*Empower. Partner. Lead.*

Ohio Supercomputer Center

# 2010 Annual Research Report

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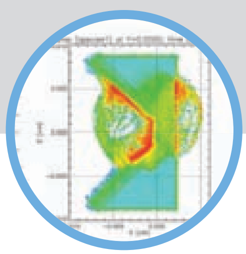

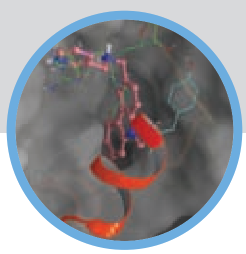

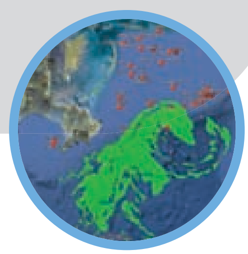
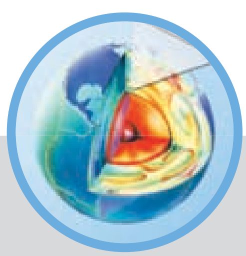

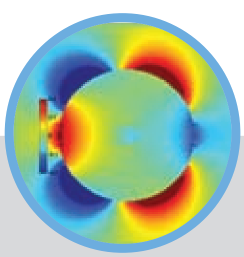

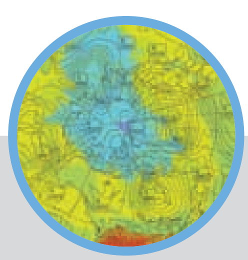


# introduction

*above:* Steven Gordon and Ashok Krishnamurthy, interim co-executive directors

## Welcome to the Ohio Supercomputer Center!

*Empower. Partner. Lead. . . . OSC's strategic vision*

To compete in a global environment, OSC depends upon powerful technology, vital services and – most importantly – talented people. We have developed a strategic vision to achieve and sustain national prominence as an academic and industrial supercomputer center that is focused on meeting and exceeding researcher needs and expectations. Our staff has the expertise, experience and flexibility to work closely with researchers to best achieve their goals using our computational resources.

Our mission is simple: empower researchers to make extraordinary discoveries and innovations; partner with industries to leverage computational science as a competitive force; and lead efforts to train Ohio's workforce on key skills to help them secure 21st century jobs.

In this report, you will find a small sampling of the research successes achieved through ready access to OSC resources – from identifying a drug that will allow the body to block brain tumors and designing solar cells with organic materials to extending the battery life of electric cars and developing algorithms to predict the likelihood of armed conflict.

Through the award-winning Blue Collar Computing program, we show industry members how to use custom web portals to design improved products and take them to market faster; and with the Ralph Regula School of Computational Science programs, we facilitate college students' pursuit of a groundbreaking minor and an associate degree curricula.

We invite you to read, enjoy and be inspired by the work of researchers and industry partners who are redefining the realms of science and even the deployment of advanced technologies like supercomputers. ■

Sincerely,

Steven I. Gordon, Ph.D.
Interim Co-Executive Director
Senior Director, Education & Client Support

Ashok K. Krishnamurthy, Ph.D.
Interim Co-Executive Director
Senior Director, Research & Scientific Development

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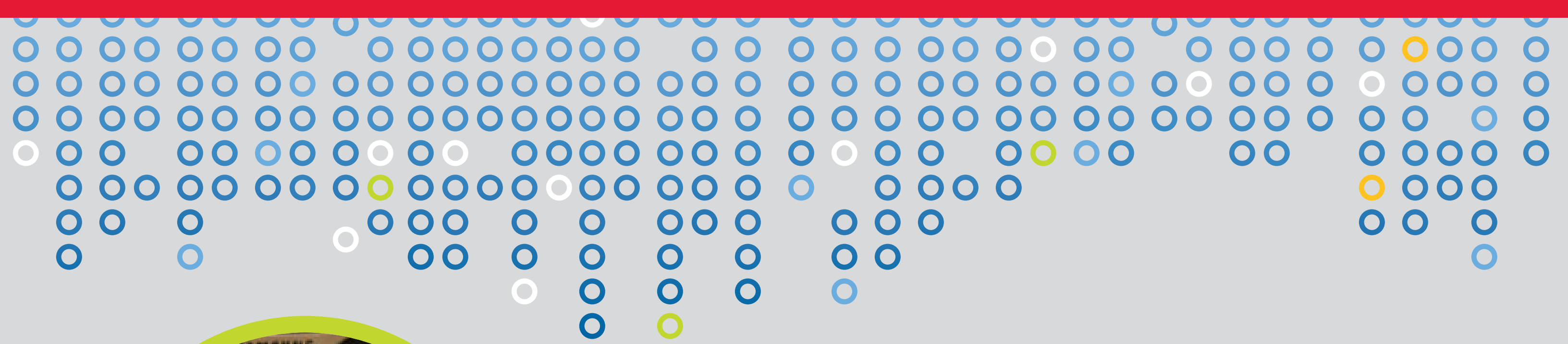
**Ohio Supercomputer Center 2010 Annual Research Report**
Published by OSC to present noteworthy research activities during the 2009–10 fiscal period.



# overview

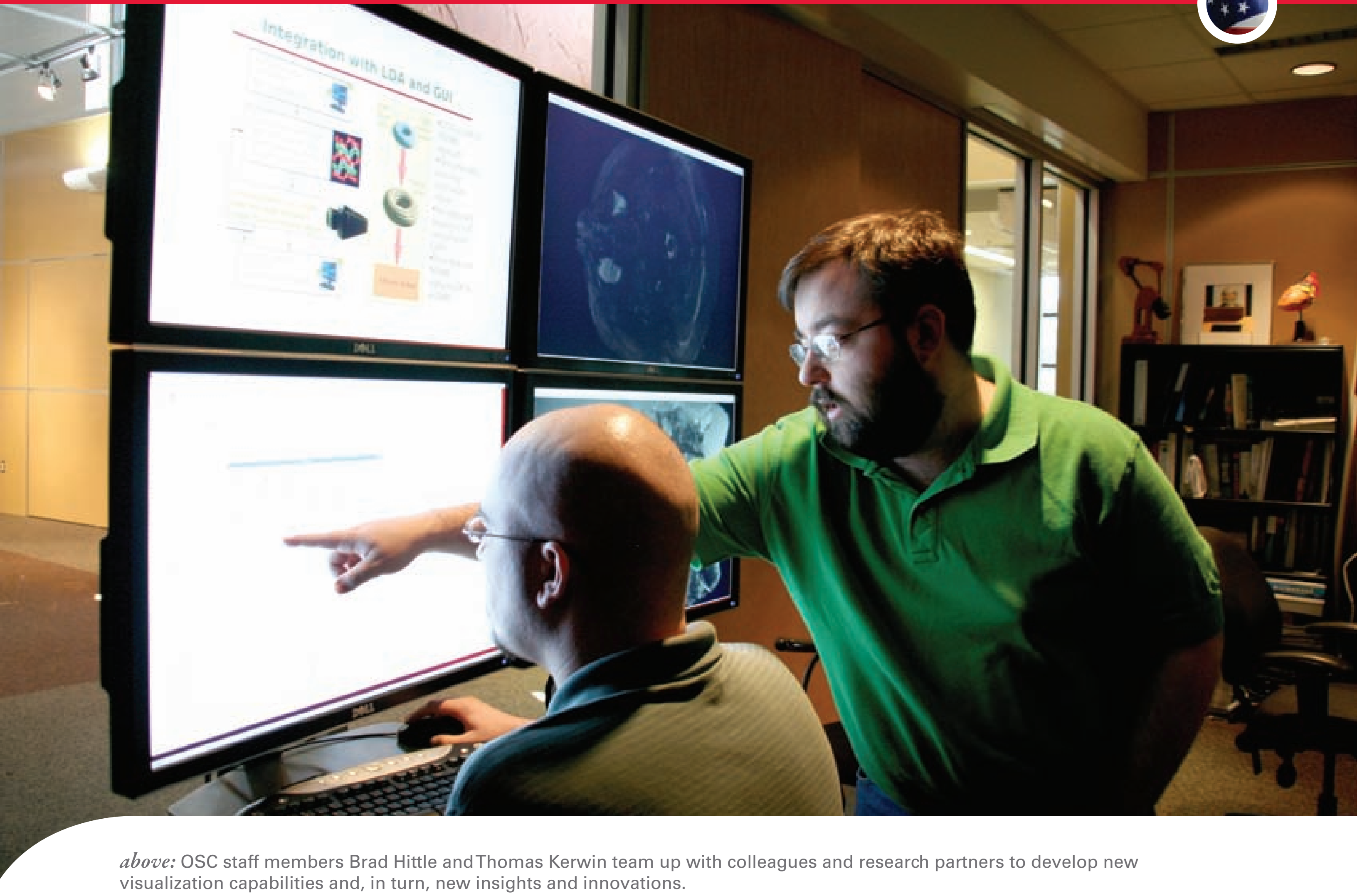
The Ohio Supercomputer Center (OSC) leverages significant investments made by the state to focus intently on our research end-users, developing the powerful tools and essential services needed to help guide scientific discoveries, classroom projects and commercial products to their culmination. OSC is renowned for demystifying the innovation process and finding novel and effective ways to exploit supercomputers for industry and academia, giving our researchers a competitive edge.

The Center effectively leverages its resources on a collaborative basis to procure significant extramural funding for a wide range of university and business collaborators in Ohio. OSC annual surveys of nearly two-dozen Ohio universities indicate that the faculty who use the Center's facilities receive more than $85 million in research funding. In addition to helping faculty win external funding, OSC helps Ohio colleges and universities attract and retain top-notch faculty and partner in new research program investments.

| | *OSC ROI* |
|---|---|
| OSC State Funds to External Funds for Ohio | 1:17 |

OSC's mission and strategic vision was strengthened in FY10 with input from its Governing Board, the Ohio Board of Regents and Center staff.

**Our vision** is to be a national center that drives research and development in computational science and the applications of supercomputing, and thus be a strategic transformative force behind Ohio's new economy: by empowering Ohio researchers to new innovations and discoveries that will lead to new products, businesses and services; by partnering with Ohio industries to use supercomputing and computational science as a competitive force; and, in collaboration with Ohio's colleges and universities, in educating Ohio's workforce in the key skills required for future jobs. The plan to realize our vision leverages the significant investments that have already been made by the Third Frontier Program. Specifically, the plan concentrates on the key areas of Advanced Materials, Biosciences and Energy & Environment and requires investments for additional technical capabilities, expertise to assist industrial clients, and staff to initiate new workforce training activities. In combination with existing programs across the state in these areas, these investments can be leveraged to position Ohio as the world leader, serving as an attractor for the brightest minds and most innovative firms to move to the state.




*above:* OSC staff members Brad Hittle and Thomas Kerwin team up with colleagues and research partners to develop new visualization capabilities and, in turn, new insights and innovations.

OSC strives to craft innovative, shared solutions for its academic and industry stakeholders. To that end, the Center's staff empowers and partners with researchers to extend their success nationally, as in the following examples:

- Staff members are working with Somnath Ghosh, Ph.D., in the Department of Mechanical Engineering at The Ohio State University (OSU) on his Teragrid Award to support development of a new multi-spatial, multi-time model for material fatigue failure.

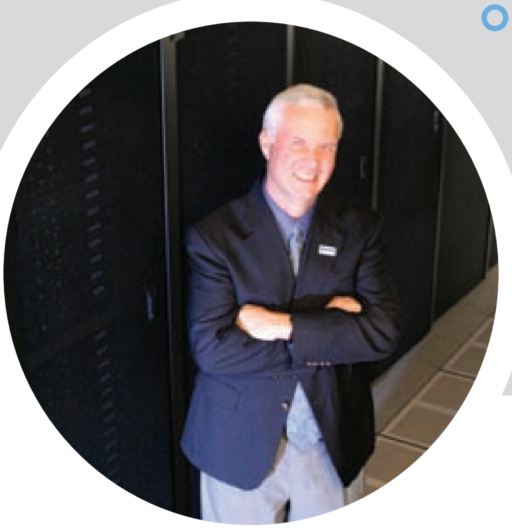
- Through our Instrumentation and Analytic Services (IAS), OSC provides new software solutions that empower researchers across institutions and disciplines to collaboratively share and use distributed instrumentation – such as electron microscopes, telescopes and spectrometers – that are expensive to buy and maintain. In addition diverse array of companies have taken advantage of the portals, shared remote instrumentation, application hosting and cycles offered by OSC through the Blue Collar Computing program.

- OSC is launching the ARMSTRONG Research Portal (A Research Management System for Training, Research Opportunities, Notices and Grants) to allow users to review system usage and track major allocations requests; post publications and grants; track customized grant opportunities; access training schedules and online tutorials; meet other OSC users to partner on research projects and grant proposals; and forge industry and academic partnerships.

OSC accomplishments for FY10 are highlighted in the following sections – hardware and software resources; visualization offerings; Blue Collar Computing; Ralph Regula School of Computational Science; and most importantly, vignettes of the innovations and discoveries achieved by researchers who take advantage of the Center's technological assets. ■

# hardware & software

*Like the innovators for whom they are named, these resources expand the research horizons for a multitude of scientific endeavors*



*above:* Kevin Wohlever, director of supercomputing operations

The Ohio Supercomputer Center offers researchers a diverse array of computer platform and software environments. The Center also provides the staff expertise to help port codes to specialized hardware configurations at OSC or national petascale centers, or to develop customized software or web portals for increased throughput on larger projects. In fact, OSC maintains more than 30 software applications and provides access to more than 70 different software packages in the areas of biosciences, computational fluid dynamics, structural mechanics and mesh generation, among others.

In August 2009, OSC more than doubled the capacity and memory of the Center's flagship IBM 1350 "Glenn" Cluster with the addition of a Biosciences Cluster. The expansion brings OSC's peak computational capabilities to 75 teraflops, boosting the machine's ranking to ninth among U.S. academic systems. The Center's capabilities were further enhanced in recent months with the addition of the robust "Csuri" Advanced GPU Visualization Environment. The deployment increased the Center's ability to serve advanced large-scale remote visualization and batch-rendering applications, as well as GPGPU and advanced visualization applications.

A prime example of recent GPU utilization involves the work of Umit Catalyurek, Ph.D., associate professor in The Ohio State University Department of Biomedical Informatics and Department of Electrical and Computer Engineering. Catalyurek accessed OSC's GPU nodes to develop a component-based runtime system for various biomedical image analyses and synthetic aperture radar image formations.

The benefits from the Csuri Advanced GPU environment also extend to the work of its namesake, Charles "Chuck" Csuri, the "father of computer graphics and animation," whose sophisticated digital art involves rendering of thousands of giant frames. Over the years, Csuri founded the Computer Graphics Research Group, the OSC Graphics Project and ACCAD, an OSU academic unit dedicated to the development of digital art and computer animation.

Other upgrades to hardware and software this past year include the addition of one petabyte of disk space to the mass storage system, as well as the following:

- **Virtual Machine Images for HPC users** – OSC VMs can share storage with OSC compute clusters in order to support production computing requests, specialized software, different operating system requirements (such as Microsoft Windows) and dedicated program development environments.
- **Core Server Infrastructure Improvements** – OSC upgraded its core system servers and streamlined administration, making the servers easier to support, expand, replace and upgrade, while reinforcing security.
- **Tivoli Storage Manager Upgrades** – Along with server upgrades, the TSM upgrade provides faster service and positions OSC to support future functionality for user home directory back up, project space and key support directories. ■


*above:* OSC's IBM 1350 Glenn Cluster, including the Csuri Advanced GPU Visualization Environment

# visualization

*"A picture is worth thousand words" – with OSC's assistance, researchers are able to visualize the results of their computation, leading to "aha" moments.*

As advanced simulations integrate progressively larger computational data sets from multiple sources, staff members of the Ohio Supercomputer Center (OSC) create intuitive methodologies to integrate these vast caches of multisensory data into a single coherent visualization that can facilitate a researcher's explorations and interactions.

To optimize the use of the Csuri GPU expansion recently installed at OSC, the Center has expanded support for the biosciences, among other modeling and simulation applications:

- **GPU Support** – OSC provides expertise and training in code optimization using CUDA™, a GPU-programming toolkit developed by NVIDIA™.
- **Remote Visualization** – OSC is actively developing remote rendering to a thin-client environment on office or lab laptops and even hand-held devices. A volume visualization application for the Small Animal Imaging Shared Resource at The Ohio State University's Comprehensive Cancer Center, in collaboration with Dr. Kimerly Powell, provides rapid dissemination of imaging results and precludes the need to transfer large data. By maintaining more standardized repositories near HPC facilities, more aggressive and complex analysis can be performed.
- **Extremely Large-Scale Rendering** – As imaging requires increasingly larger data sets at multiple scales, users are limited in efficient data handling and analysis. OSC has implemented a hierarchical volume renderer using OpenCL that is capable of handling large-scale data sets, including those that are larger than the video memory on graphics cards.

Funded projects in the biosciences include:

- **Virtual Simulation of Mouse Anatomy and Procedural Techniques** – With the OSU Center for Clinical Translational Science, OSC is creating and evaluating an interactive, 3-D volumetric atlas of a mouse anatomy that will be available on-demand for a low-cost desktop environment. The simulation will raise complex anatomy comprehension and proficiencies in procedural techniques, while limiting the need for expensive materials. The system increases model variance, promotes continuous assessment of knowledge and skills and leads to the use of "true standards" for evaluation of animal models proficiencies.
- **Virtual Reality Simulator for Canine Arthroscopy Training** – In collaboration with the OSU College of Veterinary Medicine, OSC is helping to develop and evaluate a virtual reality simulator for teaching canine arthroscopy. High-resolution digital models of the canine stifle joint will be generated by micro-computed tomography and magnetic resonance imaging. OSC's Interface Laboratory provides an integrated environment that include dexterous devices to precisely localize and track 3-D interactions with complex data, such as user movement, morphometrics and haptic (force reflecting) interaction. ■

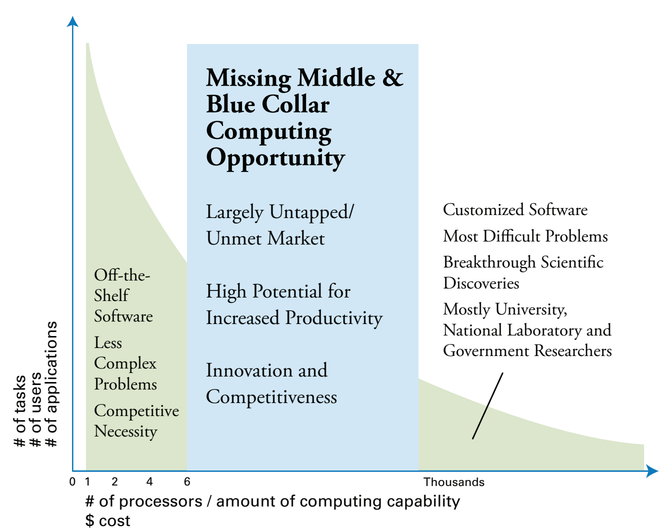
# blue collar computing

Advanced modeling, simulation and analytics is a transformative set of technologies that can impact all aspects of a business enterprise. These new technologies are used to benchmark and enhance product design, safety and performance using virtual engineering and testing that replace costly and time-consuming physical processes. They also can help to optimize plant and facility design, and promote efficiency and utilization, while reducing waste.

OSC's Blue Collar Computing™ (BCC) program represents one of the nation's first formal industrial outreach initiatives dedicated to advanced modeling, simulation and analytics. Introduced in 2004, the BCC program offers industrial clients the advanced modeling and simulation resources, training and expertise they need to compete in a global economy. To date, more than 30 companies and organizations have taken advantage of the portals, application hosting and computation offered by OSC.

BCC offers large-systems access to experienced industrial users who need peak performance for specific tasks and industry-specific web portals for users new to advanced computation. For example, the Edison Welding Institute WeldPredictor™ portal, a web-based interface created by OSC and EWI, is now offered as a free service to more than 2,800 EWI members. Information entered and retrieved from the site allows welding engineers to simulate "virtual" welds, reducing the time and material wasted with physical prototypes.


*above:* OSC's Ashok Krishnamurthy meets with representatives of Korea Institute of Science and Technology Information (KISTI), cementing a productive alliance that includes jointly developing innovative tools, web portals and expertise on open-source software deployment to industrial clients.



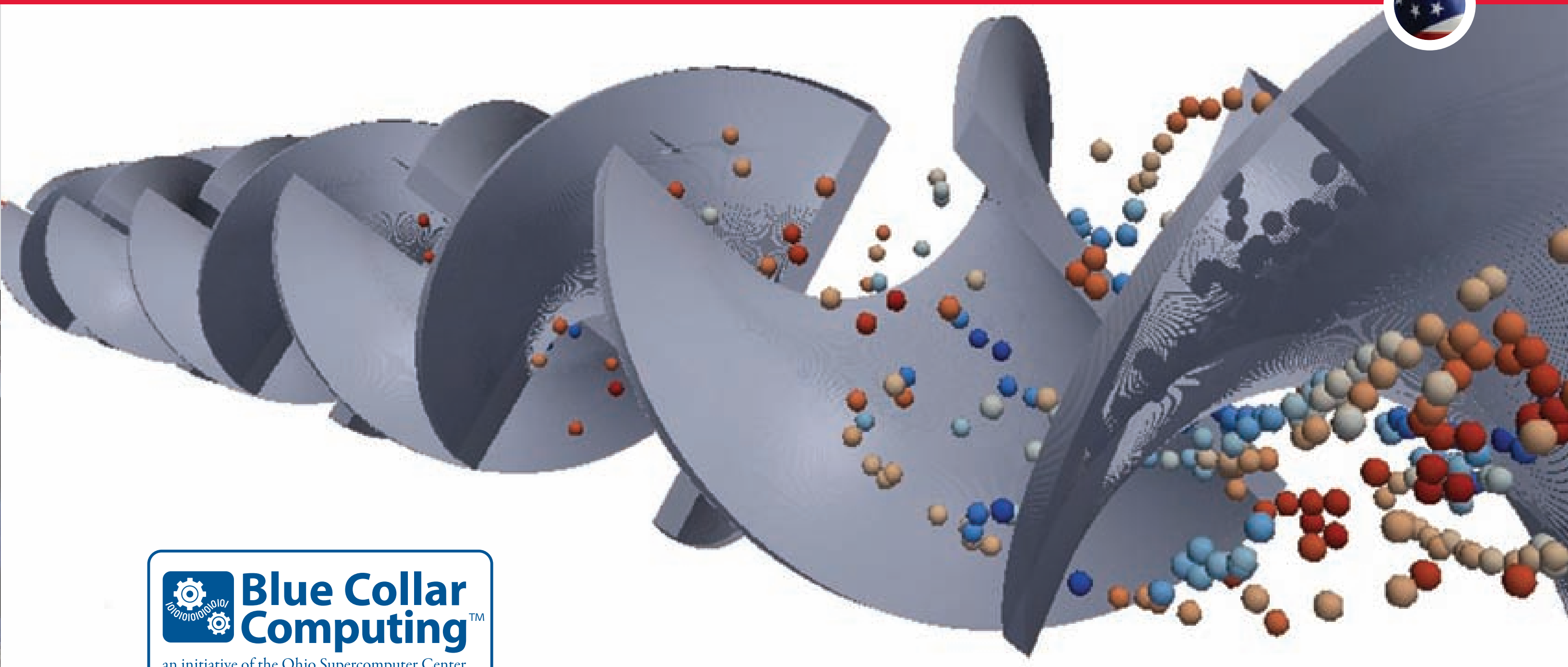

There is a fundamental gap between high-end and low-end computing usage, which is creating a drag in productivity, innovation and competitiveness.

## The "Missing Middle"

The term "missing middle" describes the large groups of industry users who do not have access to advanced modeling, simulation and analysis resources essential to their business survival. Since the Blue Collar Computing's inception in 2004, OSC has targeted this segment in its industrial outreach efforts.

While discovery-level advanced modeling, simulation and analysis tools have been used with great success by some large industries, many small- and medium-sized companies have not advanced beyond using entry-level computational systems. The gap between these two extremes, the missing middle, represents an enormous productivity opportunity for the nation. Many of these companies are desktop users who may develop simple models, at best, relying instead on traditional experimentation methods to build prototypes.

The missing middle represents an important opportunity to bolster U.S. economic competitiveness. Through advanced modeling, simulation and analysis or digital manufacturing, public and private collaborations, and federal support, this "HPC Gap" can be filled for greater productivity.



Blue Collar Computing™
an initiative of the Ohio Supercomputer Center

*above:* Sciences Computers Consultants use OSC's high performance computing systems to model and analyze particle dispersion of the Kenics© static Mixer with XimeX® software

In addition to its portals with EWI and PolymerOhio, the Center has worked hard to forge relationships with industry integrators and international companies to further extend its applications, training and services:

- OSC's agreement with the Korea Institute of Science and Technology Information (KISTI) cements a productive alliance that includes jointly developing innovative tools, web portals and expertise on open-source software deployment to industrial clients.
- As an extension of its partnership with PolymerOhio, OSC signed a memorandum of understanding with Taiwan's Cortex that will include donations of educational engineering simulation software licenses to demonstrate the performance of the firm's 3-D part/mold simulations for industry certificate use.
- In exchange for adding Sciences Computers Consultants' XimeX software to OSC's systems for scalability testing and small pilot projects, OSC has provided the French company with resources to test and scale advanced modeling and simulation software for polymer extrusion and mixing on its supercomputers with the intent of developing advanced web portals.
- Building on an earlier collaboration under a Defense Advanced Research Projects Agency contract to create real-time modeling solutions for military suppliers, Nimbis Services and OSC will provide a strategic regional customer supply-chain incubator and domain-specific web portals to serve underserved markets, coined the "HPC Gap" or "Missing Middle," where large groups of industry users have not had access to advanced computational resources.
- Building off of a successful Ohio Third Frontier award, OSC received a National Science Foundation EAGER grant to work with Fireline TCON Inc., a ceramics manufacturer, and the Center for Excellence in Advanced Materials Analysis at Youngstown State University to integrate advanced modeling and simulations into the company's processes to boost its productivity.

*"Modeling, simulation, and massive data analysis are the next huge game-changing drivers for innovation"*

*— Deborah Wince Smith, President, Council on Competitiveness*

OSC has been collaborating with industry consortia to leverage its digital manufacturing advances in the national arena. OSC and PolymerOhio received a National Institute of Standards and Technology (NIST) competitive award to build a national model from integrating computation resources into the Ohio Manufacturing Extension Partnership (MEP) system. OSC is also a member of the Alliance for High Performance Digital Manufacturing (AHPDM), supporting small- and medium-sized enterprises (SMEs) by promoting the development of a national digital manufacturing strategy and an innovation network and the Council on Competitiveness HPC Users Group that supports the need to make American manufacturing more competitive through increased use of modeling, simulation and analytics. ■

*above:* 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.

# The Ralph Regula School of Computational Science

A national leader in computational science education, the Ralph Regula School of Computational Science features collaborations and programs that take advantage of Ohio's geographically distributed centers of expertise to propel the entire state's workforce to a new level of skill and productivity.

Featured as an academic program of the future in the August 2009 edition of *The Chronicle of Higher Education*, the statewide virtual school has extended its undergraduate minor program to 13 campuses, and its associate of science concentration program has taken root at three community colleges. The Ralph Regula School is a collaborative program of the Ohio Supercomputer Center (OSC), the Ohio Board of Regents and Ohio Learning Network.

The computational science minor is a multi-institutional, interdisciplinary undergraduate program that enables science and engineering majors to apply computational tools directly to their area of study. Participating institutions instruct students on modeling and simulation applications to solve real-world problems in a wide range of fields, including medicine, engineering, mathematics and physical sciences. An associate of science degree program began in Autumn 2009. Students learn about the role of modeling and simulation in science and basic approaches to modeling needed by advanced manufacturing and research firms.

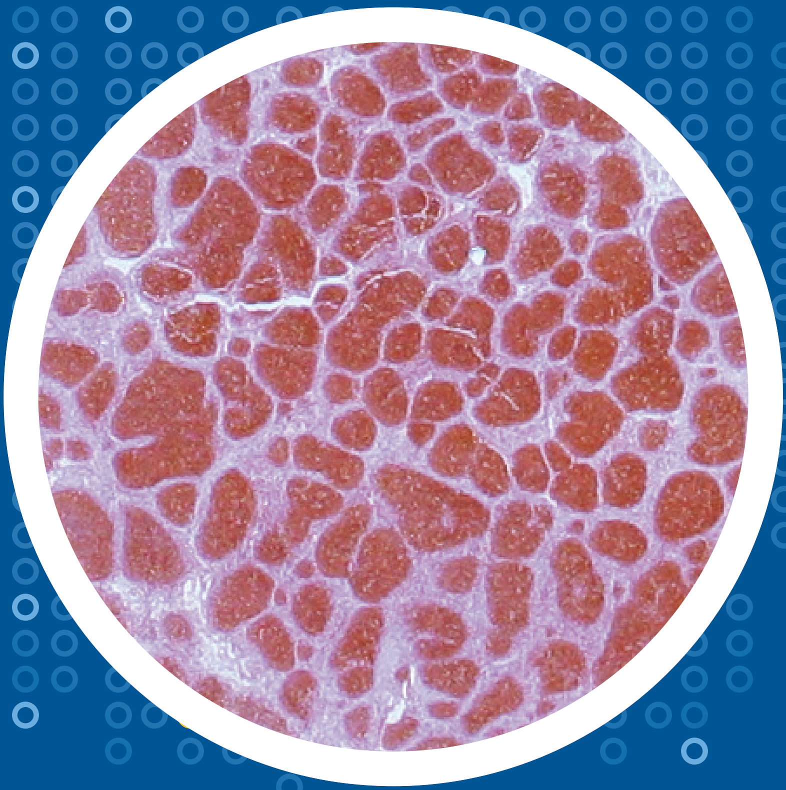
The Ralph Regula School also provides workforce training and certification in computational science and supplies computational access for businesses that currently lack the expertise or capacity to leverage these applications to improve their global competitiveness.

*Both academia and industry require people with adequate skills to apply computational science to challenging science and engineering problems*

*— Steve Gordon, Ph.D., director of the Ralph Regula School of Computational Science*

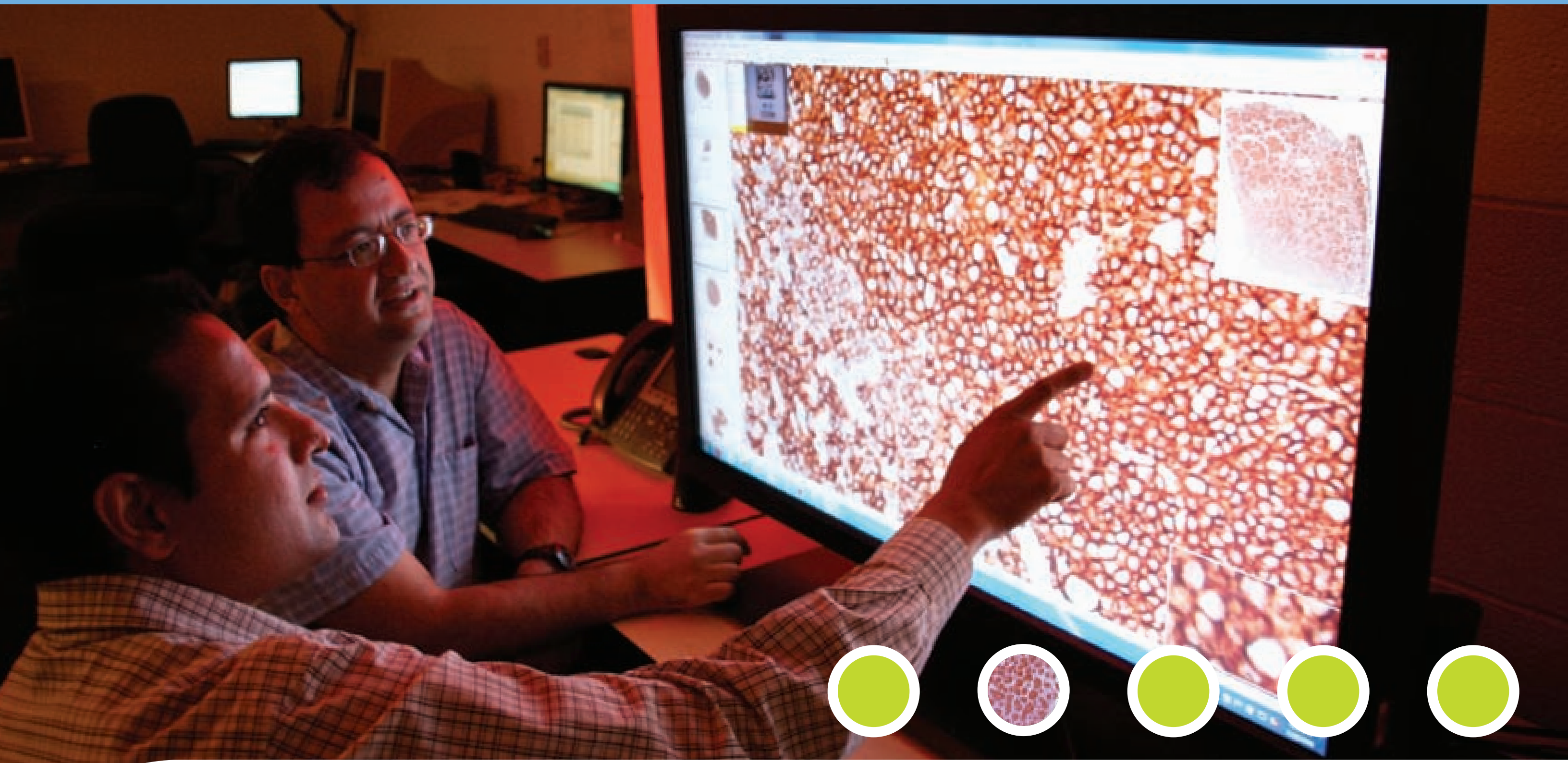
The first of several "stackable" certificates for manufacturing is offered at Sinclair Community College and Columbus State Community College, with an advanced certificate available in polymer manufacturing sponsored by The Ohio State University and the University of Akron. Working with PolymerOhio and Moldex3D, the polymer classes focus on the use of simulations in injection molding and structure-property relations in polymer systems. The School also is working with the National Association of Manufacturers on a second advanced certificate program in metal stamping. In addition, OSC instructors provide training to faculty and student researchers through scientific computing workshops, one-on-one classes, and web-based portal training.

The Ralph Regula School coordinates several K-12 outreach programs, as well. Summer Institute provides high school students the opportunity to apply modeling and visualization to research problems, while the Young Women's Summer Institute offers an environmental project-based STEM program to middle-school girls. OSC hosts student research interns from nearby Metro High School, a collaboration between Battelle, The Ohio State University and the Franklin County Education Council. And, finally, the Center serves as the OSU lead on the Ohio Board of Regents' Choose Ohio First Scholarship program for the Ohio Bioinformatics Consortium, sponsoring 12 bioinformatics students this past year. ■



# 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, oncology researchers are developing computational techniques to enhance the diagnosis of follicular lymphoma. A biomolecular engineer is generating complex computer simulations to better understand how misfolded proteins contribute to Alzheimer's disease. And, a pediatric hospital is leveraging advanced computational and storage resources to analyze data generated by their next-generation DNA sequencing machine. In addition to health care, the application of bioscience to energy, industrial products and agriculture is growing in importance. More than 1,250 bioscience-related organizations in Ohio employ over 55,000 highly-skilled workers, 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 powerful computational resources of the Ohio Supercomputer Center. ■



*above:* Metin Gurcan discusses a feature Siddharth Samsi has found on a digitized slide specimen being examined for indications of Follicular Lymphoma. Their Ohio State University Medical Center research group has been leveraging Ohio Supercomputer Center resources to develop a computer-assisted diagnosis tool to improve grading of the common, slow-growing cancer.

# Designing computer-aided analysis for Lymphoma

Follicular Lymphoma (FL) is one of the most common forms of non-Hodgkin Lymphoma occurring in the United States. FL is a slow-growing cancer of the human lymph system that usually spreads into the blood, bone marrow and, eventually, internal organs. A World Health Organization pathological grading system is applied to a biopsy sample; doctors usually avoid prescribing severe therapies for lower grades, while they usually recommend radiation and chemotherapy regimens for more aggressive grades.

Accurate grading of the pathological samples generally leads to a promising prognosis, but diagnosis depends solely upon a labor-intensive process that can be affected by human factors such as fatigue, reader variation and bias. Pathologists must visually examine and grade the specimens through high-powered microscopes. Now, computer-assisted diagnosis tools are being developed to provide pathologists with higher throughput of specimen analyses and, ultimately, quicker, accurate diagnoses.

"The advent of digital whole-slide scanners in recent years has spurred a revolution in imaging technology for histopathology," according to Metin N. Gurcan, Ph.D., an assistant professor of biomedical informatics at The Ohio State University Medical Center. "The large multi-gigapixel images produced by these scanners contain a wealth of information potentially useful for computer-assisted disease diagnosis, grading and prognosis."

Processing and analysis of such high-resolution images, Gurcan points out, remain non-trivial tasks, not just because of the sheer size of the images but also due to complexities of underlying factors involving differences in staining, illumination, instrumentation and goals. To overcome many of these obstacles to automation, Gurcan and medical center colleagues, Dr. Gerard Lozanski and Dr. Arwa Shana'ah, turned to the Ohio Supercomputer Center. Ashok Krishnamurthy, Ph.D., interim co-executive director of the center, and Siddharth Samsi, a computational science researcher there and an OSU graduate student in Electrical and Computer Engineering, put the power of a supercomputer behind the process.

"Our group has been developing tools for grading of follicular lymphoma with promising results," said Samsi. "We developed a new automated method for detecting lymph follicles using stained tissue by analyzing the morphological and textural features of the images, mimicking the process that a human expert might use to identify follicle regions. Using these results, we developed models to describe tissue histology for classification of FL grades."

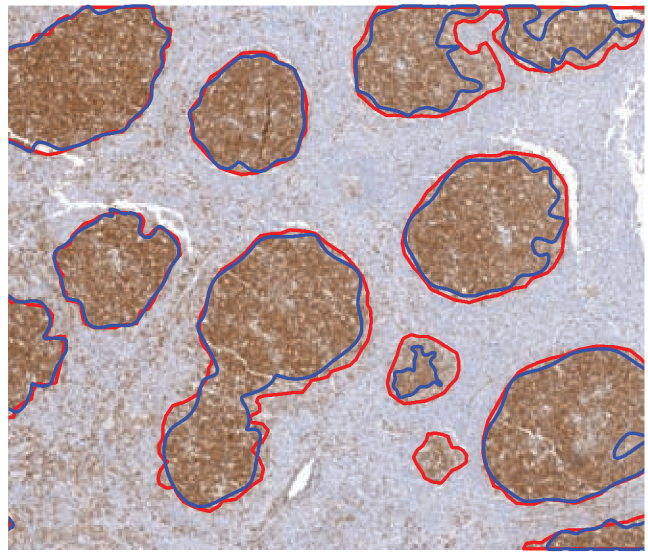
Histological grading of FL is based on the number of large malignant cells counted in within tissue samples measuring just 0.159 square millimeters and taken from ten different locations. Based on these findings, FL is assigned to one of three increasing grades of malignancy: Grade I (0-5 cells), Grade II (6-15 cells) and Grade III (more than 15 cells).

"The first step involves identifying potentially malignant regions by combining color and texture features," Samsi explained. "The second step applies an iterative watershed algorithm to separate merged regions and the final step involves eliminating false positives."

The large data sizes and complexity of the algorithms led Gurcan and Samsi to leverage the parallel computing resources of OSC's Glenn Cluster in order to reduce the time required to process the images. They used MATLAB® and the Parallel Computing Toolbox™ to achieve significant speed-ups.

Speed is the goal of the research project, but accuracy is essential. Gurcan and Samsi compared their computer segmentation results with manual segmentation and found an average similarity score of 87.11 percent.

"This algorithm is the first crucial step in a computer-aided grading system for Follicular Lymphoma," Gurcan said. "By identifying all the follicles in a digitized image, we can use the entire tissue section for grading of the disease, thus providing experts with another tool that can help improve the accuracy and speed of the diagnosis." ■



*above:* Advances in scanning technology allow researchers to automate the identification of potentially malignant regions (red boundaries) in tissue samples. The computer-aided process delivers very accurate, highly consistent results in much less time than identifications made by a trained pathologist (blue boundaries).

**Project lead:** Metin N. Gurcan, The Ohio State University
**Research title:** Computer-aided analysis of immunohistochemical slides of follicular lymphoma
**Funding source:** National Cancer Institute

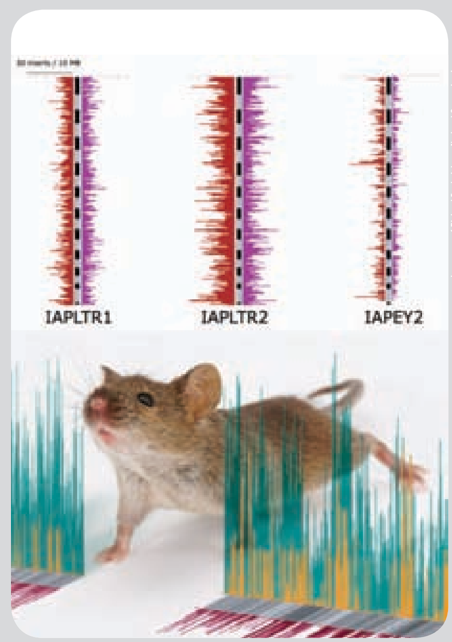
# Modeling retrotransposons' role in cancer

Recently, large-scale sequencing projects have described the complete DNA blueprints for humans, the mouse and other organisms. This work highlighted the surprising fact that almost half of all mammalian DNA genomes is made up of mobile genetic elements called retrotransposons. These virus-like retrotransposons, sometimes called "jumping genes," can move from one chromosomal location to another, causing variation between individuals or lineages and occasional genetic disruptions resulting in diseases including cancers.

The controls and consequences of movement by these mobile elements are a focus of research for David Symer, M.D., Ph.D., and Keiko Akagi, Ph.D., in the Department of Molecular Virology, Immunology and Medical Genetics and the Human Cancer Genetics Program at The Ohio State University Comprehensive Cancer Center.

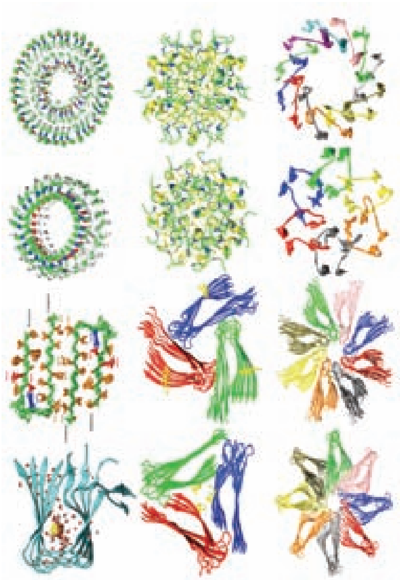
Symer and Akagi access OSC's Glenn Cluster to run various genomic alignment programs to align hundreds of millions of short sequence genomic traces – massive datasets generated from previously unsequenced individuals or cells – against the enormous reference genome assemblies for human, mouse and other organisms. They also utilize RepeatMasker and other data-intensive bioinformatics programs.

"Our long-term goal is to understand the biological and evolutionary roles played by transposons. These 'jumping genes' are major drivers of genomic variation. They can affect gene expression and structure, chromatinization and chromosomal structures," said Symer. "We'd like to exploit practical applications of this new knowledge, to improve diagnosis and treatment of human cancers and other diseases, and by modeling such processes in other organisms." ■




artwork courtesy of Richard Frederickson, National Cancer Institute

**Project lead:** David E. Symer, The Ohio State University
**Research title:** Identification and analysis of genomic polymorphisms that distinguish mouse and human lineages and populations
**Funding sources:** National Cancer Institute (National Institutes of Health); The Ohio State University



*above:* Using computer simulations, Jie Zheng can predict and validate several molecular models of Aβ oligomers to bettter understand how they are formed and accumulate in Alzheimer's disease.

# Simulating misfolded proteins in Alzheimer's

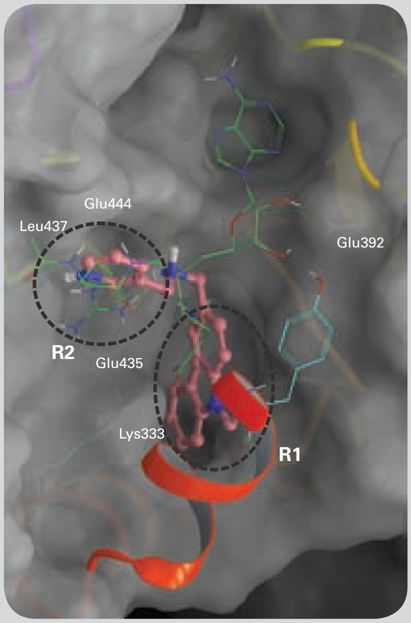
Alzheimer's disease is the most common human neurodegenerative disorder, affecting as many as 5.1 million people in America alone. Alzheimer's leads to progressive and irreversible memory loss, disability and, eventually, death through a complex series of events that take place in the brain over a period of many years.

In the nucleus of nearly every human cell, long strands of DNA are packed tightly together to form chromosomes. To deliver these instructions to various other cellular structures, the chromosomes dispatch very small protein fibers – called oligomers – that fold into three-dimensional shapes. Misfolded proteins – called amyloid fibrils – cannot function properly and tend to accumulate into tangles and clumps of waxy plaque, robbing brain cells of their ability to operate and communicate with each other.

"The exact mechanism of amyloid formation and the origin of its toxicity are not fully understood, primarily due to a lack of sufficient atomic-level structural information from traditional experimental approaches," explained Jie Zheng, Ph.D., an assistant professor of chemical and biomolecular engineering at the University of Akron. "Molecular simulations, in contrast, allow one to study the three-dimensional structure and its kinetic pathway of amyloid oligomers at full atomic resolution."

Zheng's research group is leveraging the computational muscle of the IBM Cluster 1350 system at the Ohio Supercomputer Center to develop a multiscale modeling and simulation platform that aims to establish a direct correlation between the formation of oligomers and their biological activity in cell membranes. ■

**Project lead:** Jie Zheng, University of Akron
**Research title:** Exploring kinetics and structures of Alzheimer's amyloid ß-protein formation
**Funding source:** National Science Foundation




*above:* Chenglong Li is creating complex molecular dynamics simulations involving the PRMT5 enzyme to help discover a drug that will allow the human body to better suppress invasive brain tumors.

# Discovering drugs for cancer therapies

Chenglong Li, Ph.D., an assistant professor in the College of Pharmacy at The Ohio State University, is using computational chemistry to help develop a genetically targeted drug that could surpass current approaches to treating a type of aggressive brain tumor called glioblastoma multiforme (GBM).

The survival outcome of patients diagnosed with a GBM is relatively poor and has improved only marginally over several decades. Combinations of surgery, radiation and chemotherapy remain the most common therapy, yet surgeons often can't completely remove the tumors without causing serious damage, radiation is rarely effective and chemotherapy usually produces serious side effects.

"My group has been conducting molecular dynamics simulations of the PRMT5 enzyme to gain insights on its catalytic mechanisms," said Li. "We then conduct virtual screenings of more than 100,000 pharmaceutical compounds to identify drugs that prevent that enzyme from blocking the body's cancer suppression genes. This novel approach is called epigenetic cancer therapy, where molecular compounds 'reawaken' natural human tumor-fighting genes that stay dormant in many types of cancers."

Kiran Mahasenan, a graduate student on Li's research team, developed molecular models using the IBM Cluster 1350 system at the Ohio Supercomputer Center, which the team also used to screen drug candidates. Once the most promising drug candidates are identified, the data is passed along to Dr. Robert A. Baiocchi, an oncologist at The James Comprehensive Cancer Center, who conducts clinical tests to evaluate the effectiveness, toxicity and dosage of each drug. ■

**Project lead:** Chenglong Li, The Ohio State University
**Research title:** Pursuing drugs to 'reawaken' nature's cancer-fighting genes
**Funding source:** National Institutes of Health, The Ohio State University College of Pharmacy

# Implementing DNA sequencing technology

The first human genome took 15 years and about $3 billion to complete. Soon, doctors at The Research Institute at Nationwide Children's Hospital will be able to sequence two human genomes in just over one week for a fraction of that cost. The institute's recent acquisition of a next-generation HiSeq 2000 sequencing system supports whole-genome DNA sequencing analysis, transcriptome and epigenome analysis, along with multiple other genomic applications.

"We are among the first laboratories in the nation to establish this new instrumentation," said Dr. Peter White, director of the insitute's Biomedical Genomics Core. "This will allow us to enhance the health of children by continuing to expand our programs in areas of strategic emphasis, namely, perinatal research, infectious diseases, congenital and acquired heart conditions, digestive diseases and childhood cancer. Access to this instrument will be particularly helpful for young investigators, postdoctoral research scientists, physician scientists and clinical fellows."

In support, the Ohio Supercomputer Center (OSC) provides additional mass storage for the sequencer's immense data needs. Each eight-day run requires the computational power to align 2,000,000,000 x 100 base-pair reads, using six terabytes of disk space and 600 gigabytes of storage space, plus two additional terabytes if the raw input data is retained.

"OSC also will provide computational backup for local pipeline analysis and resources for more advanced analysis of the datasets that require multi-node support," added Don Stredney, senior research scientist for biomedical applications and director of OSC's Interface Lab. ■

*above:* The computational power and storage capacity of the Ohio Supercomputer Center support the implementation of a cutting-edge HiSeq 2000 sequencing system by Peter White at The Research Institute at Nationwide Children's Hospital.

**Project lead:** Peter White, Nationwide Children's Hospital
**Research title:** Establishing next-generation sequencing technology at Nationwide Children's Hospital
**Funding source:** National Institutes of Health, American Recovery and Reinvestment Act

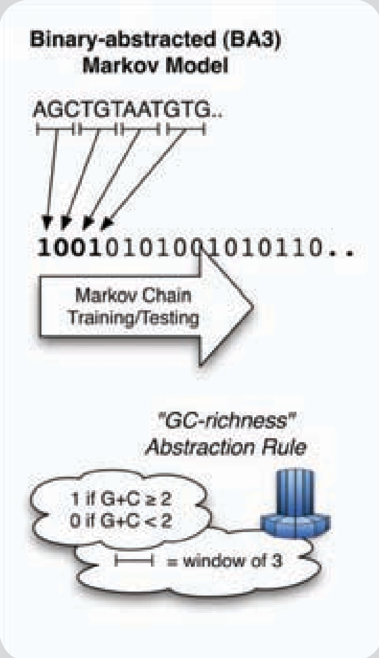
# Creating new genomic sequence predictions

Samuel Shepard, Ph.D., a researcher in the University of Toledo bioinformatics lab of Associate Professor Alexei Fedorov, recently developed an algorithm for the prediction of certain genomic sequences, known as exons and introns, using mid-range sequences of 20-50 nucleotides in length. These genomic patterns are said to display a non-random clustering of bases referred to as "mid-range inhomogeneity," or MRI. Shepard hypothesized that the MRI patterns were different for exons and introns and would serve as a reliable predictor.

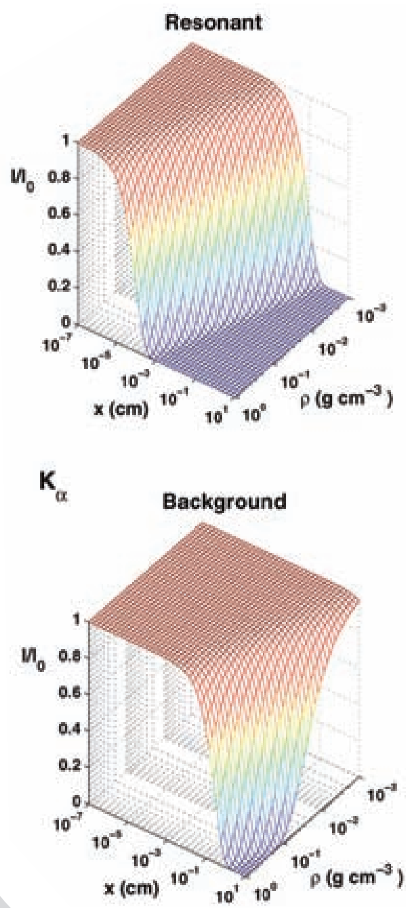
"We based our approach on Markov chain models, which are the basis for many gene prediction programs," Shepard explained. "During the project, our algorithm read 12 million nucleotides of exons and introns each, and three million each were used to test the predictions."

To circumvent the limitations of traditional Markov models, Shepard developed a technique known as binary-abstracted Markov modeling (BAMM). The procedure reduces mountains of nucleotide information into a much smaller binary code. Shepard tested abstraction rules for sequences of one or two nucleotides locally, but as larger sequences were studied, the possible abstraction outcomes increased exponentially.

Requiring far more computational horsepower, Shepard and his colleagues accessed the Ohio Supercomputer Center's Glenn Cluster to optimize the abstraction process by using "hill-climbing" techniques that determine a single, maximal value for each abstraction space, rather than each of its possible values. Shepard and his team then combined different abstraction models to achieve an exon-intron prediction accuracy of greater than 95 percent. ■




**Project lead:** Samuel S. Shepard, University of Toledo
**Research title:** The characterization and utilization of middle-range sequence patterns within the human genome
**Funding source:** National Science Foundation




# Applying high-end X-rays to cancer treatment

Two Ohio State University astronomy researchers have established an international reputation for using X-rays and supercomputers to search the vast depths of space to identify elusive black holes. Now, they and their interdisciplinary colleagues are repositioning their scientific methodology to peer into the human body to enhance cancer therapy and diagnostics (theranostics).

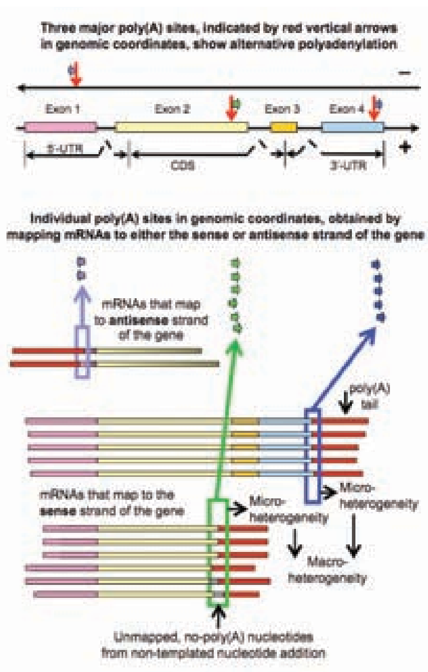
Led by OSU's Anil Pradhan, Ph.D., and Sultana Nahar, Ph.D., an international research team is using new computer-based models and high-end X-ray spectroscopy to minimize radiation risks and enhance therapeutic efficiency for cancer patients. The X-ray irradiation process causes embedded nanoparticles of iron, gold and other heavy elements to release photons and low-energy electrons to help break up the DNA in malignant tumors. The researchers are also experimenting with bromine, iodine and platinum, which are active elements in radiological contrast agents used for imaging.

"The resonant nano-plasma theranostics or RNPT could revolutionize X-ray diagnostics and therapy," Pradhan told the science magazine *Nature*. The RNPT approach would reduce radiation exposure by factors from 10 to 100, he added.

The research team accesses the IBM Cluster 1350 system at the Ohio Supercomputer Center for their modeling needs, as well as for their astrophysics research. In their study of invisible black holes, researchers collect telltale radiation readings from a plasma sea of super-hot atoms, using satellites and large telescopes. Pradhan, Nahar and their team leveraged OSC resources to perform high-accuracy energy calculations to compare with the radiation readings. ■

**Project lead:** Anil Pradhan and Sultana Nahar, The Ohio State University
**Research title:** Nanospectroscopy for nanomaterials and nanobiomedicine
**Funding source:** The Ohio State University

# Calculating disparity in RNA polyadenylation




When eukaryotic genes are expressed, precursor messenger RNA (pre-mRNA) must first be processed to become mature mRNA. One step of the maturation process is constitutive polyadenylation: the attachment of a poly(A) tail to mark and protect the end of mRNA. However, alternative polyadenylation at a different poly(A) sites on the pre-mRNA might result in information loss and sometimes can cause cancers and other diseases in humans.

A Miami University research team led by Chun Liang, Ph.D., is investigating potential regulatory mechanisms controlling alternative and constitutive polyadenylation within eight different species – two diatoms, two green algae, spikemoss, moss, Arabidopsis and human.

"It has been shown that polyadenylation is guided by regulatory elements, or motifs, known as the poly(A) signals," said Liang, an assistant professor in bioinformatics. "The process is carried out by the protein complex that recognizes and binds to those motifs, cleaves the mRNA and conducts polyadenylation."

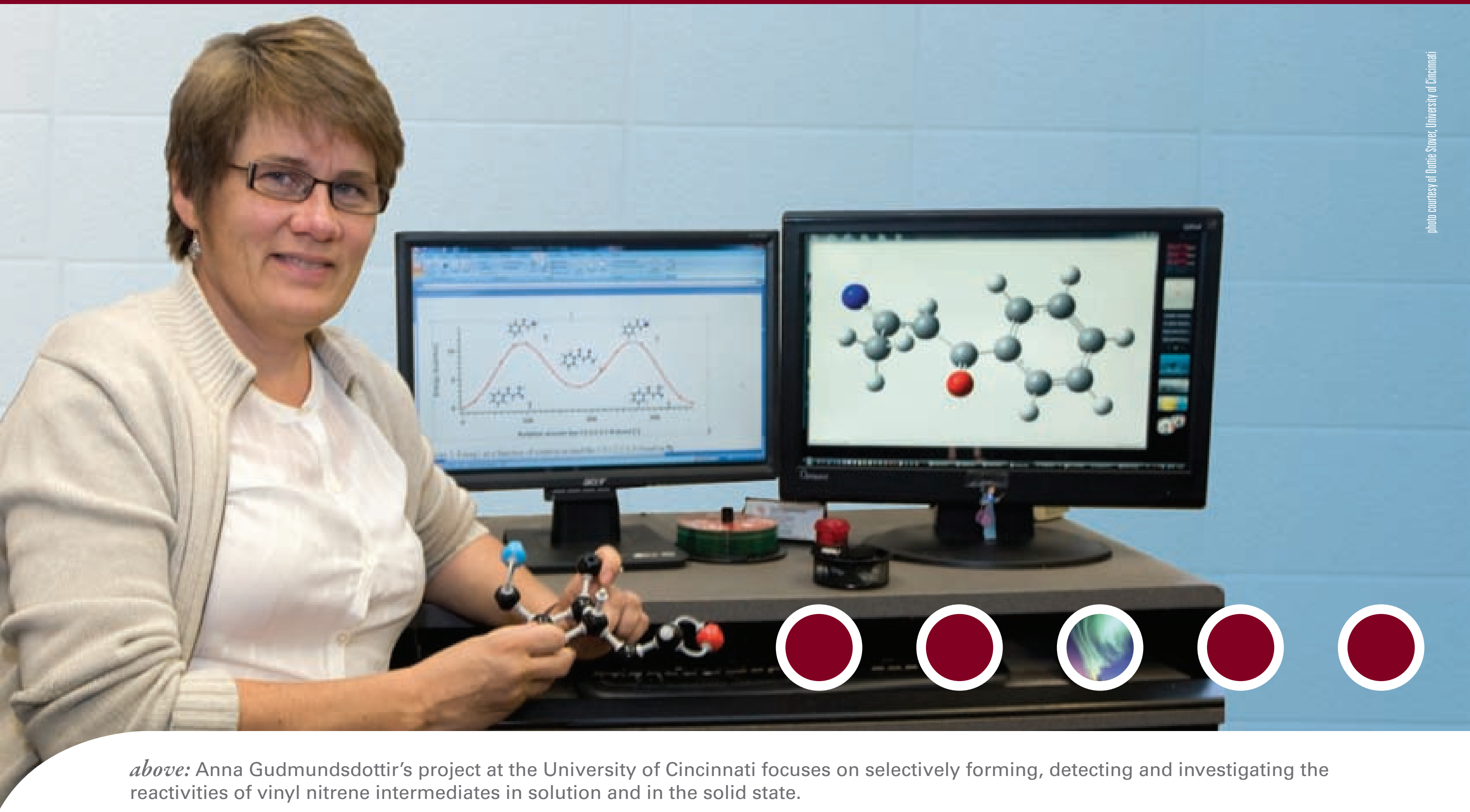
Classical genetic analysis and recent genome-wide bioinformatics analysis suggest that there are three typical regulatory elements in plants: a cleavage element, a near-upstream element and a far-upstream element.

"Using the powerful bioinformatics software package MEME (Multiple EM for Motif Elicitation), we are searching for over-represented sequence motifs from each of the regions," Liang explained. "Our preliminary data analysis reveals interesting differences among different species, but the real challenge is that we have to process a large amount of data to detect significant/meaningful patterns, while processing a large amount of data demands more computational resources." ■

**Project lead:** Chun Liang, Miami University
**Research title:** Comparative analysis of polyadenylation signals in eukaryotes
**Funding source:** Miami University

# advanced materials

Researchers and scientists in Ohio are developing exciting new classes of materials with unusual properties. Their ground-breaking 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 chemist seeks a delicate balance of compounds to create a new class of magnets that could lead to a new ways to monitor medical implants. Other researchers are unlocking the properties of a new material that could replace silicon in the computer chip industry. And, another scientist is investigating "metamaterials" that could make cloaking devices a reality. 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:* Anna Gudmundsdottir's project at the University of Cincinnati focuses on selectively forming, detecting and investigating the reactivities of vinyl nitrene intermediates in solution and in the solid state.

# Creating organic magnets from elusive compounds

Fundamental research in chemistry has laid the foundations for the discovery and design of new materials with fascinating magnetic, electrical and optical properties, prompting inventions anywhere from faster computers to lighter long-range planes.

Humans have known of magnetism for 2,500 years, finding simple magnets made from lodestone and observing the colorful aurorae in the skies of the northern and southern hemispheres. For the last thousand years, people have made use of magnetic materials in various ways: a Chinese scientist wrote in the 11th century of using a compass to improve navigation, and the concept of electromagnetism was developed in the 19th century. Today, magnets are found everywhere: credit cards, audio speakers, motors, medical imaging machines and more.

Currently, commercial magnets are based mainly on transition-metals, the 38 entries found in the center of the Periodic Table of Elements, and their corresponding oxides. Recently, however, it has been reported that magnets can be produced using certain organic molecules.

"The interest in organic materials with magnetic properties arises from their potential to be more cost effective and lighter than the more traditional metal magnets," according to Anna Gudmundsdottir, Ph.D., an associate professor of Chemistry at the University of Cincinnati. "They would be valuable in many commerical applications, such as magnetic shielding and quantum computing. Furthermore, biocompatibility of organic magnets may potentially lead to interesting biological applications, such as magnetic imaging of medical implants."

This quest for organic magnets has sparked renewed research into intermediates, called nitrenes and carbenes. Most chemical reactions involve more than one elementary step to complete, and a reactive intermediate is an unstable compound that exists only briefly in one of the intermediate steps. It normally is very difficult to isolate and directly observe a reactive intermediate.

Nitrenes are intrinsically more stable than carbenes, and researchers like Gudmundsdottir are intrigued by the possibility of linking together several molecules of intermediates. "Triplet" nitrenes are ideal candidates for researchers to investigate as potential magnets because of their high-spin properties, a condition where unpaired electrons are present and magnetism is possible.

Triplet aryl nitrenes, which have been studied extensively, have been formed by exposing a solution of chemicals called aryl azides to a source of heat or UV light – a chemical process called photolysis. While it has been difficult to stabilize triplet aryl nitrenes, researchers have found some promise in forming them in inert crystal lattices.

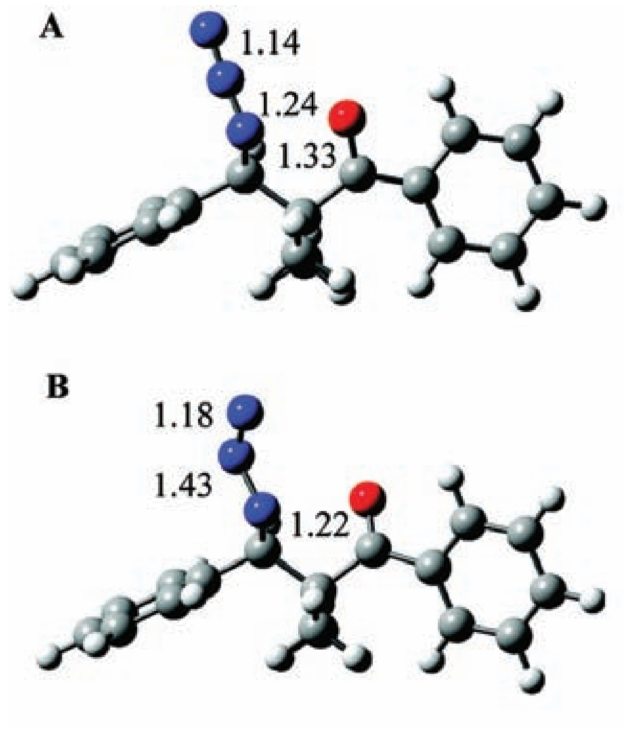
Recently, however, a pair of similar compounds – triplet alkyl nitrene and triplet vinyl nitrene – have been produced through photolysis in Gudmundsdottir's laboratory. These breakthroughs have opened up a new field in nitrene chemistry, where intermediates that have not previously been characterized can now be investigated.

"We have shown that triplet alkyl nitrenes can be formed selectively in solutions and the solid-state," said Gudmundsdottir. "Furthermore, alkyl nitrenes are highly unreactive. Currently, we are investigating the reactivity of vinyl nitrenes in solution and in the solid-state."

To aid their laboratory investigations, Gudmundsdottir's team has accessed the resources of the Ohio Supercomputer Center to conduct molecular modeling of the chemical processes that produce nitrene. To make her calculations, Gudmundsdottir leverages a computational chemistry software program called Gaussian™ to apply "density functional theory" (DFT), a quantum mechanical theory used to investigate the properties and dynamics of molecules.

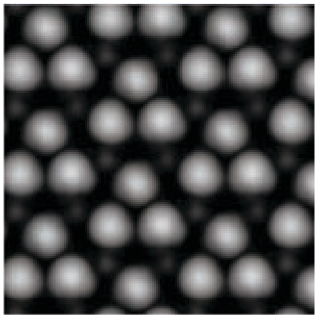
"Molecular modeling supports characterization of these intermediates and helps to probe their reactivity," Gudmundsdottir explained. "Our goal is rendering the nitrene unreactive so they can be used as building blocks for organic magnets." ■

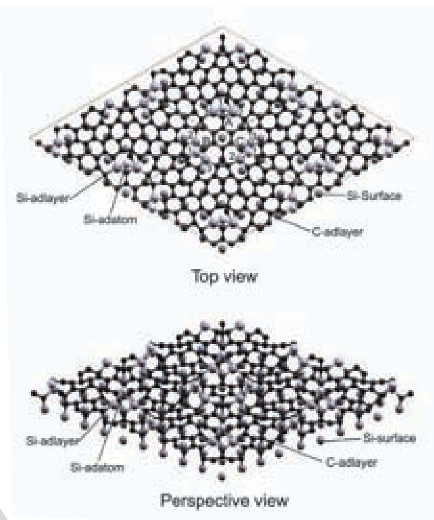
**Project lead:** Anna Gudmundsdottir, University of Cincinnati
**Research title:** Reactivity of alkyl and vinyl nitrenes
**Funding source:** National Science Foundation




*above:* An example of the molecular modeling conducted by Anna Gudmundsdottir to understand the different reactivities of vinyl azides.

*below:* Anna Gudmundsdottir's research into developing organic magnets seeks to harness the powerful physical properties behind the brilliant aurorae found in the night skies above the Earth's polar regions.






# Calculating surfaces for graphene growth

The understanding of surface reconstructions has become essential as scientists seek to develop materials with tailored properties. For instance, researchers over the past few years have been searching for a process to mass-produce circuits using a material called graphene – a one-atom-thick layer of graphite – which displays unique electronic properties.

Nancy Sandler, Ph.D., an assistant professor in the Physics and Astronomy Department at Ohio University, is investigating models for surface reconstructions of silicon carbide (SiC), a substrate material used to produce graphene. Her modeling was generated with the density functional theory-based code SIESTA on the IBM Glenn Cluster at the Ohio Supercomputer Center.

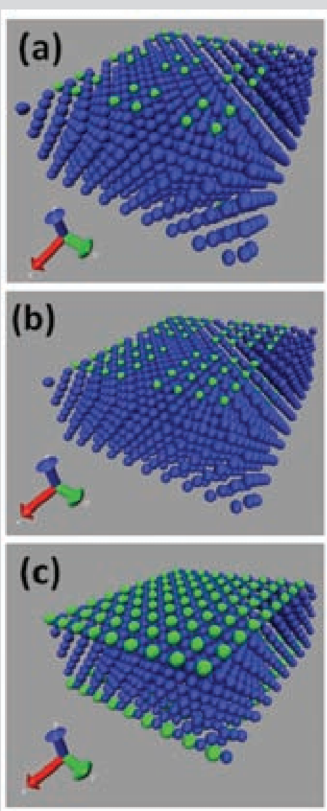
"Despite the success in the fabrication of high-quality films of graphene, there is little knowledge on the mechanisms of nucleation and growth of these films on the underlying SiC material," said Sandler. "Many of the properties of the film obtained are strongly determined by the substrate that remains after graphene separation."

Sandler and her team studied three models, each with the addition of carbon-rich layers of different coverage and electronic properties similar to that existing before graphitization. They analyzed corresponding band structures and density-of-states, comparing them to experimental scanning tunneling microscope measurements.

The model that best described the experimental observations featured an intermediate-coverage carbon-rich layer, on top of which a complex network of three-atom products, called trimers, is formed. This trimer network produces electronic properties common to both reconstructions and provides insight into graphene formation at higher temperatures. ■

**Project lead:** Nancy Sandler, Ohio University
**Research title:** Model calculations for surface reconstructions of semiconductor materials
**Funding source:** National Science Foundation

*below:* Atomic models of (a) a 2x2 island, (b) a 4x4 island, and (c) a monolayer of N atoms on Cu [001].




# Controlling nanometer-scale structures

Surprising behaviors often arise when small numbers of atoms and molecules are brought into close proximity. Such small aggregates offer a window into an intermediate state of matter between isolated atoms and bulk materials. An improved understanding and control of these nanometer-scale structures may contribute to new paradigms for technologies such as molecular circuits, spin-based electronics and quantum computation.

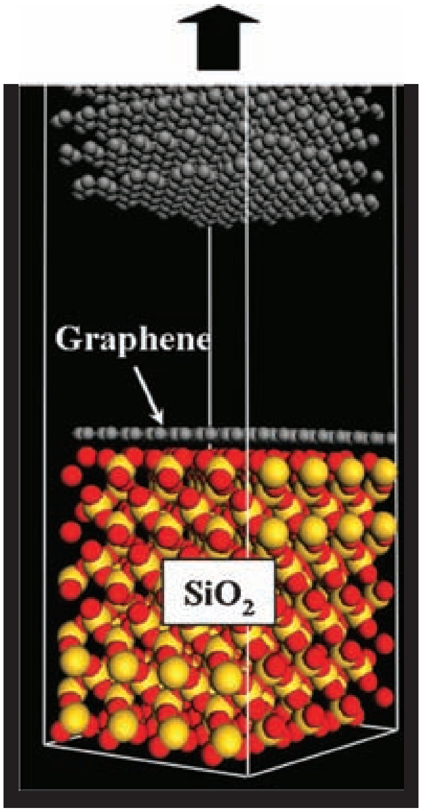
A research team led by Ohio State University's Jay A. Gupta, assistant professor of physics, and David G. Stroud, professor of physics, is using scanning tunneling microscopes (STM) to better measure the properties of nanoscale structures, whose size can vary from a few atoms to thousands of atoms.

Quantum confinement of electrons in the cluster leads to a discrete spectrum of states with a level spacing that depends on the size. By isolating the nanocluster from the underlying metal substrate by using an ultrathin insulating film of only a few atomic layers (e.g., Cu2N islands), scientists can measure this spectrum with STM. They seek to understand how these electronic structure properties depend on the dimensions of nitrogen islands.

"We have studied the electronic structure of nanoscale islands of Cu2N on the Cu [001] surface," said Gupta. "We leverage hundreds of processors on Ohio Supercomputer Center systems to perform ab-initio calculations using density functional theory. Those results are compared with our scanning tunneling microscopy measurements, and we find that our tunneling spectroscopy results are in good agreement with our computational predictions." ■

**Project lead:** Jay Gupta, The Ohio State University
**Research title:** Emergence of band structure in nitrogen islands on copper [001]: Comparison of density functional theory and scanning tunneling microscopy
**Funding source:** Center for Emergent Materials - The Ohio State University

# Devising production methods for graphene




Ohio State University researchers recently discovered potential keys to mass producing a specific pattern of graphite in a layer just one atom thick, signaling a breakthrough that could lead to "graphene" challenging silicon as the preferred material for manufacturing faster, more efficient computer chips.

While scientists have known of graphene's potential for many years, electronics industry officials became particularly excited when researchers found that thin layers of graphite are highly stable, visible under the right conditions even when only one atom thick, stronger than steel and conducts electricity quickly and in exceptional ways.

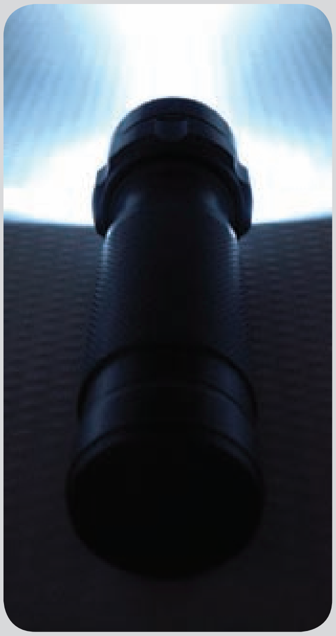
Wolfgang Windl, Ph.D., associate professor of Materials Science and Engineering, and co-workers set out to develop a method for producing very accurate, very position-specific graphene patterns in a way that industry could use to manufacture computer chips. To test their technique, Windl turned to the resources of the Ohio Supercomputer Center and the Vienna Ab-initio Simulation Package.

"The calculations are computationally very demanding for the systems under consideration due to their size and complexity," Windl explained. "Based on our initial success with these computer simulations, we currently model adhesion on different substrates along with the resulting electrical transport through the graphene to optimize the stamping process and the resulting devices."

With confirmation from their computer models, Windl's team from OSU's Center for Emergent Materials successfully sheared off graphite layers that were about ten atom-layers thick and have initiated the process of obtaining a patent on the technique. ■

**Project lead:** Wolfgang E. Windl, The Ohio State University
**Research title:** Toward site-specific stamping of graphene
**Funding sources:** National Science Foundation, The Ohio State University

# Investigating new opportunities for doping



*above:* Walter Lambrecht is investigating zinc germanium nitride as an alternative to the mixed indium-gallium nitride alloy that provides LED flashlights with their brilliant luminosity.

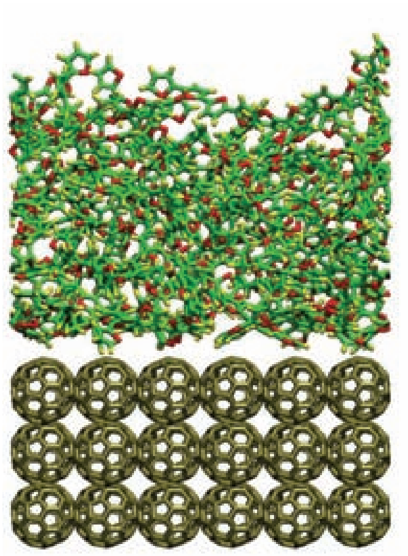
Modern flashlights with bright, white LEDs probably use a mixed indium-gallium nitride alloy as semiconductor to convert electricity into light. A Blu-ray disk system also employs a blue InGaN-based laser. However, indium is becoming scarce and costly, sending researchers scurrying to find an alternative technology. Walter Lambrecht and colleagues at Case Western Reserve University are investigating the properties of a similar, if less familiar, material – zinc germanium nitride.

"We are collaborating with Dr. Kathleen Kash's group, which is growing this and related materials by characterizing and predicting their fundamental properties," said Lambrecht, Ph.D., a professor of physics at Case Western Reserve University. He explains: "To convince people that this material is viable for opto-electronic technology, an understanding of its native defects and doping properties is essential. We think that the three-element nature of this new semiconductor provides new opportunities for doping, because one can substitute each one of these elements separately."

Lambrecht performs quantum mechanical calculations of the electronic properties of semiconductor point defects on the IBM Glenn Cluster at the Ohio Supercomputer Center. The software used for these calculations is under continuous development by an informal group of collaborators to which Lambrecht belongs and which is headed by Mark van Schilfgaarde at Arizona State University. One of the main efforts of the group is to use new approaches to remove the limitations of so-called local density approximations, allowing for a more sophisticated treatment of electronic correlations that is essential to understand defect properties. ■

**Project lead:** Walter Lambrecht, Case Western Reserve University
**Research title:** Point defects and doping in wide band gap semiconductors
**Funding source:** National Science Foundation, Army Research Office

# Evaluating organic materials for solar energy



*above:* Researchers like University of Cincinnati's Vikram Kuppa are studying the potential of combining oligothiophene and fullerene to produce viable solar cell systems.

Organic photovoltaic systems (OPVs) have generated considerable interest from researchers in recent years as materials relevant to harnessing renewable and sustainable sources of solar energy. OPVs are called "organic" because the substances are carbon-based, like the molecules of living things. The great potential of organic materials lies in their lower production costs, greater flexibility and higher optical absorption coefficients than their traditional, inorganic counterparts, such as copper or silicon.

Vikram Kuppa, Ph.D., an assistant professor of chemical and materials engineering at the University of Cincinnati, is conducting molecular dynamics simulations at the Ohio Supercomputer Center to evaluate the behavior of the carbon-based material oligothiophene when applied to a carbon-based substrate of fullerene.

"We seek to probe the effect of the surface, as well as process variables such as temperature, on the behavior of the oligothiophene," said Kuppa. "The goal is to enable a fundamental understanding of the factors that influence the properties of these hybrid systems, and their role in the transport of electrical charges that are generated in the conjugated polymers upon exposure to sunlight."

To generate these detailed simulations, Kuppa uses the classical molecular dynamics code LAMMPS, an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator, and OSC's flagship Glenn Cluster, a 9,500-node IBM 1350 Opteron system.

"The ultimate goal of this research," Kuppa said, "is to employ molecular dynamics simulations in conjunction with experimental tools to develop cost-effective and efficient materials for energy conversion." ■

**Project lead:** Vikram Kuppa, University of Cincinnati
**Research title:** Simulation of organic photovoltaic materials
**Funding sources:** University of Cincinnati

# Exploring EM wave behavior in metamaterials

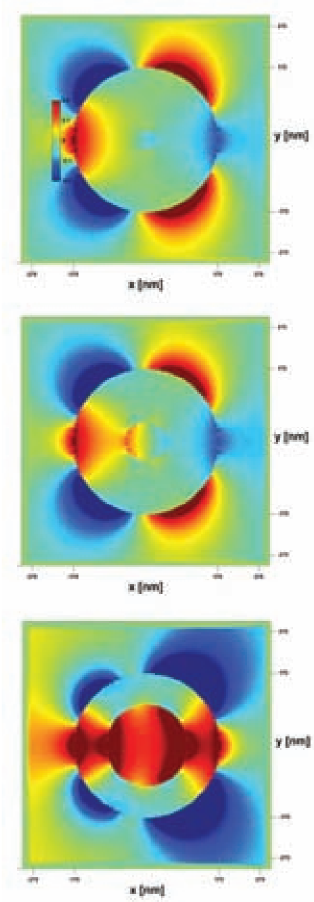
Various materials can be used to control the path of light or any other type of electromagnetic (EM) wave. For example, the lenses in a pair of eyeglasses are shaped to achieve a desired optical function. While nature and chemistry have provided many such materials, it is only in more recent years that scientists have been working at the nanoscale to create a range of "metamaterials" with novel and promising EM properties.

"Metamaterials increase the degrees of freedom for controlling EM wave behavior," according to Fernando L. Teixeira, associate professor of Electrical and Computer Engineering at The Ohio State University and a faculty member of OSU's ElectroScience Laboratory. "For example, it might be possible to create metamaterials to provide super-resolution lenses, negative refraction and electromagnetic cloaks."

The fabrication-associated design process of new metamaterial-based EM devices is expensive, time-consuming and sometimes very difficult. Manufacturers often turn to modeling and simulation to limit trial-and-error before the actual fabrication and prototyping process begins.

Teixeira and his research team have found that existing commercial codes do not have the capability of analyzing complex metamaterials with a sufficient degree of accuracy. Therefore, they are using the large parallel systems of the Ohio Supercomputer Center to develop faster, more accurate computer algorithms to investigate EM wave behavior in metamaterials, focusing especially on three types:

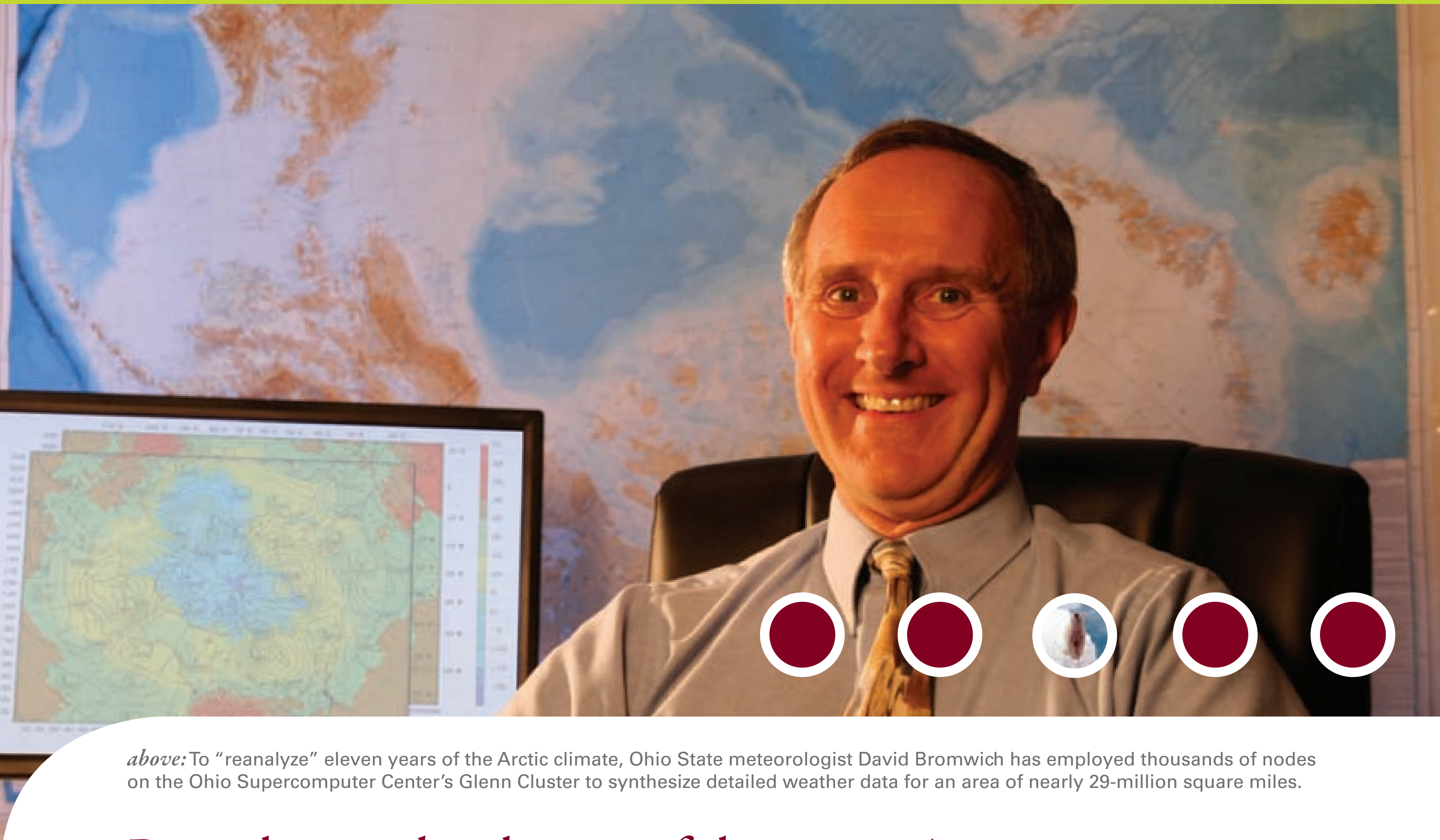
- photonic crystals (for slow pulse propagation)
- nanoscale metallic structures (for compact optical devices)
- isoimpedance metamaterials (for reflectionless waveguide bands) ■




**Project lead**: Fernando Teixeira, The Ohio State University
**Research title:** Large-scale time-domain simulations for electromagnetic wave propagation and scattering in metamaterials
**Funding sources:** National Science Foundation, Air Force Office of Scientific Research

# energy & the environment

The solution of complex global energy and environmental sustainability issues will increase demand for modeling and simulation capabilities. The Ohio Supercomputer Center is supporting ambitious researchers who are investigating various aspects of these challenges, such as synthesizing historical weather data to create large-scale polar climate models; exploiting massive volumes of satellite data to model flood patterns; simulating air flow around aircraft wings and payload cavities; modeling congested and multifaceted transportation systems; and evaluating unintended collateral threats to endangered species of wildlife. Scientists are developing new, cost-effective sources of sustainable energy by developing new materials and processes to enhance wind and solar power generation and by creating new fuel products from biomass. The Ohio Supercomputer Center provides powerful resources for researchers who today find themselves in the throes of a worldwide Green Revolution. ■



*above:* To "reanalyze" eleven years of the Arctic climate, Ohio State meteorologist David Bromwich has employed thousands of nodes on the Ohio Supercomputer Center's Glenn Cluster to synthesize detailed weather data for an area of nearly 29-million square miles.

# Reanalyzing the climate of the entire Arctic system

David Bromwich, Ph.D., and his research team are leveraging the computing and storage resources of the Ohio Supercomputer Center (OSC) to synthesize historical weather data from a region of nearly 29-million square miles – everything north of Minneapolis, Minn.; Turin, Italy; and the Black Sea.

The team is integrating multiple enormous databases containing eleven years of satellite readings and direct observations of the Arctic atmosphere/sea-ice/land-surface system. The time period corresponds to the 1999 launch of the NASA spacecraft named Terra, a polar-orbiting climate research satellite.

"The Arctic System Reanalysis (ASR), which can be viewed as a blend of modeling and observations, is ingesting historical data streams along with measurements of the physical components of the Arctic Observing Network developed as part of the global scientific project known as the International Polar Year," explained Bromwich.

Bromwich's group produced a prototype 16-month coarse-resolution version of the ASR this summer. When the full ASR is completed, the team will provide a high-resolution description of the high-latitude expanse in dimensions of altitude (71 layers), space (every 10 kilometers) and time (every three hours).

"With the introduction of space-borne measurements over the last few decades, researchers have been inundated with vast amounts of information," Bromwich noted. "Today, the trick is to figure out how to effectively use all the diverse information sources."

To generate the complex visualizations, the ASR group has processed the information using more than 1,000 cores of OSC's IBM Cluster 1350 over the last several months. The data accumulated for and generated by the model eventually will fill hundreds of terabytes of disk space on the center's IBM Mass Storage System.

"I think the model is giving very reasonable results," said Lesheng Bai, a research associate at the Byrd Polar Research Center. "We've had to resolve issues with the model physics, because some of the data types have special circumstances. But, the model is running well at the coarse-resolution stage."

OSC staff members installed on the Glenn Cluster and tested the Weather Research and Forecasting (WRF) model, a state-of-the-art numerical weather prediction and data assimilation system developed by the National Center for Atmospheric Research, the National Oceanic and Atmospheric Administration and other organizations. The Polar WRF version of the system was installed once the ASR group enhanced the program with parameters developed from data from Greenland, the Arctic Ocean and Alaska.

"The ASR is ingesting and generating about five terabytes of output per year," Bromwich said. "We will maintain the secure archive of all reanalysis data at OSC and develop web-based tools for access and analysis by the wider scientific community."

Over the final year of the four-year project, Bromwich and his team will work to complete the high-resolution version of the ASR. He hopes the detailed information generated by the study contributes to a better understanding of climate shifts in the environmentally sensitive Arctic.

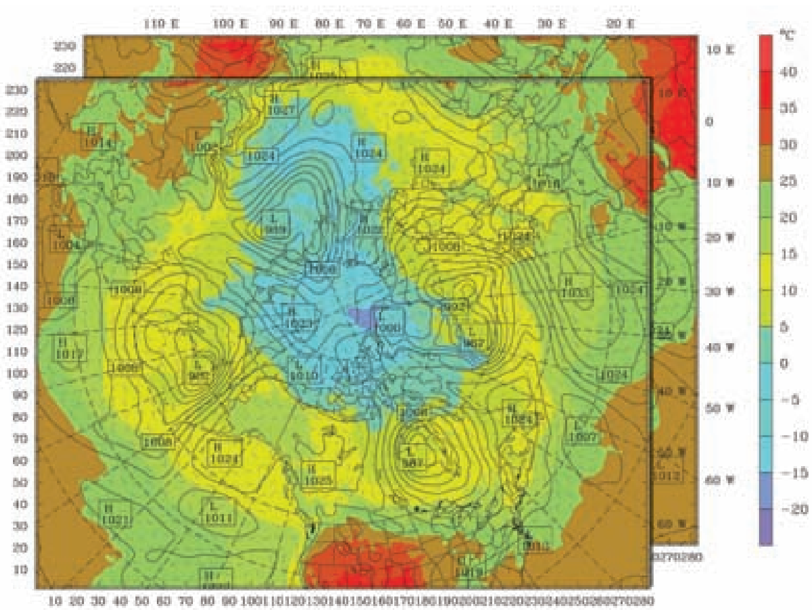
"The Arctic is in the midst of rapid change," Bromwich noted. "There have been pronounced increases in surface air temperature, especially for winter and spring over subarctic land areas, as well as over the Arctic Ocean. It's extremely important that we better understand what's happening there in order to predict the future more accurately. Through data assimilation, the ASR will serve as a state-of-the-art synthesis tool for assessing Arctic climate variability and monitoring Arctic change."

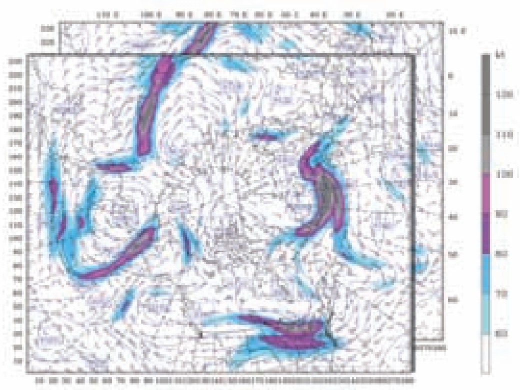
Once the initial project is completed, Bromwich sees the potential for collecting and integrating additional data into the ASR, possibly from as far back as 1957. That year signaled the beginning of a global scientific project known as the International Geophysical Year and saw the Soviet Union launch the world's first satellite, "Sputnik." ■

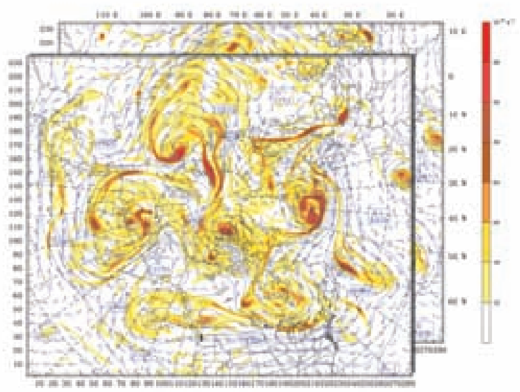
**Project lead:** David H. Bromwich, The Ohio State University
**Research title:** Arctic system reanalysis
**Funding source:** National Science Foundation

photo courtesy of NOAA.

*above:* David Bromwich hopes that his Arctic System Reanalysis provides information that will better inform the discussion of climate trends in the fragile ecosystem of the northern latitudes.

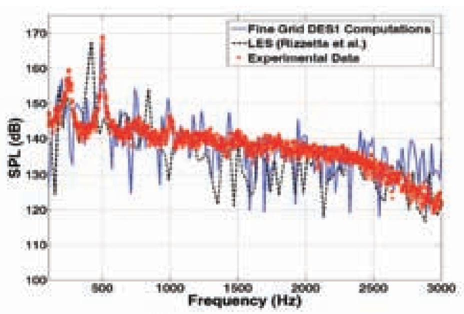






The ASR project recently unveiled coarse-resolutions mapping tools that can illustrate such climatic variables as near-surface air temperature and sea-level air pressure *(above)*, mid-level atmospheric vorticity and wind vectors *(above, right)* and high-level horizontal wind speed *(right)*.

photo courtesy of SSG Samuel Rogers, USAF




# Understanding airflow at transonic speeds

The complex unsteady airflow characteristics of certain aircraft features, such as landing gears and weapon bays, produce pressure fluctuations that reach unacceptable levels for operation and safety at transonic speeds.

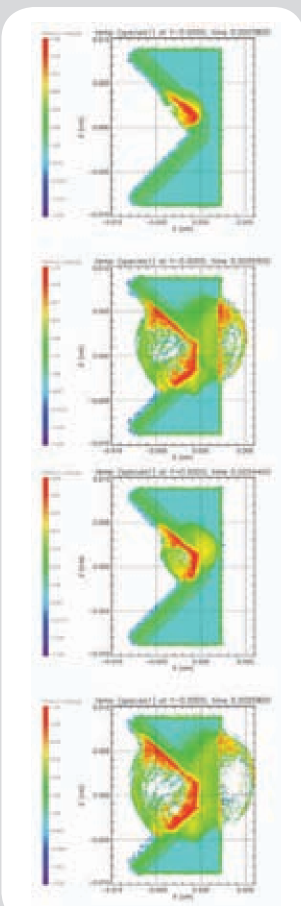
To better understand how to control the airflow for pressure fluctuations and noise reduction, Awatef Hamed, Ph.D., Bradley Jones Professor and department head of Aerospace Engineering and Engineering Mechanics at the University of Cincinnati, leveraged the computational resources of the Ohio Supercomputer Center to develop and validate a hybrid unified turbulence model for the Detached Eddy numerical simulations of the unsteady Navier-Stokes equations.

"We worked to simulate and access active flow control using steady and pulsed fluidic actuation for acoustic suppression in transonic flow over an open cavity," Hamed said. "We developed and implemented a new unified methodology to resolve both aerodynamic and aero-acoustic fields to study acoustic control."

Hamed's research team conducted high-fidelity simulations of supersonic cavity flow with active flow control and compared the results to experimental data and to LES results to assess the fidelity of the hybrid model. They also analyzed the influence of Reynolds number (the ratio of inertial forces to viscous forces) on the unsteady cavity flow and acoustic fields with and without control.

The resulting simulations illustrated that her methodology provides a useful tool for predicting complex 3-D separated unsteady flows over an expansive dynamic range at high Reynolds number and are comparable to LES predictions at one-sixth to one-tenth the CPU resources. ■

**Project lead:** Awatef Hamed, University of Cincinnati
**Research title:** Hybrid RANS/LES simuations of transonic cavity flow with control
**Funding source:** Ohio Space Grant Consortium



# Examining laser-plasma keys to fusion energy

Nuclear fusion holds the promise of sustainable, abundant clean energy. Scientists have successfully demonstrated controlled fusion in the laboratory, but have not yet been able to demonstrate useful energy production.

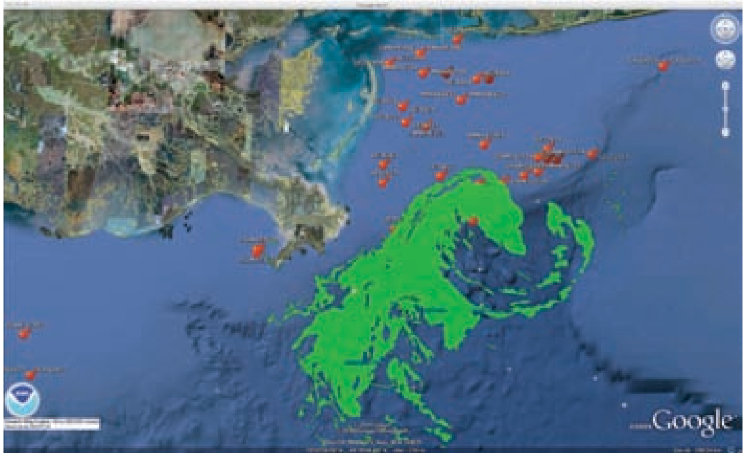
Nuclear fusion must take place in plasma, an ionized medium, and generally requires a combination of density and temperature that is difficult to achieve. As part of a worldwide effort to demonstrate the fast ignition inertial confinement approach to fusion, researchers at The Ohio State University and the Department of Energy's Jupiter Laser Facility have been examining intense laser-plasma interactions.

"We've created numerical models of an intense laser with parameters relevant for fast ignition fusion in a plasma and to determine the resulting distribution of energetic electrons excited and their subsequent propagation," said Douglass Schumacher, Ph.D., an associate professor of Physics at OSU. "Modeling also has been used to help design some aspects of the experimental program."

Schumacher's team has leveraged the computational muscle of the Ohio Supercomputer Center's Glenn Cluster to model specular reflection of an intense laser from a metallic surface, the divergence angle of a laser-generated hot electron beam, the use of $K_\alpha$ radiation as a diagnostic tool, red-shifting of reflected light due to ponderomotive compression of the plasma density profile and the spectra of escaping electrons when ultrashort laser pulses are employed. The research is helping to determine the conditions where fast ignition might work and to develop better diagnostics for fast ignition studies. ■

**Project lead:** Douglass W. Schumacher, The Ohio State University
**Research title:** Modeling intense laser plasma interactions in conjunction with an experimental program for 2010
**Funding source:** Department of Energy, The Ohio State University

# Tracking the impact of oil, chemicals on Gulf fish




When the Deepwater Horizon oil rig exploded off the Louisiana coast in April, it caused the first major deep-sea oil spill and became the first spill where chemical dispersants were used far below the water's surface. Researchers have detected toxic microdroplets spreading in concentrations that may be lethal to wildlife. Several organizations are tracking the toxins at the surface of the gulf and coastal environments, home to more than 600 species of commercially or evolutionarily important fish.

To complement these efforts, Dan Janies, Ph.D., a biomedical researcher at The Ohio State University (OSU), and Prosanta Chakrabarty, an assistant professor of ichthyology at Louisiana State University, have adapted a program to monitor infectious diseases that Janies developed with Ohio Supercomputer Center and OSU resources. Their mapping project, DepthMap, will tell scientists more about the impact of the spill on species at different stages of their life cycles and habitats.

"We combine data from historical collections of fish species with dynamic maps of the oil spill in a Geographic Information System," said Janies. "Put together, imagery on the spill and data on the pre-spill range of wildlife allow researchers a baseline from which to measure and predict the effects of the spill. We make the maps and underlying informatics tools available to a wide community of users via the web (depthmap.osu.edu), so others can leverage our work in clean-up efforts and research the impacts of the spill on any species of interest." ■

**Project lead:** Daniel Janies, The Ohio State University
**Research title:** Analysis of baseline distribution records for wildlife affected by the 2010 Gulf of Mexico oil spill
**Funding source:** The Ohio State University

# Testing battery traits in hybrid vehicles

The power needs for extended all-electric operation of plug-in hybrid electric vehicles (PHEVs) require much more on-board energy than the lower-density energy typically provided by nickel-metal-hydride batteries. The current engineering solution is to link several parallel strings of lithium-ion battery cells within a battery module and to link several modules into larger battery packs.

But, these configurations had not been empirically tested to determine how changing temperature and energy loads on individual cells affect battery life. To accomplish this, Benjamin "BJ" Yurkovich, a graduate research fellow at The Ohio State University's Center for Automotive Research, first identified the model parameters of individual cells.

"Each cell in a battery pack is unique," said Yurkovich. "They vary in manufacturing variability, cell history and existing conditions, such as temperature, current and state-of-charge. These factors must be considered by a battery management system to achieve optimum voltage equalization."

Yurkovich then used the Ohio Supercomputer Center's Glenn Cluster and Remote MATLAB Services to develop and run a battery model based on the battery cell data and simulation algorithms.

"The simulations considered two different battery pack configurations, profiles for both hybrid and plug-in hybrid vehicles, three different temperatures, two different variations of internal resistance and capacity, three different states-of-charge and three different variations for the standard deviation," Yurkovich explained.

With his results, Yurkovich was able to provide a foundation for the design of more intelligent battery management system design in PHEV battery packs. ■


**Project lead:** Benjamin Yurkovich, The Ohio State University
**Research title:** Electrothermal battery pack modeling and simulation
**Funding source:** The Ohio State University

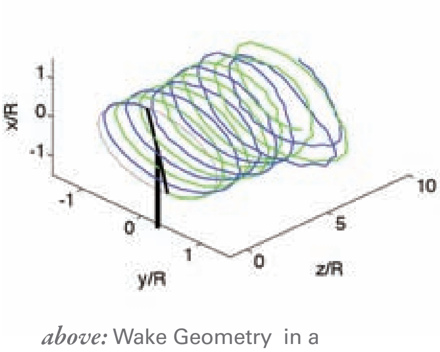
# Improving wind turbine computer models

Renewable energy is increasingly important with rising energy demands, finite fossil fuel supplies and growing environmental concerns. Over the last 25 years, wind turbine technology has increased in power output, but to meet a federal goal of generating 20 percent of the nation's energy from wind by 2030, production must increase dramatically and several significant technological advancements are needed, including improved structural and aerodynamic modeling tools.

"The inability of current state-of-the-art wind turbine design codes to accurately and reliably predict performance and loads demonstrates the need for enhanced models," said Jack McNamara, Ph.D., assistant professor of mechanical and aerospace engineering at The Ohio State University. "One issue noted in previous work is inadequate modeling of the rotor wake. For more accurate modeling of the problem, a wake model is required, where the vortex trailing the blades is tracked and its effects are included in the aerodynamic calculations."

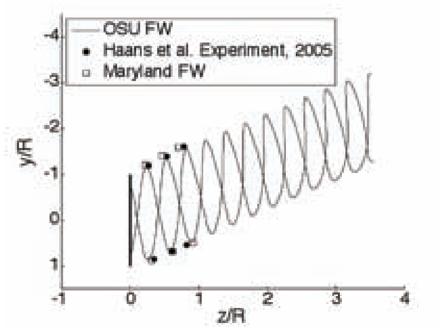
McNamara's Computational AeroElasticity Laboratory is accessing Ohio Supercomputer Center resources to study the effect of the wake on the aeroelastic response and performance of a representative wind turbine. Krista Kecskemety, a graduate student in McNamara's lab, is currently incorporating the OSU Free Wake model into the open-source NREL wind turbine aerodynamics code, AeroDyn. This will then be used in conjunction with the NREL FAST and MSC ADAMs comprehensive wind turbine codes to study of the interaction of the wake with the turbine and its impact on predicted power performance and aeroelastic blade loads. ■

**Project lead:** Jack J. McNamara, The Ohio State University
**Research title:** Impact of wake effects on the performance and aeroelastic behavior of wind turbines
**Funding sources:** Ohio Space Grant Consortium




*above:* Wake Geometry in a Turbulent Flow

*below:* Wake Verification and Validation (top view)




# Enhancing ocean surface height calculation

With more than 70 percent of the Earth's surface covered in water, studying ocean topography is vital to researchers who produce atmospheric models for forecasting hurricanes, optimizing commercial shipping routes, tracking floating debris and helping manage marine animal populations.

To measure the surface height of oceans, scientists at The Ohio State University ElectroScience Laboratory (ESL) analyze satellite altimeter data. While these instruments produce highly accurate measurements, small but important errors occur because waves are not symmetrical: wide, shallow wave troughs reflect electromagnetic energy more strongly than the narrow, sharp wave crests.

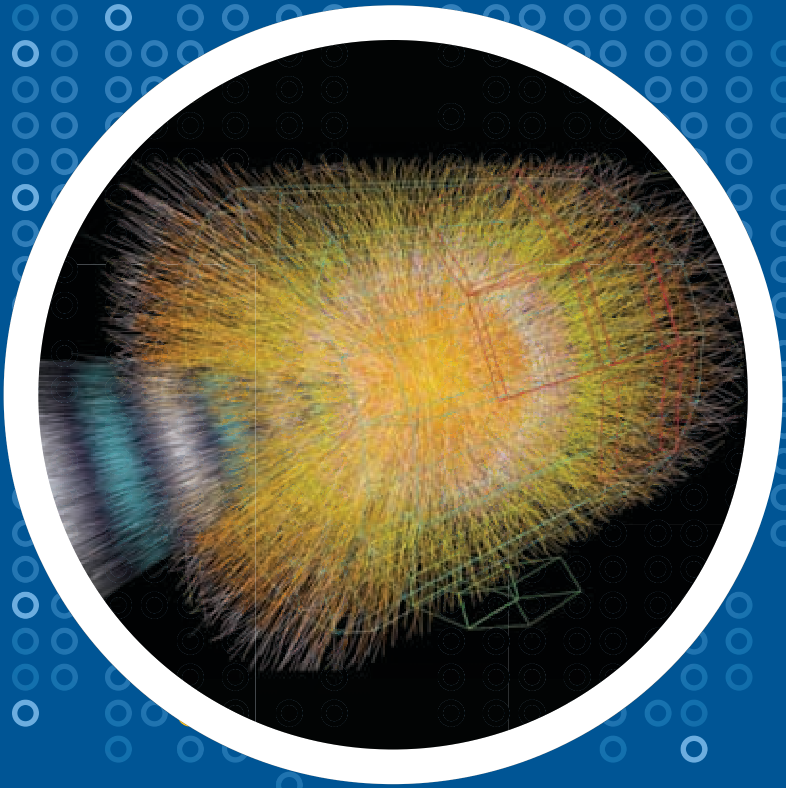
Joel Johnson, Ph.D., a professor of electrical and computer engineering, and Praphun Naenna, a graduate research assistant, have leveraged Ohio Supercomputer Center (OSC) resources to correct an "electromagnetic bias" that reports surface levels that are too low.

"Our study uses a method for hydrodynamic simulations that can better capture these effects than models previous studies employed," said Johnson. "This method, however, comes with far more computational burden, so we use supercomputing resources at OSC to produce a deterministic set of sea surface profiles and the corresponding altimeter pulse returns."

To this point, the development of EM bias simulation tools has been completed, and the numerical results have been verified.

"The focus is now on using these tools to investigate the impact of various physical effects on the EM bias, including variations with the wind speed and the radar frequency, and also the influence of short scale roughness," said Naenna. ■

**Project lead:** Joel Johnson, The Ohio State University
**Research title:** Monte Carlo simulations of altimeter pulse returns and the electromagnetic bias
**Funding source:** The Ohio State University



# 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 reveals a physicist who leverages supercolliders and supercomputers to unlock mysteries surrounding the birth of the universe. Other researchers are speeding up the world's fastest supercomputers even more by changing the way applications are developed and instructions are communicated. And, a political scientist has employed sophisticated statistical techniques to analyze the likelihood of armed conflict. 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:* Physicists such as Ohio State's Thomas Humanic are studying the immense data files created by the Large Hadron Collider and stored at the Ohio Supercomputer Center and other locations to answer fundamental questions about the basic building blocks of the universe.

# Downloading data from the European supercollider

In April, physicists working on the ALICE project (short for A Large Ion Collider Experiment) began recording data from collisions within the Large Hadron Collider, operated by the European Laboratory for Nuclear Research (CERN) near Geneva, Switzerland. More than 1,000 international physicists, engineers and technicians working on the project hope to find answers to fundamental questions about the birth of the universe, matter vs. antimatter, the nature of dark matter and maybe even the existence of other dimensions.

The ALICE scientists carefully propel and collide opposing beams of protons and beams of lead nuclei at nearly the speed of light around a 17-mile underground loop. These are the highest energy proton collisions ever produced in the laboratory – 3.5 times higher than the previous highest-energy proton collisions created at the Department of Energy's Fermilab.

The ALICE collisions expel hundreds to thousands of small particles, including quarks – which make up the protons and neutrons of the atomic nuclei – and gluons – which bind the quarks together. For a fraction of a second, these particles form a fiery-hot plasma that hasn't existed since the first moments after the Big Bang, about 14 billion years ago. Within the massive 52-foot ALICE detector, 18 sensitive sub-detectors measure the behavior of the expelled particles, recording up to approximately 1.25 gigabytes of data per second – six times the contents of Encyclopedia Britannica every second.

The massive data sets are now being collected and distributed to researchers around the world through high-speed connections to the LHC Computing Grid (LCG), a network of computer clusters at scientific institutions, including the Ohio Supercomputer Center. The LCG is composed of more than 130 organizations across 34 countries and is organized into four levels, or "tiers." Tier 0 is CERN's central computer, which distributes data to the eleven Tier 1 sites around the world. The Tier 1 sites, in turn, send data to Tier 2 sites, which provide storage and computational analysis. Tier 3 sites involve individual computers operated at research facilities.

"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., a professor of physics at The Ohio State University working on several experiments at the LHC. "OSC has been contributing computing resources to the project from the very beginning of ALICE's distributed computing efforts, starting in 2000."

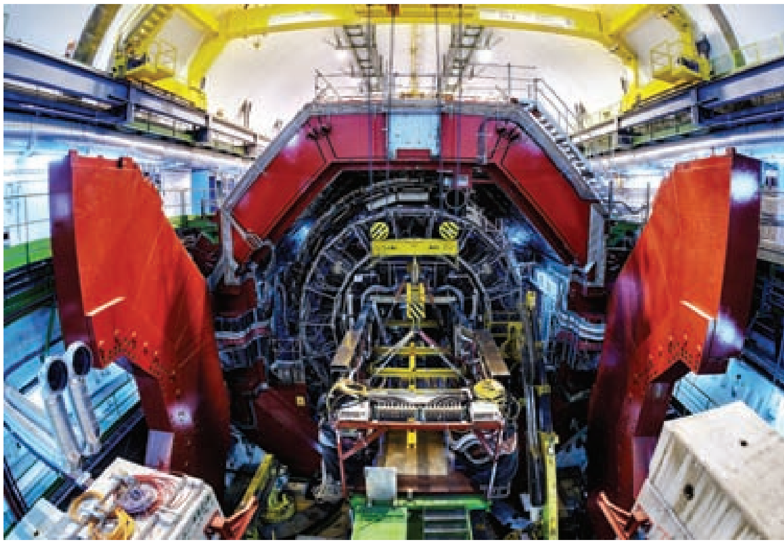
Construction of the LHC began in 1995, when much of the necessary computational and networking technologies didn't yet exist. New technologies, such as grid computing, were developed to meet the demands of the project. OSC was one of the first adopters of the ALICE-developed AliEn (ALICE Environment) grid infrastructure.

As a Tier-2 site on the LCG, OSC this year has committed, through its normal allocations process, 30 terabytes of data storage and one million processor hours, according to Doug Johnson, a senior systems developer at OSC.

"This data will be accessed by Dr. Humanic and his OSU colleagues, as well as researchers anywhere in the world, for downloading, reconstruction and analysis," Johnson said. "Researchers can sit at their laptops, write small programs or macros, submit the programs through the AliEn system, find the necessary ALICE data on AliEn servers and then run their jobs through centers such as OSC."

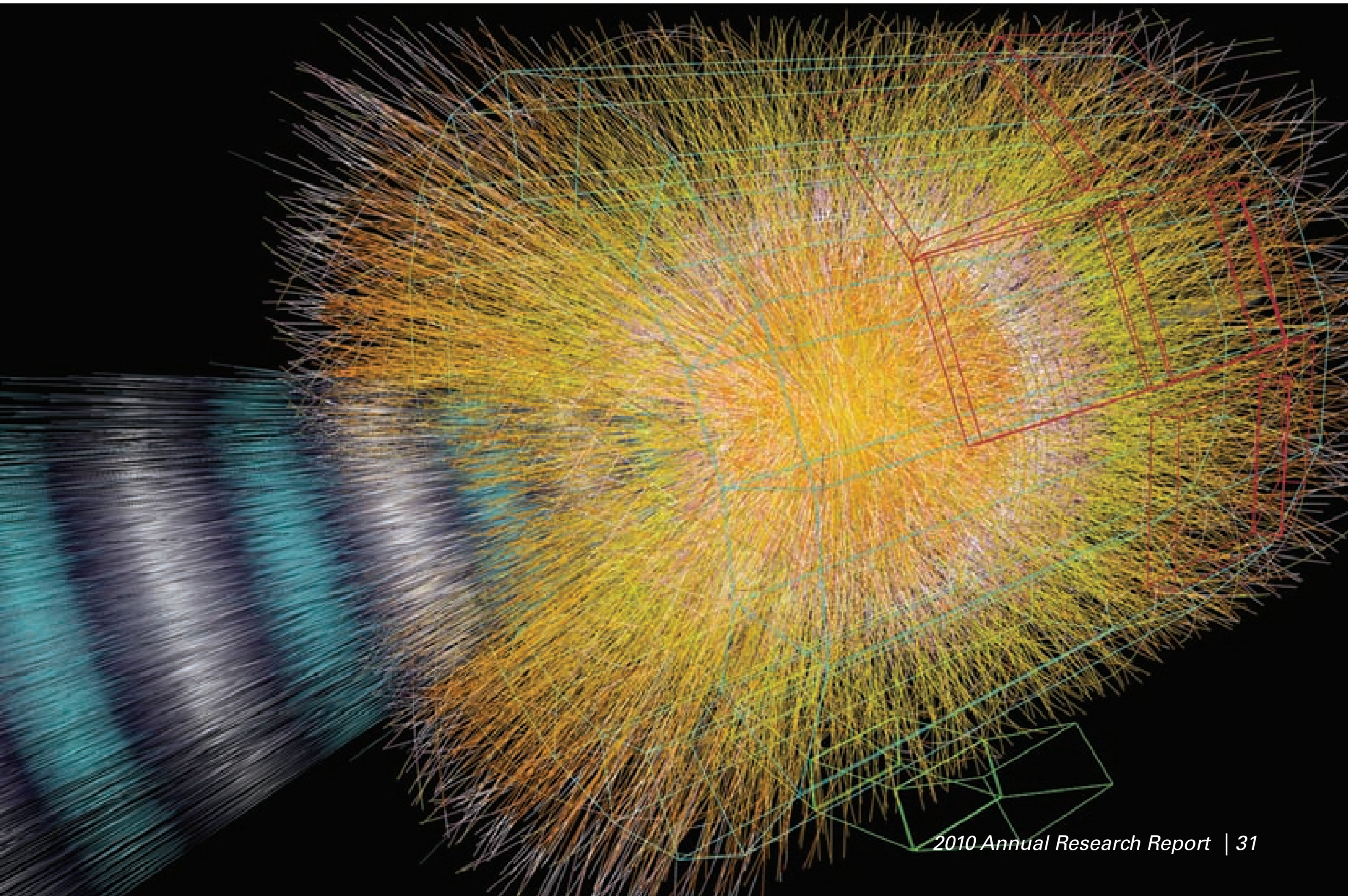
Beyond serving as a storage and analysis resource for researchers working on the project, "OSC also has been critical in the development and testing of a computing model to analyze the ALICE data," Humanic said. OSC had provided 300,000 CPU hours for data simulations prior to the actual LHC experiments. ■

**Project lead:** Thomas J. Humanic, The Ohio State University
**Research title:** Use of OSC computing resources by the Ohio State University Heavy Ion Group in support of ALICE computing program
**Funding source:** National Science Foundation



*above:* The ALICE experiments seeks to capture information about sub-atomic particles – called quarks and gluons – that will be cast aside when lead nuclei are circulated around the 17-mile underground facility and collide at nearly the speed of light.

*below:* While researchers continue to plan for lead ion collisions in the near future (simulated data capture, below), information from proton-proton collisions already is being analyzed. Thomas Humanic estimates that more than a third of the ALICE data being stored and studied in the United States is being served from facilities at the Ohio Supercomputer Center.



artwork courtesy of CERN

# Predicting the likelihood of armed conflict

A former British army officer once said, "History is littered with the Wars which everybody knew would never happen."

To better understand the likelihood of conflict, Ohio State University political science Professor Bear Braumoeller, Ph.D., and doctoral student Austin Carson recently used Ohio Supercomputer Center (OSC) resources to employ several statistical techniques relatively new to the quantitative study of international politics. Specifically, the project analyzed a handful of very large-sized datasets regarding the statistical correlates of war (350,000+ observations, 10-20 variables per observation) using a series of estimation models in the statistical program R.

"The OSC computing resources were instrumental in helping us compute the level of statistical certainty of our inferences," said Braumoeller. "The supercomputing protocol allowed us to make these inferences with a high level of accuracy; such calculations were crucial for inference."

Braumoeller and Carson found that statistical literature on conflict studies has generated strong and consistent findings on the relationship of political irrelevance (large distance between two countries) and democratic regime type on conflict. However, they found that scant attention was paid to whether these factors directly influence the likelihood of disputes or indirectly by modifying the influence of other variables.

Braumoeller's project determined that the literature to date had misunderstood the important theoretical question of how these variables influence peace and war. Greater distance between states and greater political liberalism make other war-related variables less influential and dramatically reduce the probability of conflict. ■

**Project lead:** Bear F. Braumoeller, The Ohio State University
**Research title:** Political irrelevance, democracy, and the limits of militarized conflict
**Funding source:** The Ohio State University

# Advancing network features of petascale computers

Message Passing Interface (MPI) is the dominant parallel computing model on supercomputers today, including petascale systems that are capable of executing one quadrillion operations per second. MPI allows the thousands of nodes in these large clusters to "talk" with one another over high-speed, internal networks, such as InfiniBand and high-speed Ethernet.

Dhabaleswar K. Panda, professor of computer science and engineering at The Ohio State University (OSU), is investigating how these next-generation systems can provide topology, routing and status information, network features that can improve performance and scalability for many applications.

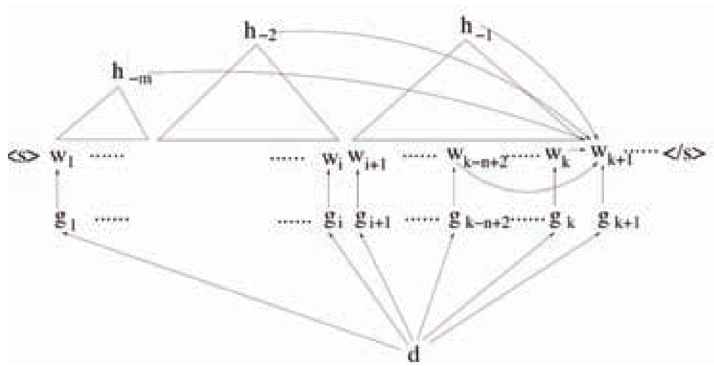
"This project will have significant impact in deriving guidelines for designing, deploying and using next generation petascale systems," said Panda. "This study involves National Science Foundation researchers from OSU, Texas Advanced Computing Center (TACC), University of California – San Diego and San Diego Supercomputer Center operating large-scale simulations on TACC's Ranger system and other supercomputers."

In another related project, the team is studying MPI-2 one-sided communication operations, to improve scaling and performance on petascale systems. The researchers are investigating methods to couple one-sided communication with hardware support from InfiniBand and leverage them in scientific applications. As a part of this project, the team is utilizing and enhancing MVAPICH2 software, a very popular MPI-2 implementation on InfiniBand, 10 GE iWARP and RoCE.

Karen Tomko, an Ohio Supercomuter Center senior systems developer/engineer, is supporting Panda's team on both projects, providing expertise with the MPI library and scientific applications and helping facilitate production-level testing. ■

**Project lead:** Dhabaleswar Panda, The Ohio State University
**Research title:** Topology-aware MPI communication and scheduling for petascale systems; and Extending one-sided communication in MPI programming model for next-generation ultra-scale HEC
**Funding source:** National Science Foundation

# Building a better statistical language model



The highly ambiguous nature of natural language presents many challenges to researchers who design software to analyze, understand and generate languages that humans use naturally. Shaojun Wang, Ph.D., an assistant professor of Computer Science and Engineering at Wright State University, is leveraging the resources of the Ohio Supercomputer Center to build a statistical language model that will capture various kinds of regularities of natural language to improve the performance of a range of natural language processing applications.

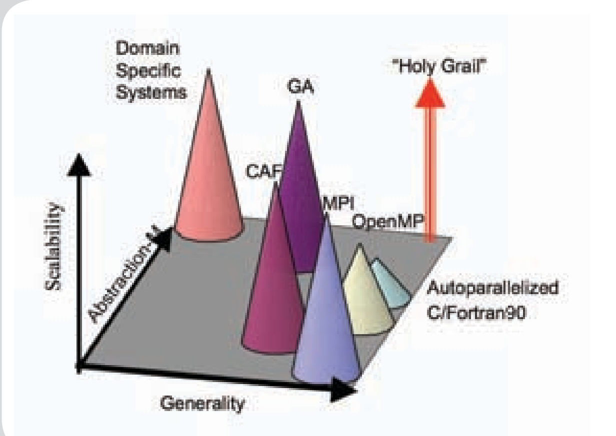
"It has long been a challenge in statistical language modeling to develop a unified framework to integrate various language model components to form a more sophisticated model that is tractable and also performs well empirically," said Wang. "Natural language encodes messages via complex, hierarchically organized sequences. The local lexical structure of the sequence conveys surface information, whereas the syntactic structure, which encodes long-range dependencies, carries deeper semantic information."

By exploiting the particular structure of various composite language models, Wang can decompose the seemingly complex statistical representations into simpler ones; this enables the estimation and inference algorithms for the simpler composite language models to become internal building blocks for the estimation of complex composite language models, thus finally solving the estimation problem for extremely complex, high-dimensional distributions.

To evaluate the performance of the composite language models in a real-world scenario, Wang and his colleagues will embed their new models in large-scale machine translation systems to remove language barriers to processing human communication. ■

**Project lead:** Shaojun Wang, Wright State University
**Research title:** Exploiting syntactic, semantic and lexical regularities in language modeling
**Funding source:** National Science Foundation, Google, Wright State University

# Promoting PGAS model for petascale computers




The Partitioned Global Address Space (PGAS) programming model has attracted considerable attention in HPC circles, primarily because it offers application programmers the convenience of globally addressable memory along with the locality control needed for scalability. This makes the PGAS models an attractive alternative for petascale computing systems, compared to the hybrid MPI/OpenMP model.

To further develop the PGAS model, Ponnuswamy Sadayappan, Ph.D., professor of computer science and engineering at The Ohio State University, is developing a collaborative research group involving his team and staff members of the Ohio Supercomputer Center (OSC).

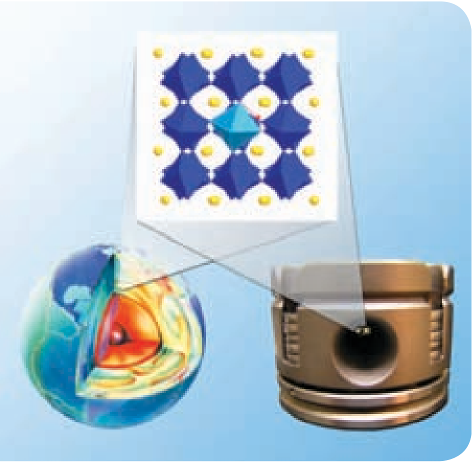
"Although some significant production applications like NWChem have been implemented using the Global Arrays PGAS model, the overall use of PGAS models for developing parallel applications has been very limited," said Sadayappan.

"Several advances are needed for PGAS to become more widely adopted, including compiler/runtime support for enabling existing sequential codes to be transformed and new parallel applications to be developed using PGAS models. The research collaboration with OSC provides significant opportunities to work with the developers of production applications to implement and evaluate our research advances in compiler/runtime systems for PGAS computing."

The group also will explore the integration of several popular HPC programming languages with the PGAS model, according to Ashok Krishnamurthy, interim co-executive director of OSC. Sadayappan has worked with OSC on a number of funded projects, including development of high-performance parallel software for electronic structure calculations and compiler/runtime optimization techniques for multicore CPUs and GPUs. ■

**Project lead:** Ponnuswamy Sadayappan, The Ohio State University
**Research title:** A Parallel Global Address Space framework for petascale computing
**Funding source:** The Ohio State University, Ohio Supercomputer Center

# Determining water capacity of the Earth's mantle



*above:* Crystal structure of a perovskite-structured magnesium and iron silicate (with one hydrogen atom in red), which makes up about 80 percent of the deep mantle.

School children learn that nearly three-quarters of the Earth's surface is covered with water, in the form of oceans, ice, rivers and lakes. However, even our brightest scientists know little about the distribution of water beneath the planet's surface or even how much total water the planet contains.

"The Earth's solid, silicate mantle has the potential to host as much as ten times the water we see on the Earth's surface," said Wendy Panero, Ph.D., assistant professor of earth sciences at The Ohio State University. "Water dissolved in the silicate mantle has dramatic effects on the physical properties and behavior of the planet, such as influencing the long-term shifting and shaping of the surface and interior, decreasing melting temperatures and slowing the speed of earthquake waves."

Evidence suggests that the main mineral of the lower mantle is considerably drier than its shallower counterparts, implying that a water filter may exist 440-660 kilometers beneath the surface. Alternatively, water may exist in the lower mantle, but only in accessory minerals. This hypothesis has important implications on how we interpret present-day sea level rise and the origin and evolution of the planet.

To test her central hypotheses and answer related questions, Panero is leveraging the computational power of the IBM Glenn Cluster at the Ohio Supercomputer Center, paired with state-of-the-art, high-pressure experiments. She performs ab-initio calculations and molecular dynamics simulations to investigate deep-water storage and its effects deep within the Earth's interior. ■

**Project lead:** Wendy R. Panero, The Ohio State University
**Research title:** Computational mineral physics: Water storage and cycling in the Earth's interior
**Funding source:** National Science Foundation

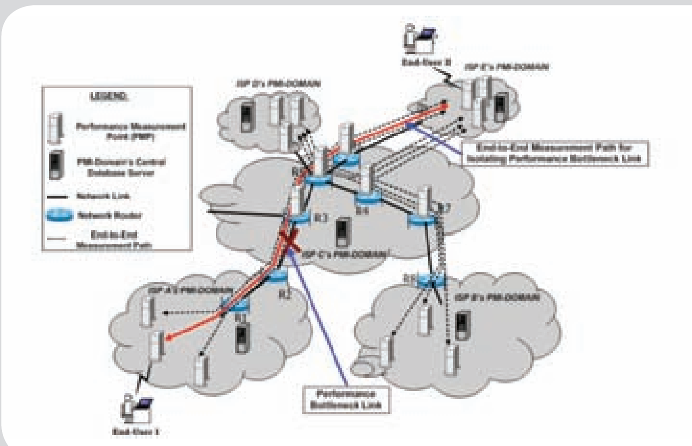
# Monitoring advanced network health status

Prasad Calyam, Ph.D., a senior systems developer and engineer for the Ohio Supercomputer Center (OSC) and Ohio Academic Resources Network (OARnet), is devising methods to improve the performance of next-generation computer networks.

"The next generation of networks will be crucial for transmitting the huge amounts of research data generated for and processed by sophisticated applications, for projects such as the Large Hadron Collider, on high performance computers at universities, Department of Energy labs and businesses," said Calyam.

"In this project, we are developing novel research methods to measure and analyze network health status. The research findings are being incorporated to extend the 'ActiveMon' network health monitoring software that was created earlier at OSC/OARnet.

In another project, Calyam and Paul Schopis, director of networking for OARnet, are creating new techniques to measure data traffic on futuristic, global networks, especially for the National Science Foundation's Global Environment for Network Innovations (GENI) project. GENI will allow researchers throughout the country to build and experiment with completely new and different designs and capabilities that will provide the basis for the creation of a 21st century Internet.



*above:* Multi-Domain PMI System showing End-to-End Measurement Path

"This project will require the integration of software for centralized and distributed orchestration of active data traffic measurements into the on-going efforts of prototype implementation and deployment of the GENI facility," said Calyam. ■

**Project lead:** Prasad Calyam, Ohio Supercomputer Center/Ohio Academic Resources Network
**Research title:** Sampling approaches for multi-domain Internet performance measurement infrastructures to better serve network control and management
**Funding source:** Department of Energy
**Research title:** OnTimeMeasure: Centralized and distributed measurement orchestration software
**Funding source:** National Science Foundation, Raytheon BBN

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**The gratitude of the OSC Outreach Team is extended to all the researchers featured in the preceding pages for their precious time, collaborative spirit and, most of all, fascinating scientific achievements.**

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