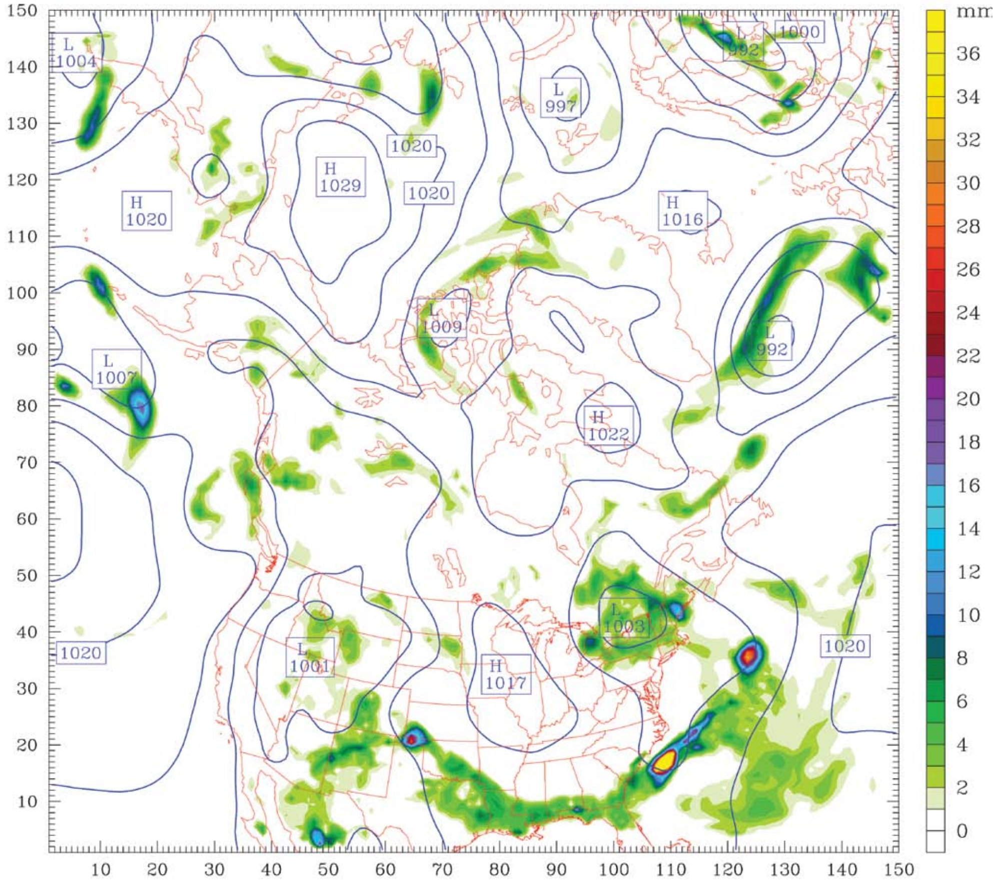
An interdisciplinary collaboration of scientists, led by David H. Bromwich, Ph.D., a senior research scientist with the Polar Meteorology Group of the Byrd Polar Research Center and a professor with the department of geography at The Ohio State University, will "reanalyze" Arctic data from the past decade at three-hour intervals, 15-kilometer distances and 70 layers from the surface of the Earth to the top of the atmosphere. The study area encompasses the Arctic Ocean, the surrounding landmasses and the rivers that drain into the ocean — an enormous area of nearly 29 million square miles.

"We used to think of places like the Arctic as 'data sparse;' they are remote, largely unpopulated with limited measurements of temperatures, winds, etc., and

A shift in climate could have serious economic and ecological implications for the shipping, fishing, mineral, gas and oil industries, as well as heighten concerns about dwindling wildlife habitat and rising greenhouse emissions.



OSU researcher David H. Bromwich (seated), graduate research associate Aaron Wilson (left) and research associate Sheng-Hung Wang are leading a reanalysis of 10 years of detailed atmospheric, sea, ice and land surface measurements of the Arctic region.



left: The Arctic System Reanalysis, powered by resources of the Ohio Supercomputer Center, will provide high-resolution visualizations in space and time of the atmosphere-sea ice-land surface system of the Arctic region.

Project lead:
David H. Bromwich, Ph.D., The Ohio State University
Research title:
Arctic system reanalysis, International Polar Year (IPY) project
Funding source:
National Science Foundation

have challenging environments," said Dr. Bromwich, who as a member of the Intergovernmental Panel of Climate Change shared a Nobel Peace Prize with former Vice President Al Gore in 2007. "With the introduction of space-borne measurements over the last few decades, researchers have been inundated with vast amounts of information. Today, the trick is to figure out how to effectively use all the diverse information sources."

To make sense of the numbers, Dr. Bromwich and his team turned to the Ohio Supercomputer Center for help with the four-year project. The scientists will fill about 350 terabytes of OSC storage space and employ 1,000 cores of the Center's IBM 1350 Opteron cluster over several months to create detailed visualizations.

"OSC is providing the project with resources that will allow us to complete our work in a limited time frame," Dr. Bromwich said. "Other computation centers likely could not have provided the CPU cycles or stored such vast amounts of data."

The National Science Foundation, as part of the International Polar Year observance, funds the Arctic System Reanalysis project, the first comprehensive environmental reanalysis project led by the academic community. IPY is a large scientific program focusing on the Arctic and the Antarctic from March 2007 to March 2009.

This observance comes "amidst abundant evidence of changes in snow and ice: reductions in extent and mass of glaciers and ice sheets, reductions in area, timing, and duration of snow cover, and reductions in extent and thickness of sea ice," according to IPY. "Changes in snow cover and sea ice have immediate local consequences for terrestrial and marine ecosystems."

Each summer, polar bears are being forced from their seal-hunting grounds on the melting sea ice, endangering their limited populations. Hundreds of thousands of acres of peat moss may decompose and begin to release higher amounts of methane and carbon dioxide, potentially accelerating the accumulation of greenhouse gases in the atmosphere, according to Dr. Bromwich.

Arctic countries are already jostling for political control of one of Earth's last remaining frontiers, he said. Russia, Denmark and Canada have claimed the Arctic sea floor in hopes of securing valuable oil, gas and mineral rights. Canada also is claiming political control over shipping lanes that pass by that country's northern islands, and Russia may follow suit, as passages near its northern shores are also nearly clear of ice.

"The summer ice melting has been advancing much faster than any of the climate models predicted," said Dr. Bromwich. "The Arctic region is a very heterogeneous environment, and it's extremely important that we better understand what's happening there in order to predict the future more accurately." ■

right: The 850 Mhz NMR spectrometer at Miami University is a good example of the sophisticated scientific instruments that can be shared through the Remote Instrumentation Collaboration Environment project.

photo courtesy of miami University

Remote use of scientific instruments expands research, education

Project leads:
Prasad Calyam, Ph.D., OSC,
Michael Kennedy, Ph.D., Miami University, &
Gordon Renkes, Ph.D., The Ohio State University
Research title:
User and network interplay in Internet telemicroscopy
Funding source:
Ohio Board of Regents

"This unique resource-sharing project will allow Ohio's colleges and universities to multiply the benefit of each strategic investment made in scientific instrumentation."
–Ohio Chancellor Eric D. Fingerhut

A researcher specializing in indentifying biomarkers for childhood obesity may wish for the insights made possible through the use of a powerful nuclear magnetic resonance (NMR) spectrometer situated on the other side of the state. Now this dream scenario is possible through special network connections over OSCnet and software being developed by members of the Cyberinfrastructure Software Development Group at the Ohio Supercomputer Center.

With funding from the Ohio Board of Regents and in partnership with The Ohio State University and Miami University, OSC is developing a statewide cyberinfrastructure to provide access over the Internet to Ohio's most valuable and expensive scientific instruments. OSC is developing web-portals that integrate the Center's Remote Instrumentation Collaboration Environment (RICE) software. The web-portal and RICE software together support multi-user session presence, user control management, live video feeds between Ohio labs, and collaboration tools such as Voice over IP and chat.

Recently, Miami University Professor Michael Kennedy, Ph.D., has partnered with OSC to "cyber-enable" the university's "only-one-of-its-size" 850-megahertz nuclear magnetic resonance (NMR) spectrometer.

"While my Miami colleagues, students and I are fortunate to have this amazingly sophisticated instrument available for our vital research projects, it's also important to make this unique NMR resource available for remote instruction and operation to my more distant research and teaching associates," said Kennedy, an Ohio Eminent Scholar in structural biology.

At The Ohio State University's Analytical Spectroscopy Laboratory, lab manager Gordon Renkes has been working with OSC to develop a RICE software variant that addresses dual-screen resolution and collaboration tool requirements of their FTIR-Raman Microprobe in order to work more closely with their partners in Alabama and California.

"OSC's ultimate goal is to develop a remote instrumentation cyberinfrastructure that fosters research and training activities that can drastically shorten the innovation process in fields such as materials modeling and cancer research," said OSC's Prasad Calyam, Ph.D. "Such a service also improves user convenience, significantly reduces costs, and, ultimately, decreases duplication of instrumentation investments." ■

Project leads:
Thomas J. Humanic, Ph.D., The Ohio State University; Paul Buerger, Ph.D., OSC; Douglas L. Olson, Ph.D., Lawrence Berkeley National Laboratory; Lawrence Pinsky, Ph.D., University of Houston; Ron Soltz, Ph.D., Lawrence Livermore National Laboratory; & Michael Lisa, The Ohio State University
Research title:
Developing extensions to grid computing for ALICE at the LHC
Funding source:
National Science Foundation

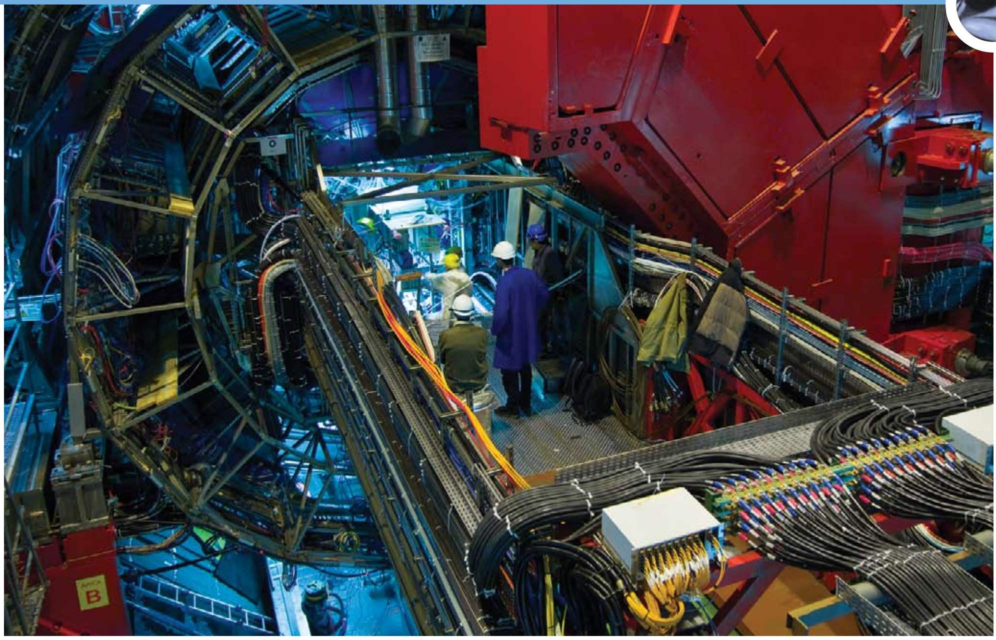
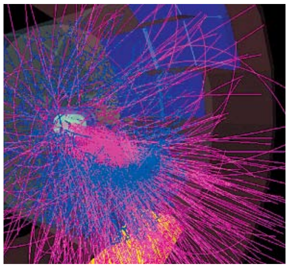


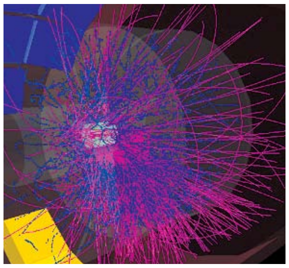
photo courtesy of CERN/Mona Schweizer

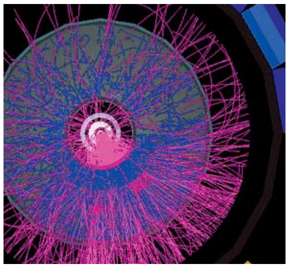
above: When the ALICE experiment collides lead atoms at nearly the speed of light, sophisticated detectors will dump data at the rate of more than one gigabyte per second into a worldwide network of research repositories, including the Ohio Supercomputer Center.

below: Physicists tracked muons from a cosmic shower event in June 2008, partly as a test of ALICE's Time Projection Chamber, which tracked similar particles when the supercollider runs the first ALICE experiments.

ALICE experiment opens a window to the creation of the universe







photos courtesy of CERN/Christian Lippman

In a lush valley on the border of Switzerland and France, more than 1,000 physicists, engineers, and technicians from 30 countries are working to answer questions about the fundamental nature of matter. The massive physics research project recreated on a small scale within the Large Hadron Collider at CERN, the European Laboratory for Nuclear Research, the explosive first moments of the birth of the universe.

As part of the ALICE experiment, short for A Large Ion Collider Experiment, physicists accelerated lead atoms to nearly the speed of light, collided their nuclei and then visualized the expelled particles that make up the protons and neutrons of the lead nuclei — quarks and gluons. Sensitive detectors measured the particles' reactions, recording approximately 1.25 gigabytes of data per second — or as much as three DVDs per minute.

To analyze tracking data from up to 8,000 collisions per second, researchers are employing a worldwide network of computing resources, including those of the Ohio Supercomputer Center.

"Traditionally, researchers would do much, if not all, of their computing at one central computing center. This cannot be done with the ALICE experiments because of the large data volumes," said Thomas J. Humanic, Ph.D., professor of physics at The Ohio State University.

The massive data sets were distributed to researchers around the world through high-speed connections to the "Grid," a network of computer clusters at scientific institutions, including the Ohio Supercomputer Center.

Beyond serving as a storage and analysis resource for researchers working on the project, "OSC has been critical in the development and testing of a computing model to analyze the ALICE data," Humanic said.

OSC already has provided 300,000 CPU hours for data simulations and has allocated up to one million hours for analysis of the first experimental data, collected in September, 2008. ALICE already has yielded many valuable second-order benefits in areas such as distributed computing, mass data storage and access, software development, and instrument design. ■

Magnifying light reveals more about the cosmos

By using the same technique that recently revealed two planets more than 5,000 light years away from Earth, Ohio State University researchers could again potentially uncover new celestial bodies.

The technique, called gravitational microlensing, is based on one aspect of Einstein's theory of relativity: gravity bends space. When two stars align almost perfectly with Earth, the gravity of the star closest to Earth temporarily bends and magnifies the light from the more distant star. The closer the stars are to a straight line the greater the magnification, and the more intricate and complex the data.

Andrew Gould, Ph.D., a professor of astronomy at The Ohio State University, and his colleagues are using the Ohio Supercomputer Center to decipher data collected by a team of international astronomers from such a microlensing event last year.

"The light curve had two sharp spikes, so we knew almost immediately there is a planet," Gould said, "because stars without planets produce smooth, bell-shaped light curves." However, after many weeks of intensive calculations, a single-planet model just didn't fit.

"That means there must be a second object orbiting the star," Gould said. To identify the object, Gould and Ohio State graduate student Subo Dong are testing more than 100 million different models on OSC's supercomputers.

"No matter what our answers turn out to be, this is exciting," Dong said. "We just need to figure out if the second orbiting object is another star, or a new planet." ■

Project lead: Andrew Gould, Ph.D., The Ohio State University
Research title: High magnification microlensing: Theory & planet detection
Funding source: National Science Foundation

Computer models predict traffic accident 'hot spots' for Ohio

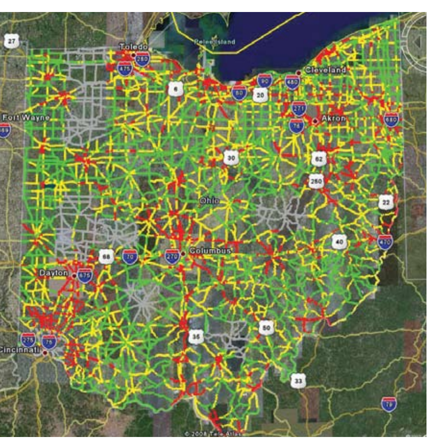
Project lead:
Christopher Holloman, Ph.D., The Ohio State University
Research title:
Predicting crashes and crash causes on Ohio roadways
Funding source:
Statistical Consulting Service at The Ohio State University Department of Statistics

An Ohio State University statistics expert used the powerful machines of the Ohio Supercomputer Center to design a program that identifies traffic accident hotspots on Ohio's roadways. Christopher Holloman, Ph.D., produced color-coded computer models to tell state troopers where fatal and injury accidents, especially those from speeding and drunk driving, are most likely to occur.

"We started out evaluating a couple of hundred miles worth of roadway in five major cities in Ohio," said Dr. Holloman. "The Highway Patrol found the information I provided extremely helpful, so it asked me to include all of Ohio."

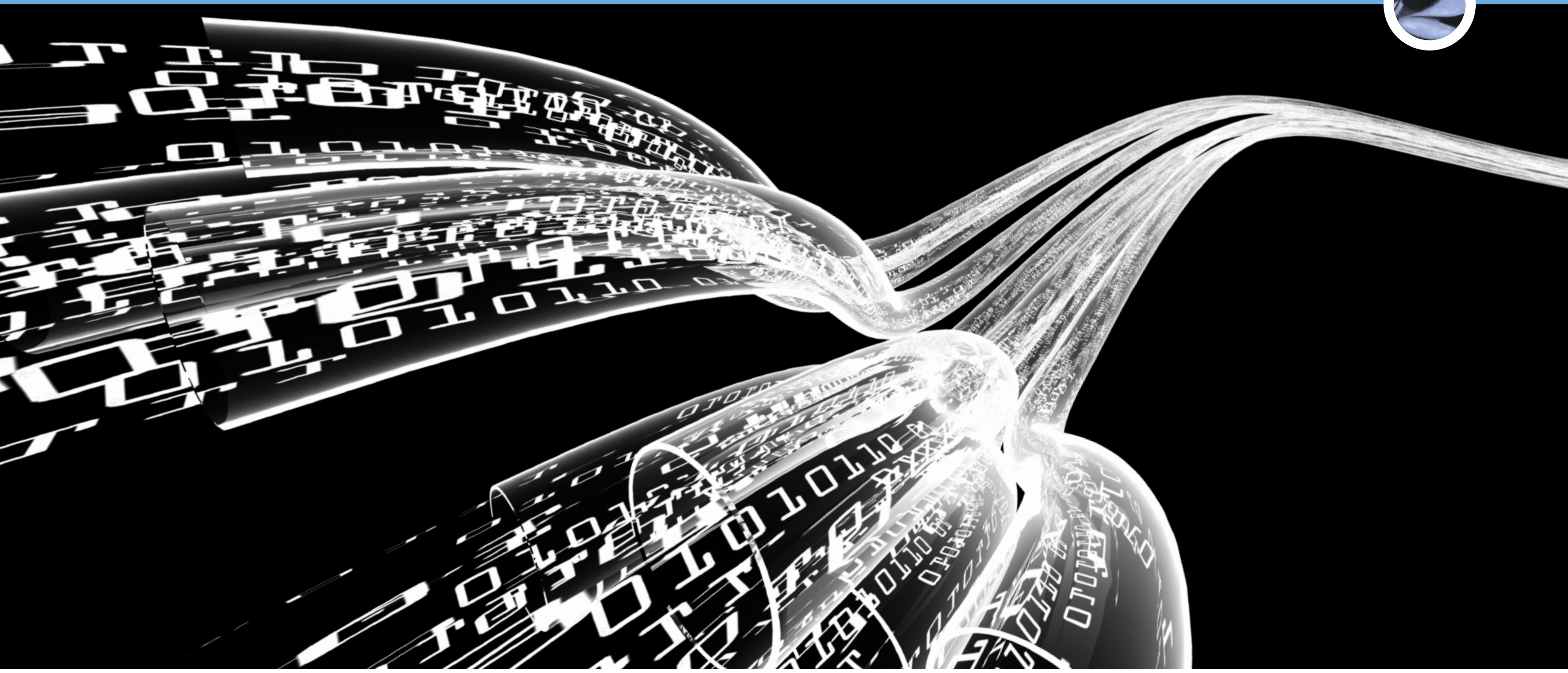
"Crashes are going to occur — it's a matter of when and where," said Lt. Anthony Bradshaw of the Ohio State Highway Patrol. "If we're able to predict a crash, then we're better able to prevent it."

> "We already had the code, we just needed a more powerful computer that would fit such a large model. We basically had two options — either go to OSC or start from scratch and rewrite the program." *–Christopher Holloman, Ph.D.*



Dr. Holloman's program analyzed every traffic accident in the Highway Patrol's databases that occurred on Ohio highways over a five-year period. Predictions were made under two types of road conditions: good or bad. Also, each roadway had predictions for each of five different categories of days: Monday through Thursday, Friday, Saturday and Sunday, the day before a long weekend, and holidays. In addition, Dr. Holloman's program breaks out results by factors such as age group, alcohol status, speed and class of vehicle.

The Ohio State Highway Patrol used the program to help position its cruisers during major holidays. The research team also combined the program with Google Earth, which Dr. Holloman said makes the tool even easier to use. ■



Supporting Defense Department security, computing needs by improving data transfer methods along multiple paths

The Department of Defense, like many companies and organizations, have leveraged the advances in supercomputing to compute increasingly complex and large computational problems. File sizes have equally expanded with the growth in computing power, especially if the files contain very large sets of data. It's not uncommon for files to occupy tens or hundreds of gigabytes, and transferring these files between supercomputing centers through standard means could take hours, or even days.

The need to transfer large amounts of data quickly led to the development of parallel file transfer software packages, which use multiple paths between computers to send the information. The military recommends the program Multiple Path Secure Copy (MPSCP) for transferring data between its supercomputing centers; however, this software package did not meet all its needs. They tasked the experts at the Ohio Supercomputer Center to improve MPSCP by improving user functions and updating the software manuals and, most importantly, adding the ability to encrypt sensitive information — without substantially sacrificing transfer speeds.

"The version of MPSCP we created not only was significantly easier to use, it also could encrypt and transfer data much faster when using more than one data stream," said Brian Guilfoos, a computational science researcher at OSC and lead developer on the project.

The OSC software development team evaluated the performance of its modified MPSCP by recording total transfer times for a directory containing 10 files, each one gigabyte in size, for different numbers of data streams and with encryption enabled or disabled. They also compared the amount of time it took for the same transfer using secure copy, which encrypts transferred data, making it functionally similar to the encryption-enabled version of MPSCP.

"As expected, encrypted file transfers are slower than non-encrypted, but multiple paths still provide a significant improvement over secure copy, even when transferring encrypted information," Guilfoos said. ■

"The Multiple Path Secure Copy program has significantly improved the productivity of our scientists and engineers who routinely require the transfer of large data sets."

–Aram Kevorkian, Ph.D., deputy director of HPC programs at the Space and Naval Warfare Systems Command, San Diego

Project lead: Jose Unpingco, Ph.D., OSC
Research title: Sharing & mining SIP (Signal Image Processing) data
Funding source: Department of Defense High Performance Computing Modernization Program

Benchmark study examines results of leading high-level languages

In the science and engineering community, three computer-programming languages, MATLAB, Mathematica and Python, are among the most popular. Called high-level languages, they let researchers focus on solving problems by cloaking the basic, yet necessary, coding that computers require. Each language also has extensions for users to access remote high performance computing systems — without sacrificing their desktop environment and the productivity that comes with it.

But is one any better than the other? Ohio Supercomputer Center researchers are currently evaluating each computing solution against four HPC Challenge benchmarks: STREAM, FFT, Top500 and RandomAccess.

"By testing the benchmarks on an OSC research cluster, we can control the configuration and system load to ensure as objective a comparison as possible. We also examine code complexity and solution time," said Alan Chalker, Ph.D., program director of computational science engineering research applications at OSC. "We'll then conduct a sampling of these test runs on Department of Defense Major Shared Resource Centers supercomputers to validate the OSC-based results."

The underlying computational analysis behind each benchmark offers a unique evaluation of whether a particular solution offers advantages in terms of performance, memory use or code complexity. These results ultimately benefit the work of researchers in all branches of the military, as many use high-level languages. ■

Project lead: Alan Chalker, Ph.D., OSC
Research title: Benchmarking of parallel high-level languages
Funding source: Department of Defense High Performance Computing Modernization Program

Processing the sounds of a battlefield to evaluate targets

The sounds of war, when accurately captured and processed, shed their cacophonous echoes and leave a trail of unique, acoustical fingerprints.

Much like sonar detects and classifies underwater resonance, acoustic signal processing sensors capture sounds in the air. By using an array of sensors, military personnel can collect the distinct auditory signatures of combat vehicles and use that information to identify and track specific targets. This type of network, though, depends on establishing the sensors' locations through triangulation of the equipment. Environmental factors such as wind, hills or air temperature can affect this process, called self-localization.

Establishing the location requires applying a number of different algorithms to the data, which, as the number of environmental factors increase, takes correspondingly more time to process. Researchers at the Ohio Supercomputer Center, in partnership with the Army Research Laboratory, ramped up the analysis phase by refining several parallel processing algorithms. Parallel processing segregates calculations across multiple computer nodes.

"We tested various parallel processing technologies on a sample data set of 63 audio files and found ways to tweak the programs' codes for better, quicker results," said Ashok Krishnamurthy, Ph.D., senior director of research at OSC. "The faster researchers can process the sounds in any given area, the faster military leaders can make critical decisions about their course of action." ■

Project lead: Ashok Krishnamurthy, Ph.D., OSC
Research title: Object detection, localization & tracking using multiple sensors
Funding source: Army Research Laboratory

OSC supports DoD's efforts to scale radar tomography analysis efforts to larger supercomputers

The Air Force Research Laboratory, Sensors Directorate, Advanced Radar Waveforms & Processing Branch recently installed a remote testing facility to gather data for radio frequency (RF) tomography technology. Because the quantity of collected data would increase exponentially once the testing site was operational, the military analysts turned to Ohio Supercomputer Center experts for assistance in adapting existing RF analysis programs to the military's high performance computing systems.

The AFRL research team already used Star-P, a commercial software platform, to seamlessly convert to parallel the programming codes written in MATLAB, a different commercial software program. However, the team members had used only Star-P on their in-laboratory Altix computer. By studying results with different sizes of problems on increasing numbers of processors, OSC staff evaluated the potential effectiveness of using Star-P for the tomography code on much larger military supercomputers.

"OSC provided valuable information about how to use Star-P to shorten time between field experiments, direction regarding the structure for existing parallel programs, and ways to shorten the time to develop a deployable system," said Kevin Magde, AFRL Sensors Directorate, Advanced Radar Waveforms & Processing Branch. "While the RF tomography effort is in relatively early stages, its eventual capability will have tremendous impacts on Department of Defense surveillance operations worldwide." ■

Project lead: Bracy Elton, Ph.D., OSC
Research title: Usability & scalability of a Star-P/MATLAB application for ultra narrow band tomography on HPC system
Funding source: Department of Defense High Performance Computing Modernization Program

Keeping pace with the world's fastest supercomputers

In the near future, the world's fastest supercomputers will incorporate millions of processing elements, a substantial increase in scale over the high performance computing systems in use at leading research centers today. At the same time, however, the rates at which users can access data storage devices, such as hard disks, are not increasing at the same rate.

In fact, the overall ability of file systems to input and output data within these high performance computers is not keeping pace with the increases in raw compute power. Even commercial file systems used on the largest cluster computers — designed for competitiveness in the larger business market — are being stretched to address the demands of the most powerful systems.

Research scientists at the Ohio Supercomputer Center are part of a team researching this issue for the Department of Energy, which, incidentally, owns and operates several of the world's most powerful supercomputers.

"A comprehensive software solution is needed to bridge the gap between processing trends and I/O systems so that leadership-class machines can most efficiently leverage the available storage resources," the DOE grant proposal states.

The team will create a software package that will operate on the IBM Blue Gene, Cray XT, Roadrunner and Linux cluster platforms and function on a variety of file systems. The package will be designed as open-source software and be available online. ■

Project leads: Rob Ross, Argonne National Laboratory, & James Nunez, Los Alamos National Laboratory
Research title: Common HEC I/O forwarding scalability layer
Funding source: U.S. Department of Energy

research landscape

Ohio's strengths in basic and applied research are broad and deep, spanning a multitude of academic, business and industrial organizations. The spectrum of clients served by the Ohio Supercomputer Center likewise encompasses many fields of study. This diversity attracts to Ohio eminent scholars and innovative entrepreneurs, as well as a breadth of regional, national and global research funding. A review of several of these projects yields a team of chemists and naturalists constructing computer simulations of forest fires that predict the dangers of controlled burns to wildlife. Researchers are measuring the water elevations of Amazon River tributaries to better understand the complexity of seasonal flooding. And, others are conducting vital studies in fields as diverse as psychology, linguistics, economics, engineering and political science. The Center strives to assist customers with basic needs, while simultaneously meeting the requirements of its most advanced customers, as evidenced by the significant projects described on the following pages. ■

above: Prescribed fires encourage new growth and reduce the risk of wildfires by intentionally burning underbrush and old wood. Foresters would like to extend the timeframe that they safely can implement prescribed fires in habitats of the endangered Indiana bat.

Healthy forests, healthy fires, healthy bats

Do no harm. In the effort to manage the forest habitats of the endangered Indiana bat, naturalists must always, always, first consider the impact on this nocturnal mammal. Bats perform a vital ecological role, feeding entirely on flying insects; a single bat can consume thousands of mosquitoes each night.

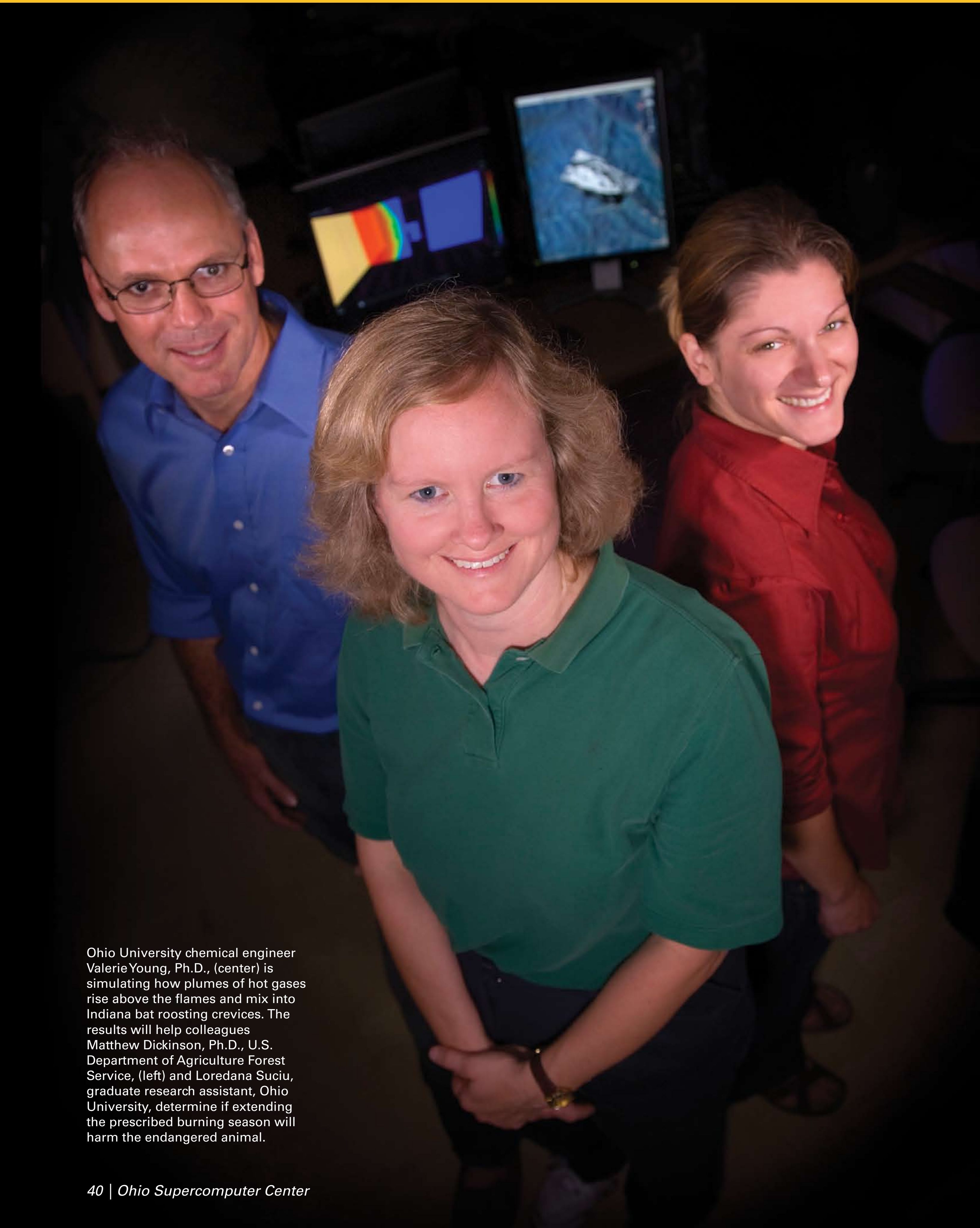
Summering in forests throughout the Eastern United States, female Indiana bats raise their young in maternity colonies. While their first choice for nurseries are dead trees with exfoliating bark, they also live in large, healthy trees such as shag hickory and oaks. Their male bats are singular creatures that choose colder microclimates; they commonly enter torpor, a hibernation-esque state, during cool or rainy days.

Ironically, one of the most effective ways to keep their ecosystem healthy could be lethal. If conducted improperly, prescribed fires — the technique of burning underbrush and old wood to encourage new growth and reduce the risk of wildfires and insect outbreak — could kill or injure both male bats in torpor and flightless young too heavy for their mothers to move. Consequently, naturalists err on the side of caution; they implement prescribed fires in known habitats of the Indiana bat only during winter months, when the bats are hibernating safely deep inside caves.

A multidisciplinary research project involving the U.S. Department of Agriculture's Joint Fire Science Program, Ohio University, University of Kentucky, Rochester Institute of Technology and several independent consultants is focusing on the potential effects of extending the burning season. The impetus for their efforts comes from Kentucky's Daniel Boone National Forest, where foresters would like to implement an aggressive prescribed burning program to restore and

below: Listed as endangered since 1967, Indiana bats play a major role in insect control. The small bats can consume up to half their body weight in insects each night.

photo courtesy of U.S. Fish and Wildlife Service



Ohio University chemical engineer Valerie Young, Ph.D., (center) is simulating how plumes of hot gases rise above the flames and mix into Indiana bat roosting crevices. The results will help colleagues Matthew Dickinson, Ph.D., U.S. Department of Agriculture Forest Service, (left) and Loredana Suciu, graduate research assistant, Ohio University, determine if extending the prescribed burning season will harm the endangered animal.

maintain oak and hickory groves and prepare for an expected invasion of gypsy moths.

Using Fire Dynamics Simulator, a version of computational fluid dynamics software, Valerie Young, Ph.D., a chemical engineer at Ohio University, is simulating how plumes of hot gases rise above the flames and mix into the roosting crevices of tree bark. She's running the data-intensive programs on the Ohio Supercomputer Center's IBM Cluster 1350.

"We suspect that the bark crevices may actually shelter bats from the fire's deadly carbon monoxide, smoke and heat," Young said. "Computational models of this kind have been used to study wildfires out West, over thousands of acres and days or weeks. As far as we can find, this is the first work that looks at the impact of fires on mammals on a microscale."

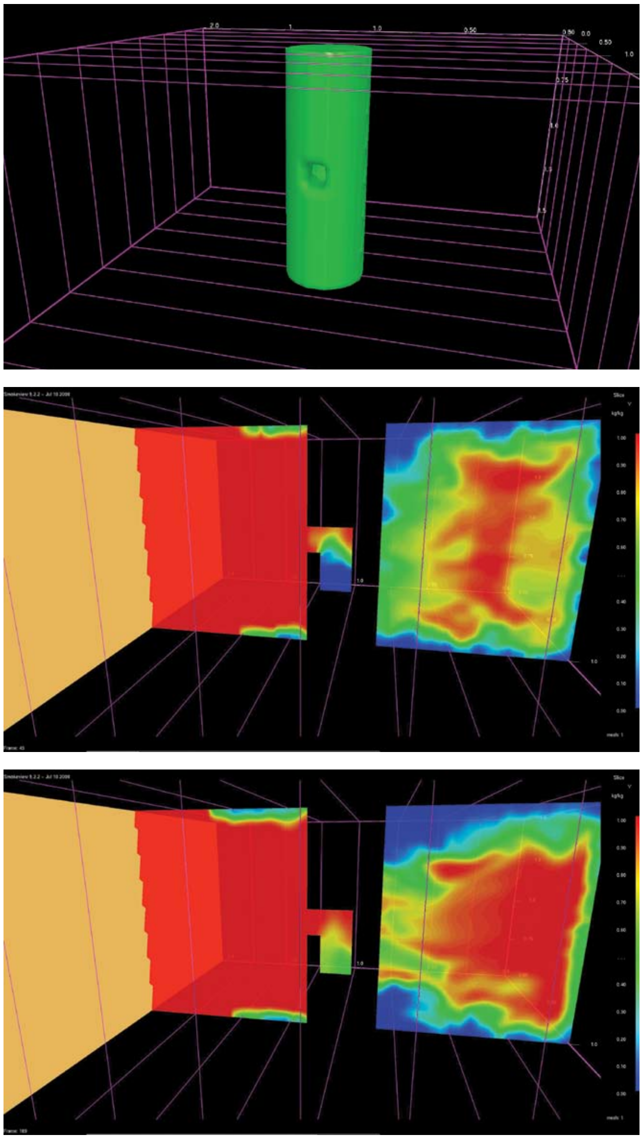
The models will help the team understand the mix of gas concentrations and temperatures for two scenarios. The first looks at the environment immediately above an active fire, when the intensity is brief, but the concentrations of smoke and heat are high. The second scenario models the low concentration of lingering smoke after the fires have subsided or been extinguished during nighttime inversions, which is when temperatures increase at higher elevations. This information will then be used to determine rates of gas and heat mixing into these crevices.

Research being conducted on OSC systems could help determine if foresters can implement an aggressive prescribed burning program that won't harm the endangered Indiana bat.

"With a better understanding of the effect of heat and smoke exposure on roosting Indiana bats, we can make better recommendations on what time of day and time of year to implement prescribed burns," said Anthony Bova, a physical scientist with the U.S. Department of Agriculture's Forest Service working on the project. "Fire obviously creates an immediate impact on the environment. We want to minimize the short term negative effects, and maximize the long term benefits."

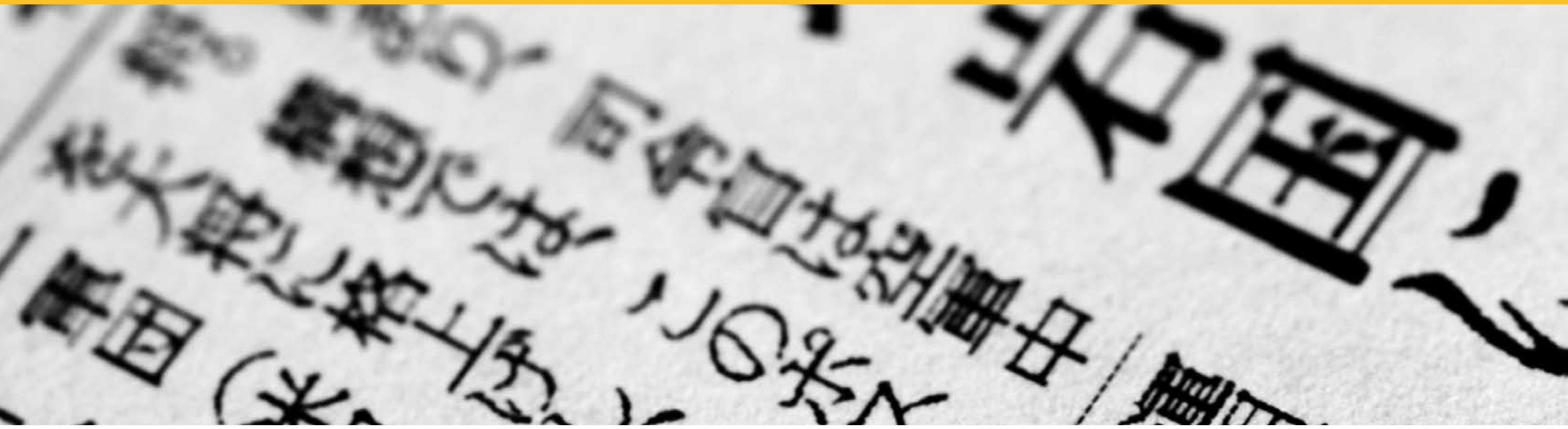
"Our goal is to determine if the foresters can expand the range of time for implementing prescribed burns, without harming the endangered Indiana bat," Young added.

Or, in essence, do no harm. ■



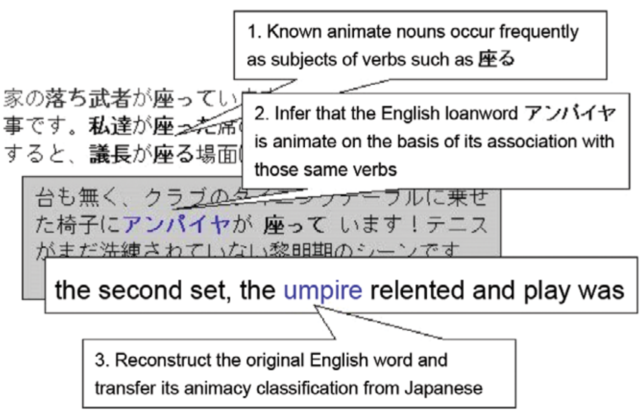
above: NIST's Fire Dynamics Simulator, a computational fluid dynamics model of fire-driven fluid flow, was used to model how tracer gas mixes into a tree cavity that might be made by woodpeckers. In the top image, the green vertical bar represents the tree; the depression in the tree represents the cavity. The subsequent images, rotated ninety degrees to the left, show the fire's gases and how they move around the tree and into this potential bat roosting area.

Project leads: Matthew Dickinson, Ph.D., U.S. Department of Agriculture Forest Service; James Norris, Ph.D., Norris Consulting Services; Michael Lacki, Ph.D., University of Kentucky; & Valerie Young, Ph.D., Ohio University
Research title: Injury & mortality risks from wildland fire smoke & heat exposures for endangered Indiana bats (Myotis sodalis) in maternity roosts
Funding source: U.S. Department of Agriculture, Joint Fire Science Program



How do we communicate?

Project lead:
Christopher Brew, Ph.D., The Ohio State University
Research title:
Hybrid methods for acquisition & tuning of lexical information
Funding source:
National Science Foundation Career Grant



above: This diagram illustrates one of the ideas developed by linguists at The Ohio State University. The technique uses information in Japanese to get at information about animacy that is missing from English.

As a computational linguist, Ohio State University Professor Chris Brew merges computer science with the scientific study of language and communication. Computational linguists create and test computational models of linguistic theories, as well as develop and apply tools for computers to complete real world tasks, such as extracting information from text, translating languages, and synthesizing and recognizing speech.

At the center of Dr. Brew's work is natural language processing, the development of ways for computers to use and understand everyday human language. In particular, Dr. Brew is working on the problem of building and maintaining dictionaries (lexicography) and grammars that reflect not only the insights of linguists and lexicographers, but also the evidence from large bodies of actual text.

"Broad-coverage dictionaries and ontologies (terms and descriptions) for natural language processing are difficult and costly to create and maintain," Dr. Brew said. "Because of the quantity of text available, computer support is essential. But while all modern lexicography is computer-based, the information used by today's systems is fairly shallow, simply because of the scale of the enterprise.

"We're working on ways of enriching the information available to lexicographers and other professionals. The challenge is to do this without losing the benefits of scale," said Dr. Brew, whose team includes graduate students Kirk Baker and Jianguo Li. "We found this is possible, and that a representation known as "dependency triples," i.e. groups of words that relate directly to each other, gives a significant boost over just counting words."

Using the Ohio Supercomputer Center systems, Baker led the effort to create these dependency triples from the Gigaword corpus, which contains a billion words of newswire text. With a supercomputer, they were able to complete in 72 hours what otherwise would have taken all summer.

"While our immediate goal is to gain a better understanding of lexical tuning and acquisition," Dr. Brew said, "the resulting dictionaries, ontologies and mapping techniques have the potential to help information professionals such as librarians navigate through data, understand their significance and incorporate insights into their working practice." ■

Psychologists decipher how we think

Psychologists increasingly wrestle with how to model one of the most sophisticated processing units of all — the human brain.

In the cognitive sciences, models are very diverse; they can range from closed-form equations with a few parameters to simulation-based models with many parameters. Selecting among competing models — for example, those of the same psychological process — can be a challenge, yet it is one of the fundamental tasks of scientific inquiry.

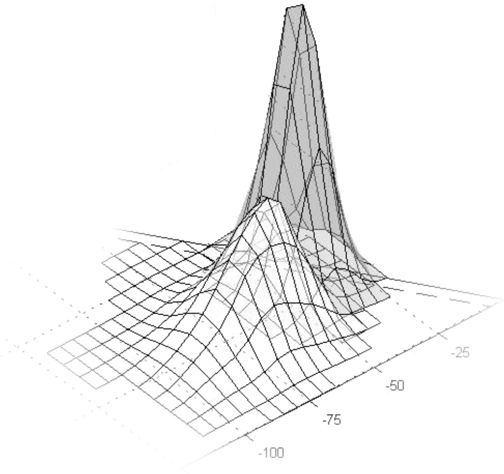
To aid the selection process, Ohio State University psychologists Mark Pitt, Ph.D., and Jay Myung, Ph.D., have introduced several sophisticated methods adapted from statistics and computer science.

"In our latest work, we're developing ways to optimize experimental design. Simulating some of the cognitive models we study requires many thousands of iterations to generate a single data point, which itself is repeated many more thousands of times to complete a full simulation," said Dr. Pitt. "By using the Ohio Supercomputer Center's supercomputers, we can complete in hours what might take days to accomplish on a PC."

They've also developed methods for analyzing model behavior called landscaping and parameter space partitioning, which, instead of comparing models on their ability to fit a single data set, takes a bird's eye view of how two models are related to each other.

"Mathematical modeling in psychology is not widespread, simply because there are not a lot of models in the field itself," said Dr. Pitt. "Our goal in developing these tools is to help researchers gain better insight into model behavior, and, ultimately, better understand how the mind works." ■

Project leads: Mark Pitt, Ph.D., & Jay Myung, Ph.D., The Ohio State University
Research title: Methods for selecting among mathematical models of cognition
Funding source: National Institutes of Health



above: Distributions depicting the representativeness of data sampled from two models of categorization. The solid line denotes the decision threshold under one criterion, and the broken line denotes the criterion when the decision is adjusted for the complexity of the model.

Analyzing politics through computation

As a political scientist, Professor Luke Keele's expertise in applying statistical techniques to social sciences serves him well.

"There's a lot more computing and statistical analysis in political science than people realize," said Dr. Keele, who teaches American politics and researches political methodology at The Ohio State University. To the uninitiated, his research appears far removed from elections, campaign trails or policy decision-making processes.

For example, Dr. Keele examines discrete choice models and time series models, and he's studying the properties of matching estimators. In political science, these are used to, respectively, predict individuals' decisions, such as voting choices; forecast the future behavior of variables, such as the influence potential running mates may have on voter appeal; and calculate probability based on a person's level of knowledge, for random variables that have discrepancies.

Recently, Dr. Keele has been developing a way to randomize experimental data collected conveniently. Because these samples of convenience do not represent the entire population, they are considered biased. However, the statistical tests most often used in political science assume that the data were generated randomly. This can lead to serious errors in the conclusions.

By running thousands of simulations using the software program R on the Ohio Supercomputer Center's Itanium 2 Cluster, Dr. Keele proved that randomized tests reduce errors when classic statistical tests are used with experimental data.

"These simulations would take several days to complete on my office computer," Dr. Keele said. "OSC's powerful resources help me get results faster while maintaining my productivity." ■

Project lead:
Luke Keele, Ph.D., The Ohio State University
Funding source:
The Ohio State University

Balancing security and performance tradeoffs for secure Internet videoconferencing

For years, experts have predicted that ubiquitous videoconferencing was just ahead. Now, several videoconferencing trends — including improved quality, reduced cost and the economy — have fueled demand. However, university network planners with H.323 and SIP videoconferencing equipment commonly deployed behind firewalls/NATs must balance trade-offs between network security for data and performance of voice and video.

"The primary challenge is in configuring firewalls to allow voice and video traffic in and out of the internal network's ports, while limiting malicious access of internal-network data," said Prasad Calyam, Ph.D., a senior system developer/engineer at the Ohio Supercomputer Center. "Improper policy decisions and misconfigurations in firewalls could result in vulnerable networks and slow data transfers, as well as voice and video performance problems."

Recently, several new standards (e.g., ITU-T H.460.18, H.460.19) and vendor (Polycom, GNU Gatekeeper, Cisco) solutions have emerged. The Ohio Board of Regents directed OSC to extensively evaluate these developments and to identify the limitations and caveats that exist in their deployment in campus and enterprise networks. The study analyzed interoperability, load tolerance and robustness-against-vulnerabilities, as well as the complex signaling-and-multimedia flow architectures that result from heterogeneous systems. Based on these studies, OSC developed a list of best practices for deploying small- to large-scale secure videoconferencing.

"OSC's experiment results clearly identify the deployment limitations and tradeoffs involved in balancing security of data and performance of video in today's networks," said Kurt Peterson, a regional director at Polycom. "The best-practices for secure video-conferencing proposed by OSC also provide sound advice to network engineers." ■

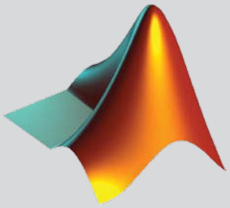
above: As the use of videoconferencing technologies swells, network planners must make important decisions to balance performance with security.

Project leads:
Prasad Calyam, Ph.D., & Steve Gordon, Ph.D., OSC
Research title:
Balancing security & performance tradeoffs in Internet videoconferencing
Funding source:
Ohio Board of Regents

Improving researcher access to Parallel MATLAB technologies

Benchmarking tests will evaluate the performance, memory use and code complexity of the leading high-level languages.

Project lead:
Ashok Krishnamurthy, Ph.D., OSC
Research title:
Applications in parallel MATLAB
Funding source:
Ohio Supercomputer Center



Researchers need look no further than the Ohio Supercomputer Center for a convenient way to access the MATLAB Parallel Computing Toolbox and ParaM, two versions of Parallel MATLAB technologies.

Parallel MATLAB enables researchers to access remote supercomputers within MATLAB, a user-friendly computer-programming language developed by The MathWorks. The Parallel Computing Toolbox is a commercial product from the MathWorks, while ParaM, an open-source addition to MATLAB, was developed by MIT Lincoln Laboratories and OSC. These technologies allow researchers to increase their productivity through the use of parallel computing without needing to re-write their MATLAB codes in a more typical parallel computing language.

"The Center's work with the Department of Defense High Performance Computing Modernization Program, combined with OSC's top-notch training programs, fortifies our national reputation as experts in deploying Parallel MATLAB. Our goal is to share our knowledge," said Ashok Krishnamurthy, Ph.D., senior director of research at OSC.

The service will support a number of concurrent remote users, offering access to multiple nodes on the Center's IBM Cluster 1350. User manuals, training courses and real-world examples of production code will round out its offerings.

"While our initial focus is serving Ohio's user community, the project will expand to businesses and national participants," Dr. Krishnamurthy added.

For example, scientists using the Teragrid, the world's largest distributed cyber-infrastructure for open scientific research, soon will have access to OSC's Parallel MATLAB services as part of Pittsburgh Supercomputer Center's pending award (Track2C) from the National Science Foundation. This prestigious grant supports acquiring, deploying and operating a high performance computing system for the national science and engineering community. ■

Examining success of empowering poor through microfinancing in rural Thailand

Over the past few decades, developing countries have increasingly used microfinance, the practice of making small loans to the working poor. TrickleUp, Kiva.org, and more than 3,6000 microfinance institutions worldwide offer hope for a more cost-effective method of empowering the poor. However, until now, little academic research has looked at the loans' actual impacts.

Ohio State University economist Joseph Kaboski, Ph.D., and his colleague, Robert Townsend, Ph.D., of the University of Chicago, examined whether the "Million Baht Village Bank" microfinance initiative helped increase consumption, investment and income growth among poor households. They also analyzed the program's impact on default rates, education, savings and job mobility in rural and semi-urban Thailand. The program, initiated in 2001, transferred one million baht to nearly 80,000 Thai villages to start local lending banks.

"The unique structure of this program gives us a laboratory for evaluating the program and also theories about how households cope when credit is limited or difficult to obtain," said Dr. Kaboski. "By using the supercomputers at OSC, we were able to efficiently solve and estimate rich models of household economic behavior and compare our predictions to the actual program."

Drs. Kaboski and Townsend found that microfinance has very large impacts on consumption, which are consistent with a model in which households build buffer stocks of savings to protect against adverse shocks when credit is unavailable, somewhat smaller impacts on investment. Still, because households bear interest costs of credit, they found transfer payments are more cost-effective than microfinance. ■

Project lead:
Joseph Kaboski, Ph.D.,
The Ohio State University
Research title:
The impact of credit: Examining a policy experiment
Funding source:
National Institute of Child Health & Human Development, National Institutes of Health, R03 HD04776801

Satellite measurements provide key to estimating Amazon River discharge

Project leads:
Doug Alsdorf, Ph.D., &
Michael T. Durand, Ph.D.,
The Ohio State University
Research title:
Assimilation of wide swath altimetry
Funding sources:
NASA Terrestrial Hydrology Program, NASA Physical Oceanography Program & The Ohio State University Climate Water Carbon program

The vast fresh-water Amazon floodplain plays an important role in climate changes, biogeochemical fluxes, wetlands ecology and flood hazards. Yet, scientists really don't know exactly how much water courses through the world's largest river.

Building on his earlier work modeling flood patterns of the Amazon, Ohio State University Earth scientist Doug Alsdorf, Ph.D., has joined colleagues at the University of Bristol, the University of Washington and the NASA Jet Propulsion Laboratory to better understand the dynamics of the Amazon.

NASA's proposed Surface Water and Ocean Topography (SWOT) satellite mission, with a launch expected 2013-16, will use radar altimetry to provide high-spatial resolution, global measurements of ocean surface topography and surface water elevations. For the terrestrial branch of the mission, SWOT will measure water storage changes in all rivers, lakes and wetlands.

Using Ohio Supercomputer Center resources, Dr. Alsdorf and fellow OSU research scientist Michael Durand, Ph.D., plan to incorporate those measurements into the LISFLOOD-FP hydrodynamic computer model to more accurately estimate river depth and slope, which are needed to calculate the waterway's discharge. OSC researcher Judy Gardiner, Ph.D., adapted the program to the parallel processing platform of the Center's IBM Cluster 1350.

"Fresh water is a basic requirement for life, yet surprisingly, our knowledge of the volume and fluxes of water on floodplains and in rivers is poor," said Dr. Alsdorf. "Using synthetically produced SWOT measurements in two proof-of-concept experiments, we found that we will be able to estimate river depth and slope to within fractions of a meter and centimeters-per-kilometer, respectively." ■

photo courtesy of NASA

Research Grants

Awarded to the Ohio Supercomputer Center 2008 Fiscal Year (July 1, 2007 to June 30, 2008)

Funding Source	Title	OSC Contact	Team *LEAD IN BOLD*
Air Force Research Laboratory Sensors Directorate/ Sensor Technology Research, Development, Test & Evaluation	Center for Automatic Target Exploitation and Recognition (CATER)	Ashok Krishnamurthy, Ph.D.	• Georgia Tech • Massachusetts Institute of Technology • **The Ohio State University** • Ohio Supercomputer Center • Rensselaer Polytechnic Institute • University of Florida • University of Michigan • Washington University • Wright Patterson Air Force Base • Wright State University
Air Force Research Laboratory Sensors Directorate/ Sensor Technology Research, Development, Test & Evaluation	SOW: Gotcha Radar Exploitation Program (GREP)	Ashok Krishnamurthy, Ph.D.	• **Ohio Supercomputer Center** • SET Corporation
Alternative Research and Development Foundation	The Integration of Simulation Technologies in Veterinary Medicine for Anatomical Review and Procedural Training	Don Stredney	• **The Ohio State University** • Ohio Supercomputer Center
Argonne National Laboratory	PVFS Portals Performance Improvements	Pete Wyckoff, Ph.D.	• **Ohio Supercomputer Center**
Department of Defense High Performance Computing Modernization Program	PET — High Productivity SIP Application Development: Development Methodology, Performance and Scalability	Alan Chalker, Ph.D.	• Mississippi State University • **Ohio Supercomputer Center**
Department of Defense High Performance Computing Modernization Program	PET — Benchmarking of Parallel High Level Languages	Alan Chalker, Ph.D.	• Mississippi State University • **Ohio Supercomputer Center**
Department of Defense High Performance Computing Modernization Program	PET — SIP Metadata Tool Improvement	Alan Chalker, Ph.D.	• Mississippi State University • **Ohio Supercomputer Center**
Department of Defense High Performance Computing Modernization Program	PET — User Friendly High Productivity Computational Workflows: Productivity and Performance Evaluation of the VISION/HPC Open Source Solution	Alan Chalker, Ph.D.	• Mississippi State University • **Ohio Supercomputer Center**
Department of Defense High Performance Computing Modernization Program	PET —TENA/HLA Gateway for HPC	Ashok Krishnamurthy, Ph.D.	• Mississippi State University • **Ohio Supercomputer Center**
Department of Defense High Performance Computing Modernization Program	PET — Physical Simulation Model of the Non-Uniform Correction (NUC) for Infrared Scene Projector (IRSP) Arrays	Judith Gardiner, Ph.D.	• Mississippi State University • **Ohio Supercomputer Center**
Department of Defense High Performance Computing Modernization Program	PET — Usability and Scalability of a Star-P/MATLAB Application for Ultra Narrow Band Tomography on HPC System	Stan Ahalt, Ph.D.	• Mississippi State University • **Ohio Supercomputer Center**

Funding Source	Title	OSC Contact	Team *LEAD IN BOLD*
Department of Energy Scientific Discovery through Advanced Computing (SciDAC)	Next Generation Multi-scale Quantum Simulation Software for Strongly Correlated Materials	Karen Tomko, Ph.D.	• Oak Ridge National Laboratory • Ohio Supercomputer Center • University of California — Davis • **University of Cincinnati**
Department of Energy National Laboratories	Common HEC I/O Forwarding Scalability Layer	Pete Wyckoff, Ph.D.	• **Ohio Supercomputer Center**
Department of Health and Human Services	Virtual Microscopy to Microarry (VM2M): Integrated Virtual Microscopy and Molecular Analysis Software for Enhanced Cancer Diagnosis	Ashok Krishnamurthy, Ph.D.	• Children's Oncology Group • Cincinnati Children's Medical Center • Nationwide Children's Research Institute • DHRS Office for Advancement of Telehealth • Ohio Board of Regents • **Ohio Supercomputer Center**
National Institutes of Health/Institutional Clinical and Translational Science Award	The Ohio State University Center for Clinical and Translational Science	Don Stredney	• **The Ohio State University** • Ohio Supercomputer Center
National Science Foundation/ Cyberinfrastructure Training, Education, Advancement, and Mentoring for our 21st Century Workforce	Improving American Competitiveness through Workforce Education in Cyberinfrastructure	Steve Gordon, Ph.D.	• Columbus State Community College Council on Competitiveness • Ohio Learning Network • The Ohio State University • **Ohio Supercomputer Center** • Sinclair Community College • University of Akron
National Science Foundation	Collaborative Research: IPY: Arctic System Reanalysis	Paul Buerger, Ph.D.	• National Center for Atmospheric Research (NCAR) • **The Ohio State University** — Byrd Polar • Ohio Supercomputer Center • University of Colorado • University of Illinois • University of Alaska
National Science Foundation/ Partnerships for International Research and Education (PIRE)	PIRE: Graduate Education in Petascale Many Body Methods for Complex Correlated Systems	Karen Tomko, Ph.D.	• ETH Zürich • Göttingen University, Germany • Max-Planck-Institute für Festkörperforschung, Germany • Oak Ridge National Laboratory • Ohio Supercomputer Center • S.N. Bose Center Basic Science, Calcutta • Technical University Darmstadt, Germany • University of Cincinnati • University of Denmark • **University of North Dakota** • University of Tennessee • University of Würzburg, Germany
NetEffect	OpenFabrics Implementation and Testing of an RDMA Module for Apache	Pete Wyckoff, Ph.D.	• **Ohio Supercomputer Center**

Research Grants

Awarded to the Ohio Supercomputer Center 2008 Fiscal Year (July 1, 2007 to June 30, 2008)

continued

Funding Source	Title	OSC Contact	Team *LEAD IN BOLD*
Department of Energy	Nuclear Magnetic Resonance (NMR) Spectroscopy	Ashok Krishnamurthy, Ph.D.	• **Ohio Supercomputer Center** • Miami University
Ohio Board of Regents	Visualization, Imaging and Modeling; Shared Instrumentation in Materials Research and Education	Ashok Krishnamurthy, Ph.D.	• **Ohio Supercomputer Center**
Ohio Board of Regents	Ralph Regula School of Computational Science — Short Courses	Steve Gordon, Ph.D	• **Ohio Supercomputer Center** Ralph Regula School of Computational Science • Ohio Aerospace Institute • ACES • Ohio Resource Center
Ohio Board of Regents/STEM (Science, Technology, Engineering, Mathematics and Foreign Language Academy)	Summer Academy in Computational Science and Engineering	Steve Gordon, Ph.D.	• **Ohio Supercomputer Center**
Ohio Board of Regents (Choose Ohio First Scholarship Program)	Ohio Consortium for Bioinformatics	Steve Gordon, Ph.D.	• Bowling Green State University • Case Western Reserve University • Central State University • Clark State Community College • Kent State University • Miami University Dayton • The Ohio State University • **Ohio University** • Ohio Supercomputer Center Ralph Regula School of Computational Science • University of Akron • University of Cincinnati • University of Toledo • Wittenberg University • Wright State University
Ohio Department of Education/2008 Summer Honors Institute Office for Exceptional Children	Summer Institute	Elaine Prichard	• **Ohio Supercomputer Center**
Ohio Third Frontier Wright Projects Program FY 2008	Center for Excellence in Advanced Materials Analysis	Tim Wagner	• **Youngstown State University** • Fireline TCON • Ohio Supercomputer Center
Ohio State University/Public Health Preparedness for Infectious Diseases Pilot Research Grant	Development and Evaluation of Immersive Simulations for use in Response Training for Outbreaks of Infectious Disease	Pete Carswell Don Stredney	• Ohio Supercomputer Center • **The Ohio State University**
Robert Wood Johnson Foundation	ALR Round 7: Environmental Perception, Evaluation, and Desirability for Physical Activity among African-American Families of Different Incomes	Steve Gordon, Ph.D.	• Advanced Computing Center for the Arts and Design (ACCAD) • **The Ohio State University** • Ohio Supercomputer Center

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Ohio Supercomputer Center

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