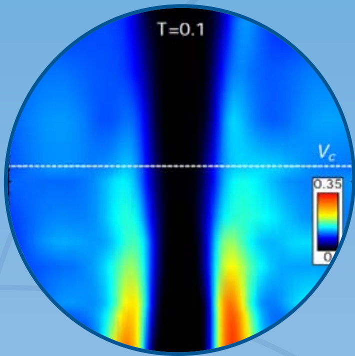

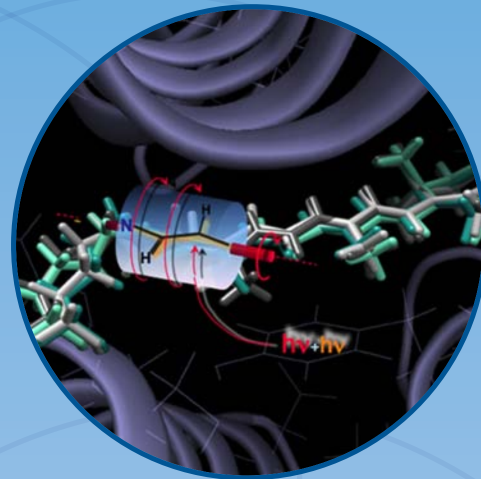


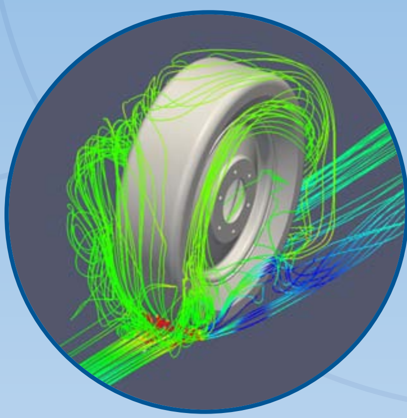



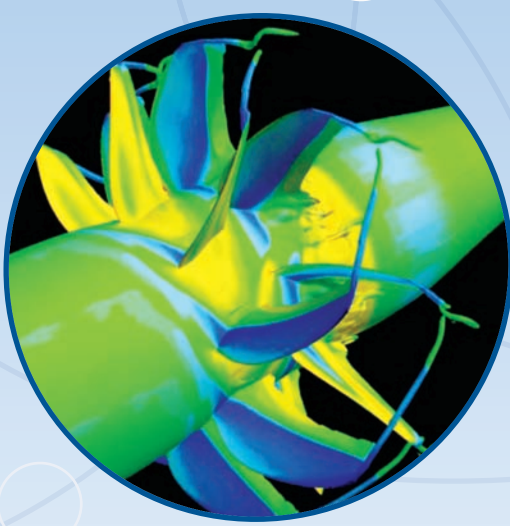

Empower. Partner. Lead.

Ohio Supercomputer Center

2011 Annual **Research** Report

Introduction

Welcome to the Ohio Supercomputer Center!

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

Ashok Krishnamurthy and Steven Gordon, interim co-executive directors

As the supercomputing world has evolved and become increasingly essential and available to industry, government and academia, these powerful resources are being used in ways that influence everyday life, from the cars we drive and the food we eat, to life-saving medical advances we now perceive as commonplace.

As we look ahead to the 25th anniversary of the Ohio Supercomputer Center next year, we both have observed that no matter the changes in computational power or the diversity of applied science projects conducted on our systems over the years, the mission OSC established in 1987 still applies today. Quite simply, we have focused our efforts on maintaining a high level of service to our academic and industrial clients to empower their research and innovation efforts, while advancing projects that support our major strategic goals to partner and lead on projects that generate scientific discovery.

In the last few years, we have made significant strides by prioritizing our efforts in the following areas:

- Focused research in the biosciences, advanced materials and energy and environment
- Application of modeling and simulation in industry to make Ohio more competitive
- Workforce education and training in computational science and engineering

Along the way, we have garnered recognition and respect for the support we have provided to thousands of researchers, the partnerships forged with industry and the national leadership role exhibited in boosting workforce competency through computational science education.

These success stories are evident in this report's highlighted researchers who, by tapping OSC's resources and expertise, have been empowered to tackle a diverse number of projects: analyzing the genetic causes of speech impairments in children; developing warfare nerve agent antidotes that reverse an aging problem; creating evolutionary algorithms that best explain economic phenomena; simulating the formation of micro-thin materials, solar cells and pharmaceuticals; and even helping an electric vehicle set a new land speed record.

Our industrial and workforce development programs – Blue Collar Computing and the Ralph Regula School of Computational Science, respectively – have made great strides this year in bringing small- and medium-sized companies up to speed with the global economy by providing the computational tools and trained staff they needed. As we observe our silver anniversary next year, please join us as we celebrate our path to prominence. From the Ohio Board of Regents to the faculty who advocated for our existence, we – and our clients – owe many of you sincere thanks.

For continuous updates on all OSC activities, please sign up on Facebook or Twitter or engage us at ARMSTRONG.osc.edu, the portal we developed to meet your needs throughout the year.

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

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Ohio Supercomputer Center 2011 Annual Research Report
Published by OSC to present noteworthy research activities during the 2010-11 fiscal period.

Overview

As Chancellor Jim Petro of the Ohio Board of Regents recently stated: "*[We] can no longer delay taking bold action to allow our public universities to drive economic development through innovation.*" In keeping with that vision, the Ohio Supercomputer Center (OSC) accelerates the efforts of universities and industries for prosperity-driven collaborations with innovative results, both statewide and nationally.

OSC's impact on Ohio's economy is most evident in its provision of supercomputing resources to academic and industry researchers, through its ground-breaking Blue Collar Computing industry support program and by way of the innovative, virtual Ralph Regula School of Computational Science. Petro recently created the Ohio Technology Consortium to further strengthen and streamline several related statewide technology initiatives: OSC, the Ohio Academic Resources Network and e-Student Services. The directive aims to "*leverage existing strengths of each organizations and trim administrative costs, technological and management duplication and inefficiency.*"

According to a 2011 report by the Alliance for Science & Technology Research in America, federal research and development spending spur growth and job creation by creating an investment foundation in innovation. For its part, 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.

The most recent survey of nearly two-dozen Ohio universities indicated that faculty members who leverage the center's facilities receive more than $140 million in research funding. OSC contributes to Ohio's ninth place standing in federal R&D spending (2009 figures) and offers the state a significant return on investment.

ARMSTRONG

The Ohio Supercomputer Center launched ARMSTRONG (A Research Management System for Training, Research Opportunities, Notices & Grants) this year to provide Ohio researchers and partners a valuable online research portal. As a 'one-stop digital shop,' ARMSTRONG permits users to:

- Review system usage and track major allocations requests
- Post publications
- Track customized grant opportunities from a feed of relevant federal, state and private postings
- Monitor training schedules and view online tutorials
- Meet other OSC users to partner on research projects and grant proposals
- Match expertise of academic researchers and manufacturers with research needs
- Access a customized portal interface with a dashboard of available applets

Based on user input, OSC staff members have developed additional new features, such as a Twitter feed for HPC notices and events registration. Upcoming versions will connect HPC user account databases directly to the ARMSTRONG portal for instant access to enhanced usage statistics.

In addition to helping faculty win external funding, the Ohio Supercomputer Center (OSC) helps colleges and universities in the state attract and retain talented faculty and partner in new research program investments. Many researchers who work with OSC are able to extend their success nationally in the biosciences, advanced materials and energy/environment. In addition to the many projects detailed throughout this report, two other outstanding examples include:

Hendrik Heinz, Ph.D., an assistant professor of polymer engineering at the University of Akron, leverages OSC's modeling and simulation resources to study the process of biomineralization, nature's ability to form complex structures, such as bones, teeth and mollusk shells, from peptides. He uses this knowledge to bond organic and inorganic material for the purposes of replacing bone, generating energy efficient products and treating diseases.

In addition to tracking the movement and evolution of the avian and swine flu viruses, Dan Janies, Ph.D., an associate professor of Biomedical Informatics at The Ohio State University, leveraged computer systems at OSC to help a national team unlock the evolution of a new class of animals that are actually starfish, but have lost the large star-shaped, adult body from their life cycle.

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 providing support to a Teragrid award received by Somnath Ghosh, Ph.D., professor of civil and mechanical engineering at Johns Hopkins University. His OSU research group is developing a new multi-spatial, multi-time model for material fatigue failure.

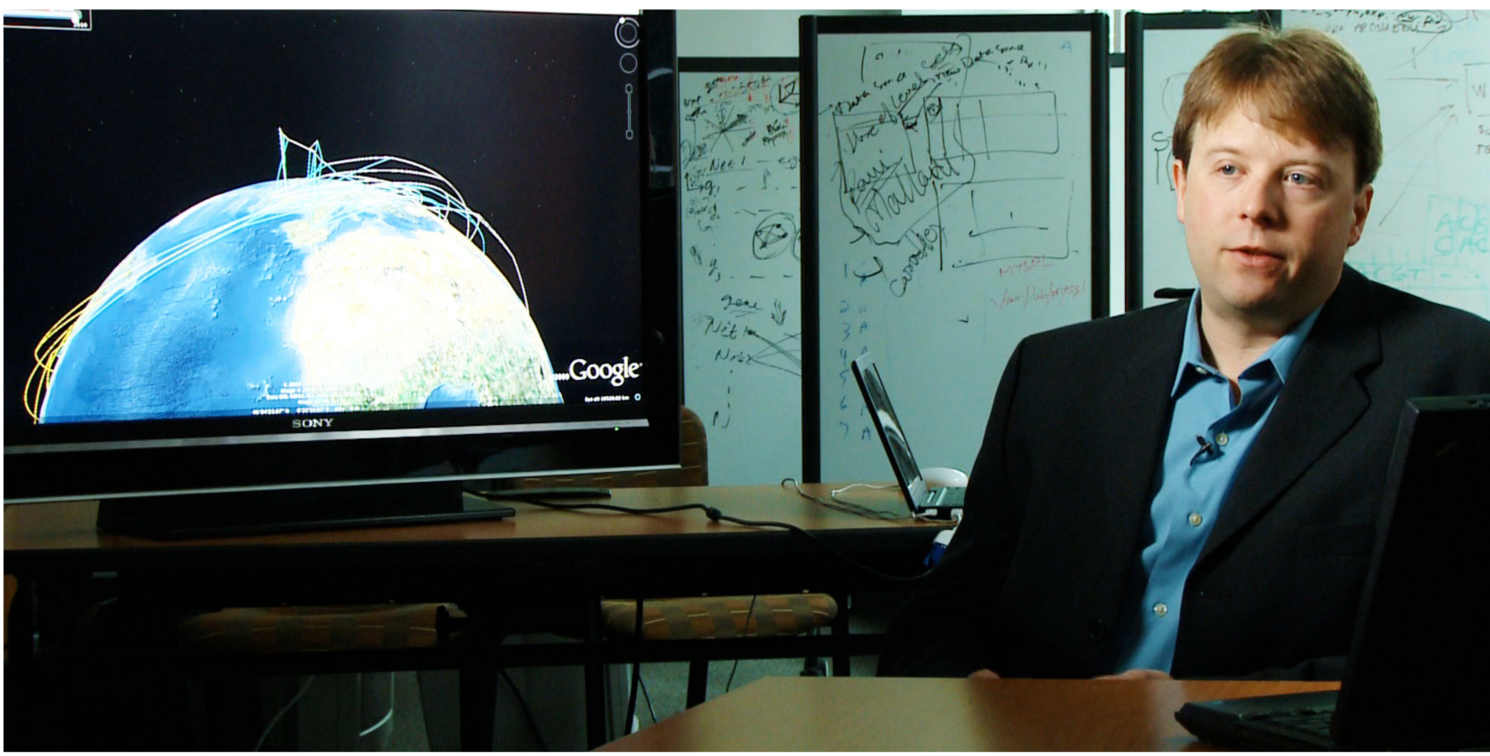
Through our Instrumentation and Analytic Services, OSC provides new software solutions that empower researchers across institutions and disciplines to collaboratively share and use distributed instrumentation – such as electron microscopes, telescopes and spectrometers – that are expensive to purchase and maintain.

A diverse array of companies have taken advantage of the portals, shared remote instrumentation, application hosting and cycles offered through OSC's Blue Collar Computing program.

OSC's accomplishments in 2011 are highlighted in the following sections — hardware and software resources (including the new Oakley Cluster); visualization offerings; Blue Collar Computing; Ralph Regula School; and, most importantly, vignettes of the innovations and discoveries achieved by researchers who use OSC's resources and expertise to create innovative research here, in the state of Ohio. ■

A National Science Foundation (NSF) study found that 73 percent of science papers cited in industry patents were funded by taxpayers through the federal government, especially those involving university research operations.

below: Ohio Supercomputer Center resources have helped Ohio State's Dan Janies analyze the genetic variations and geographic movements of world-wide viruses and track various species of fish that were impacted by oil and chemicals in the Gulf, as well as define the phylogenic placement of Xyloplax, a deep-sea starfish that is evolutionarily "stuck" in its armless, juvenile body plan.



Hardware & Software

As the Ohio Supercomputer Center (OSC) staff prepares to power down Phase I of the Center's flagship IBM Opteron 1350 "Glenn" Cluster in 2012, they are anticipating the installation of a new OSC system slated for late autumn: the Hewlett-Packard "Oakley" Cluster, which features more cores on half the nodes, nearly twice the memory, three times the GPUs and 20 percent more power efficiency. OSC officials selected a system that would fit in the same power envelope as Phase I of the Glenn system with the following specifications:

- A theoretical system peak performance of more than 88 teraflops, plus an additional 65.5 teraflops from GPU accelerators, for a total of 154 teraflops of total peak performance
- A reduction from 500 kilowatts per hour of power consumption from the existing system to 300 kilowatts per hour on the new system
- An increase of more than 600 terabytes of storage space

OSC offers invaluable supercomputing and storage resources to all institutions of higher education in the state, providing support for major research endeavors and saving significant local resources a state-of-the-art, shared facility. This past year, OSC delivered almost 41.5 million CPU hours to researchers, offering a significant portion of the center's computing resources to industrial clients. And, as always, OSC continued to provide a variety of software applications to support all aspects of scientific research.

In addition to the brilliant researchers profiled in this report, OSC supports approximately 2,000 active researchers across the state. Many correspond with staff to indicate their appreciation of the facilities available to them, as in the following examples:

> *"I appreciate the flexibility of OSC in meeting the differing needs of various educational users across the state."* — Stephen Harnish, Ph.D., chair and professor of mathematics at Bluffton University.

> *"I'm glad to report that our collaborative paper has been published this week in Science magazine. Using high throughput sequencing, we found mutations in a non-protein coding, very small RNA gene that result in a severe human developmental disorder called MOPD I. This disorder has been observed in the Amish population in Ohio, along with other populations elsewhere. We thanked the Ohio Supercomputer Center in the acknowledgments. Keiko and I sincerely appreciate the computational resources provided by your center. This sort of state-of-the-art biomedical and bioinformatics research would not be possible without it."* — David E. Symer, Ph.D., M.D., assistant professor of bioinformatics, hematology and oncology, molecular virology, immunology and medical genetics at The Ohio State University Comprehensive Cancer Center. ■

Annie Oakley

"For me, sitting still is harder than any kind of work." — Annie Oakley

Recent Ohio Supercomputer Center systems have been named after important Ohio pioneers. The Glenn Cluster honors astronaut and statesman John Glenn, while the Csuri Advanced GPU environment recognizes computer artist Charles "Chuck" Csuri. The center's next system has been dubbed Oakley, to pay tribute to sharpshooter Annie Oakley.

Oakley was born in a log cabin in eastern Ohio's Darke County in 1860, and died in Greenville 66 years later. She learned to shoot a gun at the age of eight and leveraged that skill to become one of the most famous sharpshooters in American history. She could strike a small metal coin thrown in the air twenty-seven meters away, hit the thin edge of a playing card and shoot it six more times as it fell to the ground, and remove the ashes from a cigarette her husband would hold in his mouth.

For 16 years, Oakley performed as a celebrated markswoman in a traveling Wild West show with "Buffalo Bill" Cody and was introduced to kings, queens and Indian chiefs. She met the famous Native American chief, Sitting Bull, at a performance with her husband, Frank Butler. The chief liked her skill in shooting and her personality so much, he gave her the nickname "Little Sure Shot."

After retiring from the traveling show, Oakley offered to help the military during World War I by training a group of women volunteers who would become soldiers in the war. Her request ignored, she instead visited many training camps to give shooting demonstrations and raise money for medicine and supplies.

In her storied life, Annie overcame poverty, mistreatment and physical injury, helped to break barriers for women with her talent and accomplishments and showed great compassion and generosity to orphans, widows and other young women.

Visualization & Interface

Scientific visualization is based on the synthesis and modeling of three-dimensional phenomena, where vast amounts of clinical, imaging and environmental data can be manipulated in real time to determine the best solution. For instance, researchers may employ a tool in the fight against cancer in the form of a web portal that correlates tumor images with their corresponding genetic codes.

The benefits of visualization extend from bioscience and agriculture to energy and industrial products. The following examples illustrate the wide array of funded modeling and simulation projects the Ohio Supercomputer Center (OSC) supports:

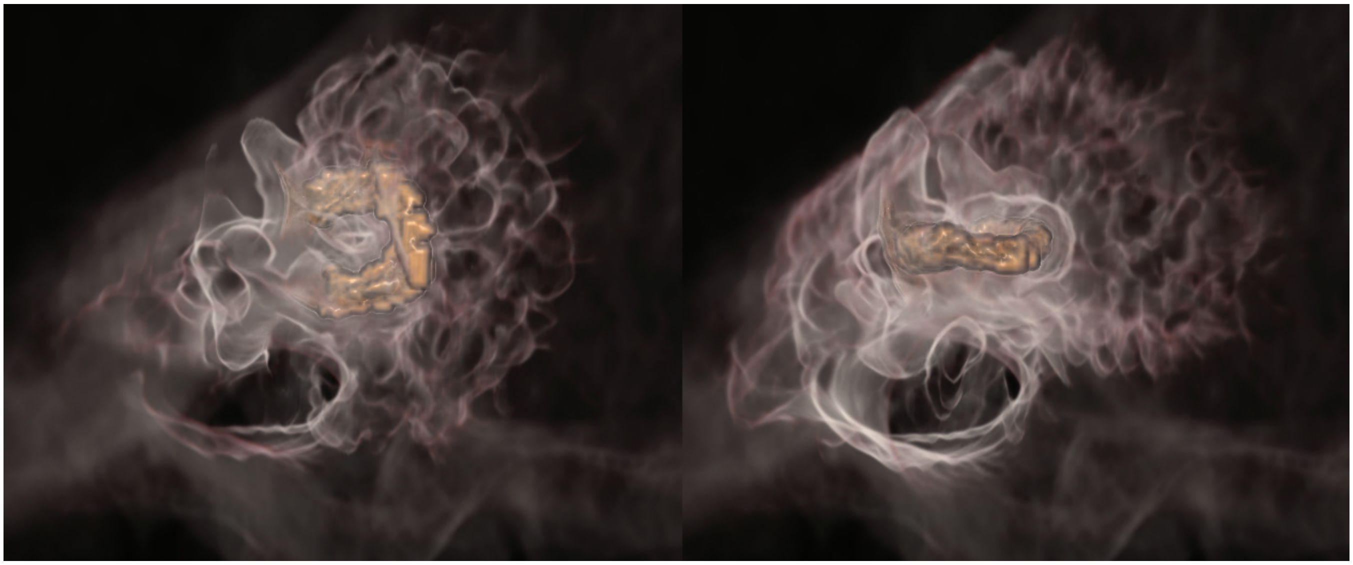
- A research team led by visualization experts at OSC received funding from the National Science Foundation to create an interactive virtual interface of Mammoth Cave so that geoscience students with mobility impairments may explore the geological structures and thereby meet the degree requirements of field-based research (please see page 28 in the Research Landscape section for more detail).
- A temporal bone surgical simulator from OSC was recently used by Nicaraguan ear/nose/throat (ENT) surgical residents as part of a humanitarian initiative to ensure that patients there have access to highly specialized clinical treatment. During a trip to Escuela Hospital Antonio Lenin Fonseca in Managua, Nicaragua, in January 2011, Dr. Greg Wiet of Nationwide Children's Hospital and The Ohio State University (OSU) and his team delivered touch-enabled training to otolaryngology residents using the simulator, which integrates stereo graphics, audio and force-feedback (haptics).
- A joint project with the OSU Veterinary School supports the effort to create digital models of animal anatomy through non-invasive, in-vivo imaging acquisition. OSC experts are working with vet students, surgical faculty and computational technologists to promote the adoption and adaptation of simulation technologies for use in the veterinary surgical teaching curriculum.

above: Otolaryngology residents in Nicaragua recently honed their surgical skills with a simulation system developed at Nationwide Children's Hospital, The Ohio State University and the Ohio Supercomputer Center.

In addition, the Center has developed new modeling and simulation services for a wide constituency of researchers:

- For Kun Huang, Ph.D., associate professor of biomedical informatics at OSU, OSC specialists are mirroring the University of California, Santa Cruz, genomics database, installing and supporting the SOLID/Lifescope software required for analysis of generated data by running PhemoLIMS, a lab information system. Being able to combine clinical results with other medical markers and microscopic data results in high-impact projects in translational medicine.
- Working with Dave Billiter, director of the Research Informatics Core at the Research Institute at Nationwide Children's Hospital, OSC staff members are providing data storage and remote visualization of histo-pathological images for the Children's Oncology Group. OSC experts are creating a set of services relating to the capture, analysis and remote visualization of image data from high-resolution microscopes (such as multi-photon microscopes) and histo-pathological tissue scanners.

below: These images of the posterior and lateral semicircular canals are generated with a distance field renderer that highlights the anatomical structure in the context of the bone in which it is embedded. The semicircular canals are part of the inner ear and give people their sense of balance.



Posterior

Lateral

Blue Collar Computing

Through its Blue Collar Computing™ program, the Ohio Supercomputer Center has taken a leading role in promoting the use of computational modeling to make industry more competitive, serving more than 55 individual industrial clients through access to OSC's hardware, software, expertise, training and customized portals. In FY2011, industry consumed almost 1.5 million CPU hours, about 3.4 percent of the total usage of OSC's flagship Glenn Cluster. This percentage is expected to grow as staff members implement several new projects aimed at providing digital manufacturing services to the 'missing middle,' promoted by national groups like the Alliance for High Performance Digital Manufacturing (AHPDM).

In addition to collaborations with AHPDM, a group of HPC industries, economic-development organizations and supercomputing centers dedicated to changing the way America manufactures by bringing the power of high performance computing (HPC) to the value chain, OSC is one of four solution providers working with the National Digital Engineering and Manufacturing Consortium (NDEMC). NDEMC was established by the Council on Competitiveness and is funded by the U.S. Economic Development Administration to introduce modeling, simulation and analysis to small- and medium-sized manufacturers (SMEs) who do not have resources to bring this technology into their workflow. In addition to an improved and diversified product base of manufacturers, such as Procter & Gamble, Lockheed Martin, GE and John Deere, expected outcomes include job-retention, new exports and reshoring. OSC's subject-matter experts plan to offer specialized web portals based on requirements from these large companies to assist manufacturing suppliers. A manifold flow predictor is already in development to determine the consistency and properties in the spread of liquids, such as the glue used for cardboard packaging.

A grant from National Institute of Standards and Technology Manufacturing Extension Partnership (NIST MEP) program was renewed for a second year to expand the scope and reach of the Polymer Portal, a "one-stop" resource that bundles access to OSC's supercomputers, software and training in computation and 3-D modeling. OSC is partnering with PolymerOhio to provide, on a short-term licensing basis, access to an injection-molding package called Moldex3D, allowing SMEs to use that sophisticated software. The site also features web-based applications designed to help increase productivity for polymer companies, including those in the plastics, rubber and advanced materials sectors. Once the advantage of larger companies, supercomputing through the Polymer Portal now offers a pay-per-use model that provides a scalable and immediately accessible alternative, opening the door for smaller companies to aggressively create new products and enter favorable global markets.

above: Ohio Supercomputer Center Co-executive Director Ashok Krishnamurthy (far right) recently met at the White House with administration, technology and manufacturing officials to help announce a nearly $5 million public-private initiative to help small- and medium-sized manufacturers in the Midwest compete in the 21st century global economy.

Also this year, OSC's entry on the EWI WeldPredictor was selected as one of nine winners in the first round of International Data Corporation's HPC Innovation Excellence Awards. This award recognizes major HPC-supported achievements in industry, government and academia toward the goal of demonstrating the close link between HPC and economic/scientific innovation and competitiveness.

All of these activities help to reinforce the national goals outlined by the President's Council of Advisors on Science and Technology in their Report to the President on Ensuring American Leadership in Advanced Manufacturing of June 2011:

- Invest in shared infrastructure facilities, including Federal and university laboratories, which could be easily accessed by small and medium-sized firms and would facilitate significant productivity gains by allowing those companies to rapidly prototype, customize, test and produce new products.
- Support the development of advanced manufacturing processes that cut across multiple industry sectors and could be used by an array of companies to dramatically reduce product development time and increase entrepreneurs' ability to design and transition their inventions into products made in the United States.
- Participate in partnerships with industry and academia that identify and invest in broadly applicable, precompetitive, emerging technologies that have the potential to transform the manufacturing sector. ■

"The missing middle really isn't missing — it is poised on the brink of a manufacturing renaissance." – John Kirklen, Editor, Digital Manufacturing Report

Polymer Portal

The Polymer Portal is a "one-stop resource" that bundles access to commercial software modeling and simulation services with training in computation and 3-D modeling.

Developed by PolymerOhio, Inc. and the Ohio Supercomputer Center (OSC), the portal features web-based applications designed to help increase productivity for polymer companies, including firms from the plastics, rubber and advanced materials segments. The applications featured on the site transparently access OSC's supercomputing systems and software to accelerate product and process development, as well as problem-solving, by allowing engineers to quickly conduct "what-if scenario" calculations.

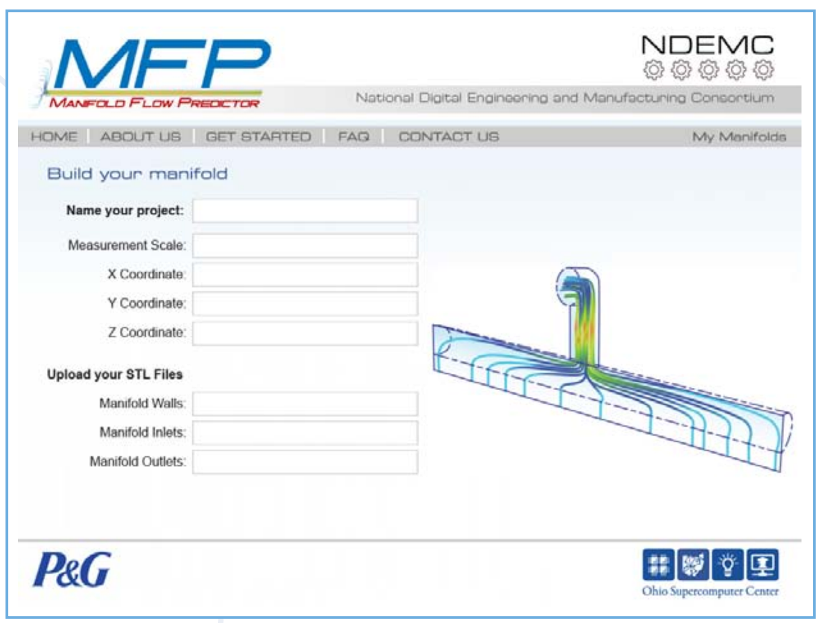
The site targets smaller polymer companies to help them address the technical barriers, costs and training necessary to effectively use this technology. Large companies have long seen competitive advantages from high performance computing and modeling & simulation applications. For example, General Motors uses parallel computing to simulate crash testing automobiles and claims that it can reduce the number of full-size crash vehicle tests by more than 85 percent. Similarly, supercomputing simulations have reduced the cost that Goodyear spends on physical tire prototypes from 40 percent to 15 percent.

Manifold Flow Predictor

Manifolds involve a large category of industrial applications that uses pipes, hoses, sprinklers or vacuums to move either air or fluids through several openings, from spraying glue on a cereal box lid to capturing smoke from a boiler.

Large manufacturers require advanced modeling and simulation to predict the properties of manifolds through computational fluid dynamics (CFD). Creating the algorithms that make these predictions currently requires computational experts, software and high performance computing.

The Ohio Supercomputer Center (OSC), Procter & Gamble and TotalSim, Inc. have created an application called the Manifold Flow Predictor (MFP) as part of an effort by the National Digital Manufacturing Consortium (NDEMC) to extend CFD capabilities to smaller manufacturers. To use the MFP web portal, an engineer enters a CAD file describing the manifold, selects the fluid (e.g., water, air, glue, hydraulic fluid) and enters an input pressure. The CFD and visualizations are calculated using OSC resources and displayed to the user. MFP is currently in development and a release is planned for 2012.



above: OSC's Manifold Predictor can be used by manufacturers to reduce variations in a fluid's spread, such as filling liquid into a detergent bottle.

The Ralph Regula School of Computational Science

"We hope to work with universities around the country to formalize computational science education programs and prepare a future workforce that can apply computational modeling to solve challenging science and engineering problems."

— Steven Gordon, Ph.D., Ralph Regula School director and XSEDE education program lead

Supercomputing is the technological foundation for large-scale, data-intensive science and engineering. Computational science is the application of this type of high-end modeling and simulation that enables researchers to "see" the unobservable – phenomena that are too small (atoms and molecules), too large (galaxies and the universe), too fast (photosynthesis), too slow (geological processes), too complex (jet engines) or too dangerous (toxic materials). A knowledgeable workforce that understands what supercomputers can do, as well as how to use computational science effectively, is needed to improve our lives.

Through the virtual Ralph Regula School of Computational Science and in cooperation with Ohio's colleges and universities, the Ohio Supercomputer Center (OSC) continues to be recognized as a national leader as it makes major strides in developing a computationally skilled workforce.

Based on the Ralph Regula School's strong reputation in workforce development, Steven Gordon, Ph.D., interim co-executive director at OSC, was selected to lead the National Science Foundation's Extreme Science and Engineering Discovery Environment (XSEDE) project. Part of the XSEDE support infrastructure for NSF's national supercomputing program, the education and outreach mission is to answer a critical need to advance computational science and engineering by recruiting, preparing and sustaining a large and diverse scientific academic and industrial workforce using the XSEDE cyberinfrastructure ecosystem.

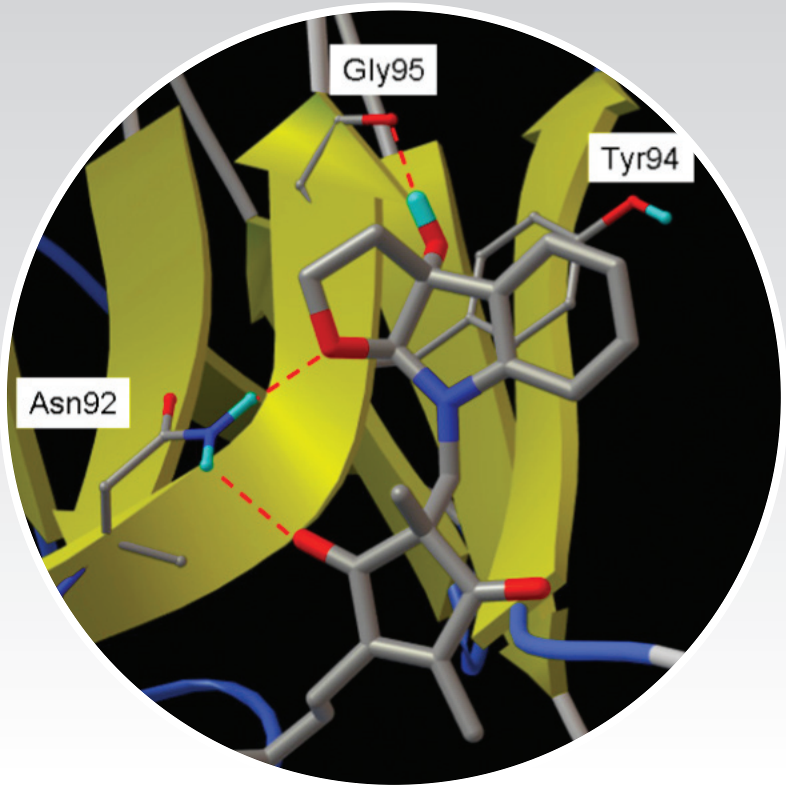
Others are taking note of the Ralph Regula School industry certificate programs funded by the National Science Foundation and the National Institute for Standards and Technology Manufacturing Extension Partnerships (NIST MEP) in conjunction with PolymerOhio. Moldex3D and OSC have agreed to jointly support the center's efforts to train Ohio's workforce in advanced modeling and simulation skills required for polymer manufacturing, such as simulations in injection molding. And OSC staff members associated with the National Digital Engineering and Manufacturing Consortium (NDEMC) help industrial clients with the required training needed to develop advanced manufacturing production.

During the past year, OSC has engaged in the following workforce development activities:

- Developed a Ralph Regula School Internship Portal to connect educators, employers and students looking for computational science opportunities to each other
- Conducted workshops for dozens of faculty and graduate students to assist in their use of OSC's computational resources
- Continued OSC's high-school Summer Institute for the 22nd year and middle-school Young Women's Summer Institute for the 12th year
- Led the OSU effort supporting the Ohio Bioinformatics Consortium, providing Choose Ohio First scholarships to students in bioscience-related fields
- Hosted more than 13 student interns from Metro High School, a collaborative initiative of Battelle, The Ohio State University and Franklin County Education Council, to conduct in-depth research projects at OSC

Gordon also was selected as president-elect of the Great Lakes Consortium for Petascale Computation, a collaboration of colleges, universities, national research laboratories and other educational institutions facilitating the widespread and effective use of petascale computing. ■

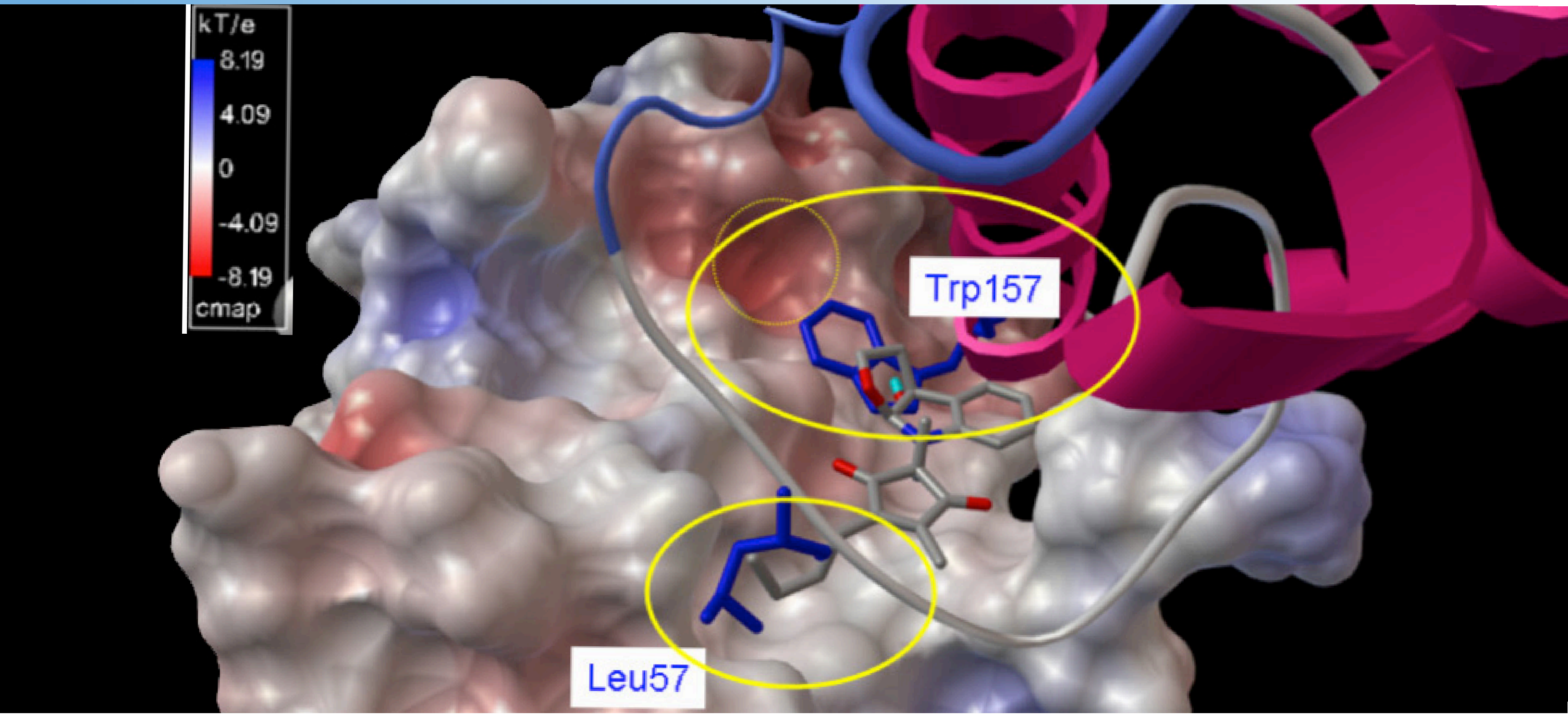
below: Through the Ralph Regula School of Computational Science, the Ohio Supercomputer Center and its partners offer a continuum of science, technology, engineering and mathematics (STEM) educational opportunities, from junior-high summer institutes to college-level programs to workforce certificates.



A simulation created at the Ohio Supercomputer Center by Chenglong Li illustrates MDL-A (ball-and-stick) binding with a section of GP130 (yellow ribbon). Li is using fragment-based drug design to find potential solutions to suppressing Interleukin-6.

Biological Sciences

Ohio's bioscience researchers are gathering and analyzing vast amounts of genetic, molecular and environmental data to target diagnosis and treatment of disease, improve understanding of intricate systems and optimize valuable biological traits. For example, a biophysicist is manipulating simulated enzyme fragments to create potent, new cancer-fighting drug candidates. Another scientist is studying a strain of bacteria that has the potential to provide light in alternative environments. And, a chemist is developing techniques to help combatants fight off the deadly effects of neurotoxins. More than 1,345 bioscience-related organizations call Ohio home, employing more than 62,000 highly skilled workers, according to BioOhio, a nonprofit industry association. The following pages illustrate just a few examples of cutting-edge biosciences research supported by Ohio Supercomputer Center resources and services.



above: An electrostatic representation (red: negative; blue: positive; white: hydrophobic) created at the Ohio Supercomputer Center by Ohio State's Chenglong Li shows the immune-response messenger IL-6 in ribbon representation. Two yellow ellipses indicate binding "hot spots" between IL-6 and the common signal-transducing receptor GP130.

Li leverages fragment-based drug design to **block cancer precursor**

The human body normally produces an immune-response messenger known as Interleukin-6 (IL-6) to combat infections, burns and traumatic injuries. Scientists have found, however, that in people who have breast or prostate cancer, the body fails to turn off the response and overproduces the protein molecule IL-6, causing inflammation.

"There is an inherent connection between inflammation and cancer," explained Chenglong Li, Ph.D., an associate professor of medicinal chemistry and pharmacognosy at The Ohio State University (OSU). *"In the case of breast cancers, a medical review systematically tabulated IL-6 levels in various categories of cancer patients, all showing that IL-6 levels elevated up to 40-fold."*

In 2002, Japanese researchers found that madindoline A (MDL-A) could be used to mildly suppress the IL-6 signal. About the same time, Stanford scientists constructed a static image of the crystal structure of IL-6 and two related proteins. Li recognized the potential of these initial insights and partnered with an organic chemist and a cancer biologist at OSU's James Cancer Hospital to investigate further, using Ohio Supercomputer Center systems to construct malleable, three-dimensional color simulations of the protein complex.

Li simulated IL-6 and the two additional helper proteins: receptors IL-6R and GP130. Two full sets of the three proteins often combine to form a six-sided "hexamer" to transmit signals that will, in time, cause cellular inflammation. Li defined the interactions between those proteins and the strength of their binding at five 'hot spots' found in each half of the IL-6/IL-6R/GP130 hexamer.

By plugging small molecules, like MDL-A, into any of those hot spots, Li would be able to identify the most effective binding site for blocking the formation of the hexamer. So, he examined the binding strength of MDL-A at each of the hexamer hotspots, identifying the most promising location, which turned out to be between IL-6 and the first segment, or modular domain (D1), of the GP130 protein.

To design even more effective derivatives of MDL-A that would dock with D1 at that specific hot spot, Li searched through more than 6,000 drug fragments, identifying two potential solutions by combining the "top" half of the MDL-A molecule with the "bottom" half of a benzyl or a pyrazole fragment. These candidates preserve the important binding features of the MDL-A, while yielding molecules with stronger molecular bindings that also are easier to synthesize than the original MDL-A.

"We're making excellent progress," said Li. *"The current research offers us an exciting new therapeutic paradigm: targeting the tumor microenvironment and inhibiting tumor stem cell renewal, leading to a really effective way to overcome breast tumor drug resistance, inhibiting tumor metastasis and stopping tumor recurrence."*

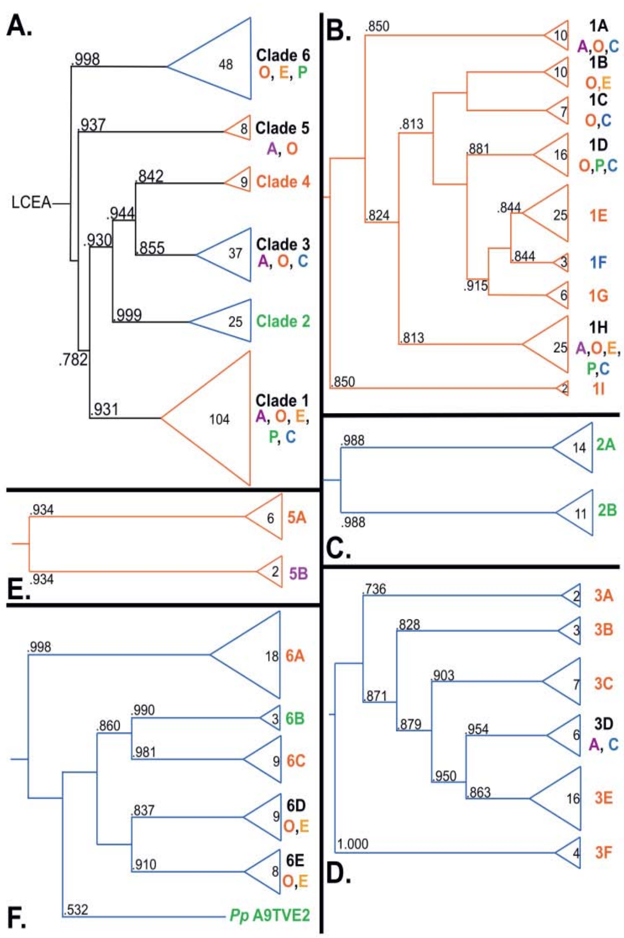
Project lead: Chenglong Li, The Ohio State University

Research title: Designing drugs to stop IL-6 signaling for anti-cancer therapy

Funding source: Department of Defense

Web site: pharmacy.osu.edu/programs/medchem/faculty/chenglong_li/

Lamb analyzes evolutionary history of **enzyme behind diseases**



above: Ohio State's Rebecca Lamb analyzed the evolutionary history of the poly(ADP-ribose)polymerase (PARP) enzyme superfamily, a protein group implicated in a wide range of human diseases and, therefore, serve as important targets for anti-cancer therapies.

A group of enzymes implicated in a wide range of human diseases are important targets for anti-cancer therapies and the targets of a study by a molecular biologist to more fully understand the enzymes by helping to better define the group's family tree.

Along with several of her Ohio State University colleagues, Rebecca S. Lamb, Ph.D., an assistant professor of molecular genetics, recently analyzed the evolutionary history of the poly(ADP-ribose)polymerase (PARP) superfamily. These proteins are found in eukaryotes, a wide range of organisms – animals, plants, molds, fungi, algae and protozoa – whose cells contain complex structures enclosed within membranes. While PARP proteins can be found within any of these 'supergroups,' they have been studied most extensively in mammals.

*"In these organisms, PARPs have key functions in DNA repair, genome integrity and epigenetic regulation," said Lamb. "*More recently it has been found that proteins within the PARP superfamily have a broader range of functions than initially predicted."

The researchers used computers to identify 236 PARP proteins from 77 species across five of the six supergroups. Lamb then accessed systems at the Ohio Supercomputer Center to perform extensive phylogenetic analyses of the identified PARP regions, computationally intensive work that would have been impossible without such resources, according to Lamb. In particular, the ability to try a variety of tools that require a great deal of CPU and memory capabilities was essential. Among the software tools she employed was the PhyML3.0 package, which fit a statistical model to the aligned sequence data and provided estimates for the model's parameters.

"PARPs are found in all eukaryotic supergroups for which sequences are available, but some individual lineages within supergroups have independently lost these genes," said Lamb. *"The PARP superfamily can be subdivided into six branches or 'clades.' Two of these clades were likely found in the last common eukaryotic ancestor. In addition, we have identified PARPs in organisms for which they have not previously been described."*

Three main conclusions were drawn from the study. First, the broad distribution and pattern of representation of PARP genes indicated to the researchers that the ancestor of all existing eukaryotes encoded proteins of this type and may have had multiple members. Second, the ancestral PARP proteins had different functions and activities. One of these proteins likely functioned in DNA damage response. Third, the diversity of the PARP superfamily is larger than previously documented, suggesting as more eukaryotic genomes become available, this gene family will grow in both number and type. ■

Project lead: Rebecca S. Lamb, The Ohio State University
Research title: Evolutionary history of the poly(ADP-ribose) polymerase gene family in eukaryotes
Funding sources: Ohio Plant Biotechnology Consortium, The Ohio State University
Web site: www.biosci.ohio-state.edu/pcmb/osu_pcmb/faculty_sites/rebecca_lamb/index.html

Bartlett looking for genetic key to

specific-language impairments

Of all the American school children receiving special education services, the largest number suffer from learning language impairments, including a subset of children that have language as their only deficit. Specifically Language Impaired (SLI) children have weakened language ability but otherwise possess normal hearing, education and intelligence.

"My laboratory staff examines DNA from families that have multiple persons with specific language impairment," said Christopher W. Bartlett, Ph.D., an assistant professor at The Research Institute at Nationwide Children's Hospital and The Ohio State University (OSU). *"The laboratory of my collaborator, Dr. Stephen A. Petrill, a professor of human development and family science at OSU, works directly with the families to enroll them in the study.* Then we work together to understand how the DNA data and analysis from my group can be understood in the context of language difficulties."*

Bartlett points out that while several studies consistently have shown that SLI can be inherited, only a handful have begun discovering specific molecular genetic causes of the disorder. Bartlett's group found strong evidence of a genetic variation associated with SLI, located on the human chromosome 13q21; however the specific version of the gene that increases susceptibility to SLI, he noted, has not yet been identified. The work is greatly complicated since language involves many underlying biological processes in the brain, including multilevel interactions of many genes.

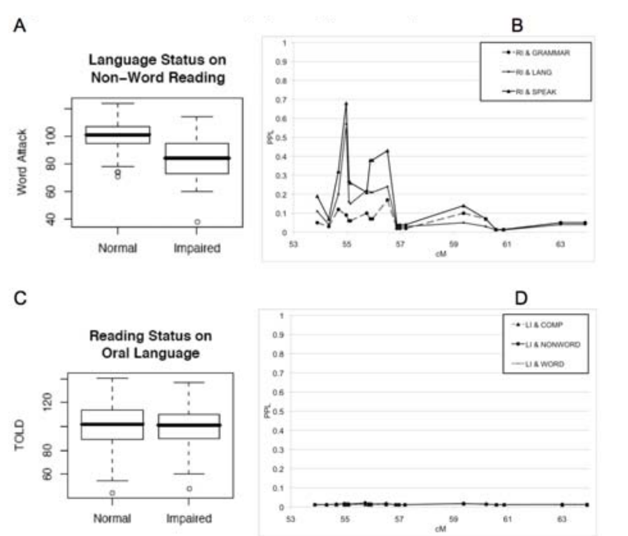
This type of genetic analysis typically involves millions of likelihood calculations at each genetic position linked to the trait under investigation. To speed up this process, Bartlett applied algebraic computation that achieved a speed-up factor of around 20 to 40.

"The gain of speed-up comes at the expense of memory demand, as large polynomials are stored in the memory for fast access," Bartlett said. *"For complex pedigrees, the memory consumption can go as high as 64 gigabytes, if not more. Once the polynomial is built, the evaluation process is highly parallelized, and we have been able to utilize the high memory and multi-core nodes of Ohio Supercomputer Center clusters to the full extent to complete our important research, which would otherwise be impossible or too slow to conduct."*

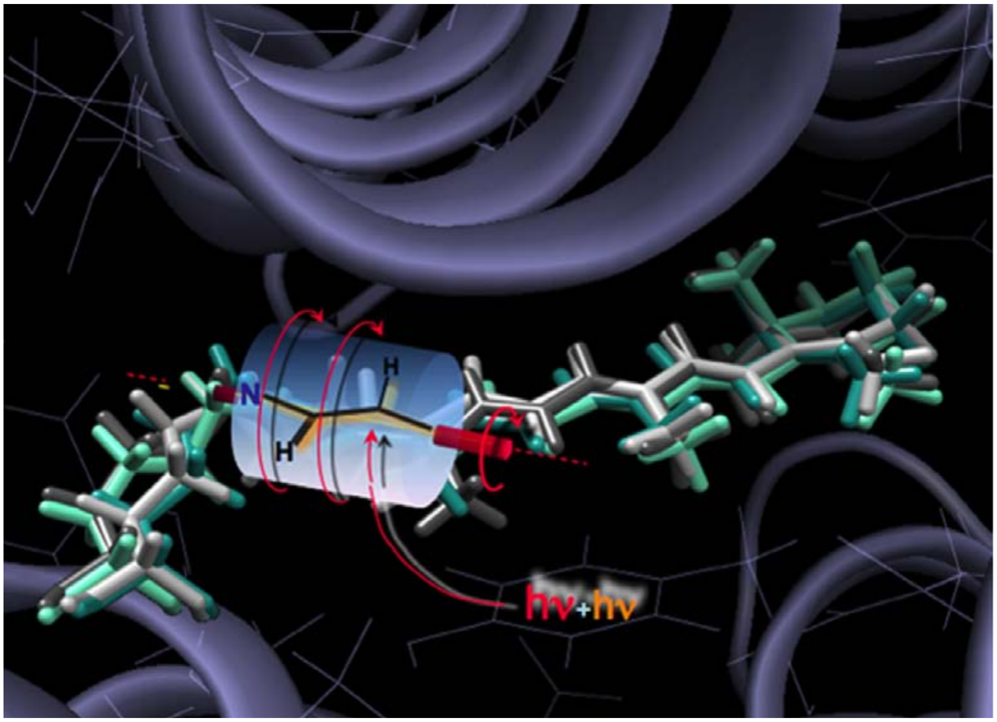
The aims of the project are important, according to Bartlett, because they link genetic analysis with the multiple cognitive pathways that may lead to SLI in the hopes of earlier identification in patients and earlier intervention with the goal of much better language outcomes for the children. ■

*Families interested in finding out more about the study can email bls@ehe.osu.edu for details.

Project lead: Christopher W. Bartlett, Research Institute at Nationwide Children's Hospital and The Ohio State University
Research title: The biology of language study
Funding source: National Institutes of Health
Web site: www.mathmed.org/#Christopher_Bartlett



Leveraging Ohio Supercomputer Center resources, Christopher Bartlett at the Research Institute at Nationwide Children's Hospital (left) employed a unique statistical model to clarify relationships between clinical diagnosis and quantitative variation (above).



left: In a simulation created at the Ohio Supercomputer Center by Bowling Green's Massimo Olivucci, a short fragment of the long retinal chromophore backbone of Anabaena Sensory Rhodopsin undergoes a complete clockwise rotation powered by the energy carried by two photons.

Olivucci assesses potential, **implications of bacterial photoreceptors**

Blue-green algae are causing havoc in Midwestern lakes saturated with agricultural run-off, but in a northwest Ohio lab, researchers are studying how to harness the positive properties of a closely related strain of bacteria – *Anabaena*.

"An in-depth understanding of light sensing, harvesting and energy conversion in Anabaena may allow us to engineer this and related organisms to thrive in diverse illumination conditions," said Massimo Olivucci, Ph.D., a research professor of chemistry at Bowling Green State University. *"Such new properties would contribute to the field of alternative energy via the microbial conversion of water and light to oxygen and hydrogen. Biophysical studies of the bacterial photoreceptor and its underlying molecular mechanisms can help us to understand its biotechnological potentials and the associated environmental implications."*

Olivucci's research focuses on a sensory protein found in the Anabaena sensory rhodopsin (ASR) bacteria. ASR senses light of two different colors and behaves like the "eye" of Anabaena, which serves as a model for cyanobacteria, the scientific term for freshwater blue-green algae. Cyanobacteria use sunlight as an energy source, and ASR controls sensing green light to activate a cascade of light-sensitive reactions.

"We are constructing quantum-mechanical and molecular-mechanical models on Ohio Supercomputer Center systems," Olivucci explained. *"Past simulations have revealed that light induces a molecular-level rotary motion in the protein interior. Now, the same computer models will be used to engineer hundreds of mutants that display programmed spectroscopic, photochemical and photobiological properties and identify which mutants should be prepared in the laboratory. This new approach constitutes a unique opportunity for developing computational tools useful for understanding the molecular factors that control the spectra of proteins and their photo-responsive properties in general."*

Olivucci noted that protein mutants displaying properties, such as high-binding affinities and novel catalytic activities, have been designed using computational tools based on molecular mechanics. He pointed out, however, that the design of mutants with specific responses to light represents a more complex problem. In these cases, he employs ab initio complete-active-space self-consistent-field method and multi-configurational second-order perturbation theory computations – quantum chemical methods capable of describing both ground and electronically excited states of the ASR.

Olivucci's research will lead to an unprecedented tool by which hundreds to thousands of mutant models can be screened for wanted properties, such as color, excited state lifetime or photochemical transformations. This will provide tailored genetic materials for generating organisms that, for instance, can thrive under alternative light conditions and modulate biomass production or be used in engineering applications. ■

Project lead: Massimo Olivucci, Bowling Green State University

Research title: Computational engineering and predictions of excited state properties of bacterial photoreceptor mutants

Funding sources: Ohio Board of Regents, Bowling Green State University

Web site: www.bgsu.edu/departments/photochem/people/molivuc.html

Hadad **developing reagent solution** to deadly nerve agent exposure

Scientists at The Ohio State University (OSU) are working to develop a drug that will regenerate a critical enzyme that "ages" after a person is exposed to deadly chemical warfare agents. To help develop a more effective antidote to organophosphorus (OP) nerve agents, Christopher Hadad, Ph.D., professor of chemistry, is combining findings from the biochemical studies of his partners with synthetic and computational organic chemistry his research team is conducting at OSU and the Ohio Supercomputer Center.

OP nerve agents inhibit the ability of an enzyme called acetylcholinesterase (AChE) to turn off the messages being delivered by acetylcholine (ACh), a neurotransmitter, to activate various muscles, glands and organs. After exposure to OP agents, AChE undergoes a series of reactions, culminating in an "aging" process that inhibits AChE from performing its critical biological function. Without the application of an effective antidote, neurosynaptic communication continues unabated, resulting in uncontrolled secretions and muscle spasms, which, if untreated, result in death.

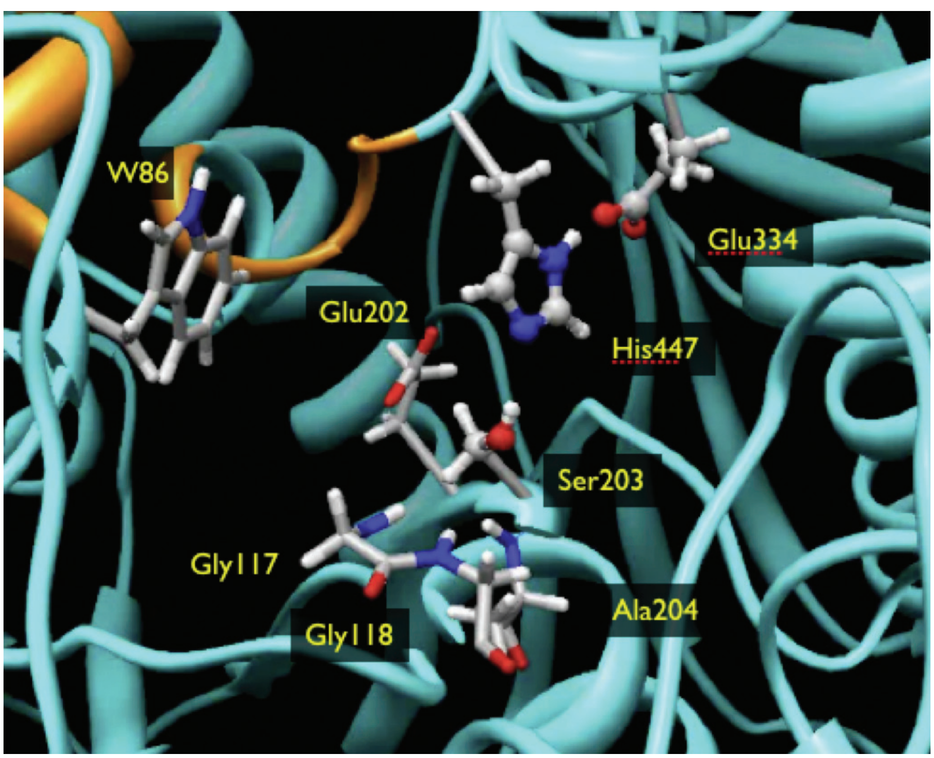
Conventional antidotes to OP nerve agents block nerve agent activity by introducing oxime compounds, which have been the focus of several studies. These compounds attach to the phosphorus atom of the nerve agent, after the OP is bound to AChE, and then split it away from the AChE enzyme, allowing the AChE to engage with receptors and finally relax the tissues.

However, in some cases, the combined nerve agent/AChE molecule undergoes a process called aging, in which groups of single-bonded carbon and hydrogen atoms called alkyl groups are removed from the molecule, and a phosphonate residue is left behind in the AChE active site. Relatively unstudied in nerve agents, this "dealkylation" process, makes the nerve agent/AChE molecule unreceptive to oxime treatments – an unfortunate situation, considering that certain nerve agents (e.g., soman) can undergo aging within minutes of exposure to AChE.

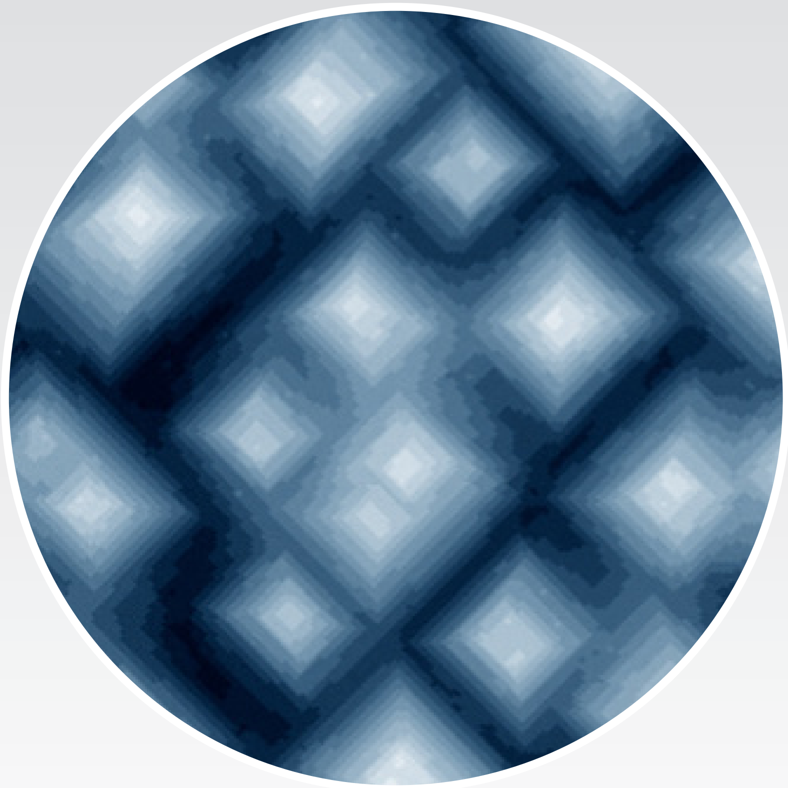
Hadad is studying compounds that would return an appropriate alkyl group to the aged nerve agent/AChE molecule, thus allowing treatment with oximes to provide for complete recovery. The project is focusing on numerous common OP nerve agents, which take on a similar molecular structure upon aging.

"Computational studies of the interaction of the alkylating compounds with AChE were used to provide insight for the design of selective reagents," Hadad explained. *"Ligand-receptor docking, followed by molecular dynamics simulations of the interactions of alkylating compounds with aged OP-AChE, was carried out in conjunction with experimental studies to investigate the binding of alkylating compounds to AChE. These results were then used to suggest interactions that aided in the orientation of alkylating compounds for maximal efficacy."* ■

Project lead: Christopher Hadad, The Ohio State University
Research title: Design of an alkylating agent with specificity for acetylcholinesterase to reactivate the aged enzyme following nerve agent exposure
Funding source: Defense Threat Reduction Agency
Web site: hadad.group.chemistry.ohio-state.edu/



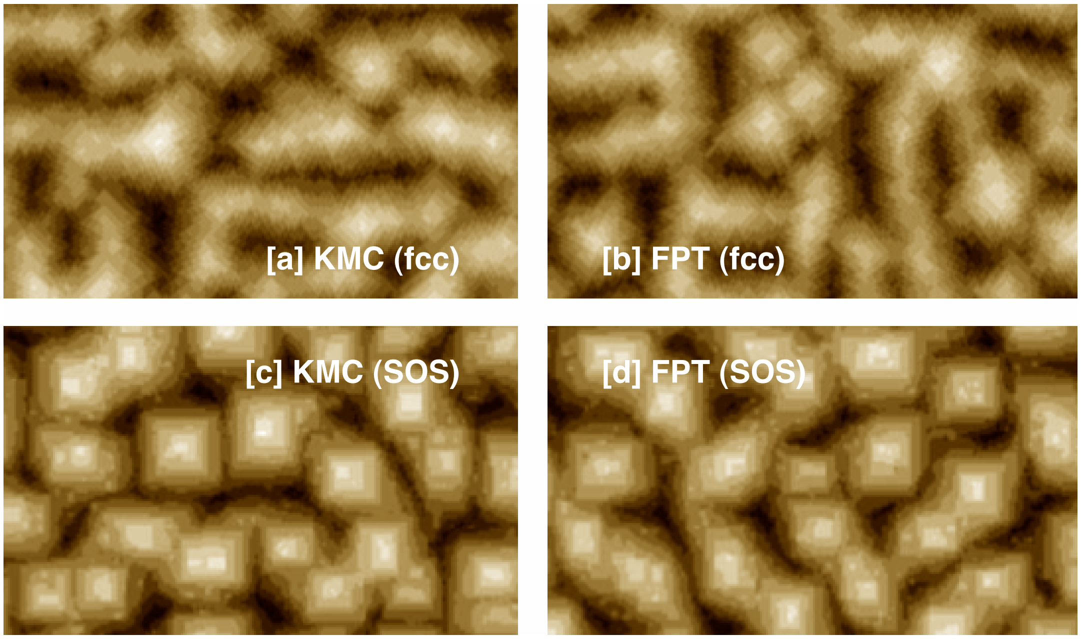
left: Preliminary simulations conducted by Christopher Hadad identify catalytic amino acid residues and other critical binding residues in the active site of AChE.



Jacques Amar accessed Ohio Supercomputer Center systems to investigate a new mathematical approach that accelerates some complex computer calculations used to simulate the formation of micro-thin materials.

Advanced Materials

Ohio's world-class polymer and advanced materials industries have long driven the state's economy, employing more than 81,000 people, according to the Ohio Department of Development. Materials researchers here are conducting ground-breaking studies of polymers and various other advanced materials, such as composites, nanomaterials, liquid crystals and bio-based materials. For example, an engineer is collaborating with industry experimentalists to study value-added composite materials. A chemist is investigating molecular systems that play a key role in drug delivery and the release of fragrances from household goods. And, a scientist is investigating how polymers age, experiencing mechanical deformation and cracks. 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.



left: The University of Toledo's Jacques Amar leveraged Ohio Supercomputer Center systems to test an accelerated approach to simulating thin film growth. Using two different models (labeled fcc and SOS), Amar compared the regular Kinetic Monte Carlo method (figures a and c) with a first-passage-time approach coupled with the KMC method (figures b and d).

Amar's approach **speeds computer simulations** of thin film growth

Thin films are used in industry to create a variety of products, such as semiconductors, optical coatings, pharmaceuticals and solar cells. A new mathematical approach developed by Jacques Amar, Ph.D., professor of physics at the University of Toledo, accelerates some complex computer calculations used to simulate the formation of micro-thin materials.

Employing Ohio Supercomputer Center systems, Amar implemented a "first-passage time approach" to speed up simulations of materials being created just a few atoms thick. He used Kinetic Monte Carlo (KMC) methods to simulate the molecular beam epitaxy (MBE) process, where metals are heated until they transition into a gaseous state and then reform as thin films by condensing on a wafer in single-crystal thick layers.

"One of the main advantages of MBE is the ability to control the deposition of thin films and atomic structures on the atomic scale in order to create nanostructures," explained Amar. *"The KMC method has been successfully used to carry out simulations of a wide variety of dynamical processes over experimentally relevant time and length scales. However, in some cases, much of the simulation time can be 'wasted' on rapid, repetitive, low-barrier events."*

While a variety of approaches to dealing with the inefficiencies have been suggested, Amar settled on using a first-passage-time (FPT) approach to improve KMC processing speeds. FPT, sometimes called first-hitting-time, is a statistical model that sets a threshold for a process and then estimates certain factors, such as the probability that the process reaches that threshold within a certain amount time or the mean time until which the threshold is reached.

"In this approach, one avoids simulating the numerous diffusive hops of atoms, and instead replaces them with the first-passage time to make a transition from one location to another," Amar said.

In particular, Amar and his colleagues targeted two atomic-level events for testing the FPT approach: edge-diffusion and corner rounding. Edge-diffusion involves the "hopping" movement of surface atoms – called adatoms – along the edges of islands, which are formed as the material is growing. Corner rounding involves the hopping of adatoms around island corners, leading to smoother islands.

Amar compared the KMC-FPT and regular KMC simulation approaches using several different models of thin film growth: Cu/Cu(100), fcc(100) and solid-on-solid (SOS). Additionally, he employed two different methods for calculating the FPT for these events: the mean FPT (MFPT), as well as the full FPT distribution.

Amar's FPT-KMC approach accelerated simulations by a factor of approximately 63 to 100 times faster than the corresponding KMC simulations for the fcc(100) model. The SOS model was improved by a factor of 36 to 76 times. For the Cu/Cu(100) tests, speed-up factors of 31 to 42 and 22 to 28 times were achieved, respectively, for simulations using the full FPT distribution and MFPT calculations. ■

Project lead: Jacques Amar, University of Toledo
Research title: First-passage-time approach to kinetic Monte Carlo simulations of metal (100) growth
Funding source: National Science Foundation
Web site: astro1.panet.utoledo.edu/~jamar/ph/jga.html

Trivedi analyzes superconductor-insulator transition of thin film

A superconductor is an amazing state of matter in which a macroscopic number of electrons pair up and condense into a coherent state exhibiting remarkable properties, such as zero resistance and perfect diamagnetism. Experiments suggest that upon tuning the film thickness or magnetic fields, there is an unusual phase transition from a superconductor to an insulator, driven by quantum effects.

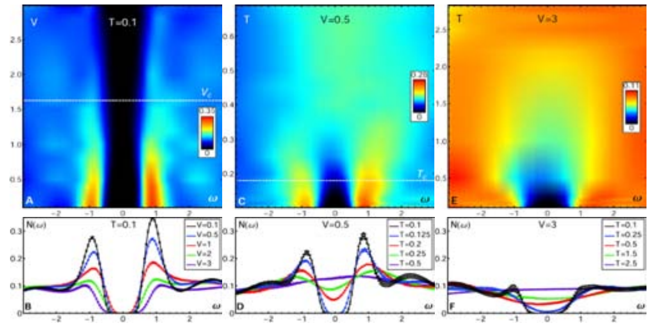
"When a superconducting material is deposited as a thin film, it may behave as an insulator due to disorder and quantum fluctuations," said Nandini Trivedi, Ph.D., a professor of physics at The Ohio State University. *"There has been considerable theoretical work in the last decade, including our own work, on the superconductor-insulator transition (SIT), but many fundamental questions remain unanswered. These approaches have proved to be inadequate to capture the transition, let alone characterize the nature of the phases."*

According to one school of thought, electrons that are bound together at low temperatures – known as Cooper pairs – break apart, leading to a metallic phase near the SIT. An alternative viewpoint holds that the Cooper pairs remain bound and that the SIT is caused by phase fluctuations that destroy long-range phase coherence between superfluid patches.

Trivedi's team is enlarging upon previous studies by including quantum and thermal phase fluctuations and calculating frequency-dependent quantities, such as the density of states. Whereas early experiments focused on the resistance of different films as a function of temperature, recent developments have allowed measurements of local and/or dynamical quantities.

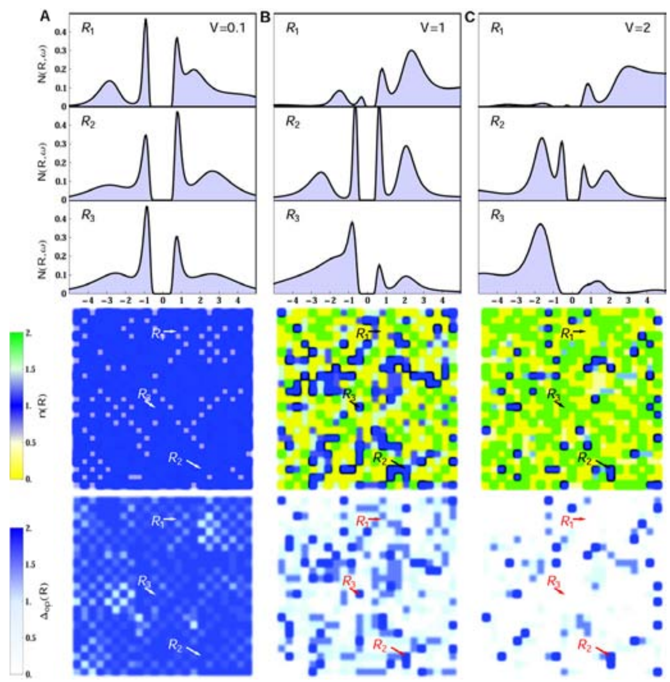
"Quantum Monte Carlo (QMC) techniques are computationally expensive and require a high statistical accuracy in order to extract dynamical quantities via analytic continuation, but they are necessary for a unified explanation of the experiments," she explained. *"With the resources of the Ohio Supercomputer Center, we are able to conduct determinant QMC studies of the disorder-driven superconductor-insulator transition. By including thermal and quantum fluctuations we now can obtain a complete understanding of the superconductor, the insulator and the quantum phase transition."*

Previous studies conducted through the Ohio Supercomputer Center helped Trivedi to develop a phase diagram and show the emergence of a new type of insulator, different from previously known insulators. Now, her team is working to calculate for the first time the frequency-dependent conductivity and pair susceptibility – the tendency of pairs – as functions of disorder and temperature. Trivedi's simulations include both thermal and quantum phase fluctuations, which are crucial to understanding some of the recent, puzzling experimental data showing low frequency absorption, well within the gap, in a disordered superconductor. ■



above: Using Ohio Supercomputer Center systems, Ohio State's Nandini Trivedi modeled energy and temperature scales to determine the superconducting transition temperature as a function of disorder.

below: Trivedi then calculated local density of states (top row), spatial local occupation (middle row) and local parameter order (bottom row) for increasing disorder (from left to right).



Project lead: Nandini Trivedi, The Ohio State University

Research title: Elucidating the role of quantum phase fluctuations across the disorder-driven superconductor-insulator transition

Funding source: National Science Foundation

Web site: www.physics.ohio-state.edu/~trivedi/

left: University of Cincinnati's Anna Gudmundsdottir employed Ohio Supercomputer Center resources to better understand how to tether fragrance molecules to a photoremovable protecting group (A) and release the fragrance molecules by exposure to sunlight (B).

Project lead: Anna Gudmundsdottir, University of Cincinnati
Research title: Reactivity of 1,2-biradicals and their applications
Funding source: American Chemical Society – Petroleum Research Fund
Web site: www.che.uc.edu/annag/

Gudmundsdottir studying mechanisms behind **PRPG photorelease**

In the past decade, a series of useful molecular systems – known as phototriggers, photoswitches, photocaging groups or photoremovable protecting groups (PRPGs) – have been used in a wide variety of applications, playing a key role in the release of fragrances from household goods, as an aid in multi-step syntheses and in drug and gene delivery.

PRPGs also make it possible for biochemists to release bioactive compounds in living tissue with both high temporal and spatial accuracy, thus making it possible to study physiological events, such as enzyme activity, ion channel permeability and muscle contraction. The choice of PRPG is critical, depending upon the system, and must be tailored to the application.

"We have designed several new PRPGs and studied the mechanism for the photorelease," said Anna Gudmundsdottir, Ph.D., professor of chemistry at the University of Cincinnati. *"The photoremovable protection group acts as a sort of cap, containing the fragrance until the cap is pried off by a photon of light. For this purpose, it is important to design a 'photoprotection group' that was somewhat difficult to pry off. For household products, such as a scented cleaning fluid, consumers want fragrance to be released slowly over a long period of time. That requires what is known as a low 'quantum yield.' "*

The goal of one of Gudmundsdottir's latest research projects has been to discover how to selectively form reactive intermediate compounds, such as triplet 1,2-biradicals, and use them to release alcohols from PRPGs, as well as to form triplet vinyl nitrenes, another reactive intermediate compound. While somewhat short-lived, these compounds hold great potential as PRPGs due to their high-energy properties.

She and her research team are leveraging computational resources at the Ohio Supercomputer Center and the electronic structure modeling capabilities of Gaussian and Turbomole software packages to: characterize the intermediates formed upon photolysis of simple vinyl phenyl ketones, determine the mechanism and the rate of photorelease from 4-hydroxyl-4-phenylcrotonate ester derivatives and characterize the intermediates formed from photolysis of vinyl azides.

"The research is both creative and original because it uses a simple sensitization technique to selectively form 1,2-biradicals that can be used to initiate fast photorelease of alcohols and form vinyl nitrene intermediates," Gudmundsdottir noted. *"These studies will result in a better understanding of the reactivity of triplet 1,2-biradicals and vinyl nitrenes. Furthermore, the results will lead to new PRPGs and the elucidation of the mechanism for release from these PRPGs, which will contribute to the advantage of fundamental photochemistry and reactive intermediates."*

Jana investigating the potential of **carbon nanotubes for industry**

Carbon nanotubes (CNTs) attract great attention for their strong potential in applications involving aerospace/naval materials, nano-electrical products, optical devices, chemical sensors, catalyst supports, water/gas treatments, drug carriers and artificial tissues. These future applications are spurred by the extraordinary mechanical, optical, thermal and electrical properties and chemical sensitivity to small molecules of CNTs.

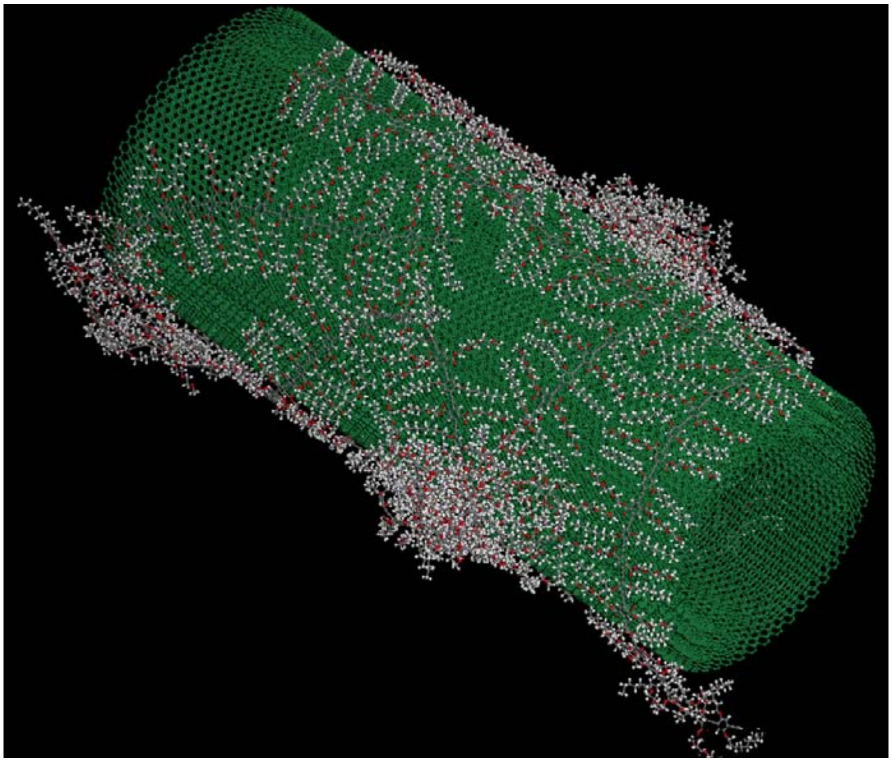
"The biggest obstacle in realizing the full potential of CNTs is agglomerate formation owing to van der Waals and electrostatics interactions between individual CNT particles," explained Sadhan C. Jana, Ph.D., professor and chair of Polymer Engineering at the University of Akron. *"Researchers have devised several methodologies to weaken such interactions. Of these, the chemical functionalization is an effective method when dispersion and stabilization CNTs are sought in polar liquids, including polymers."*

Two major approaches are followed for functionalization of CNTs — covalent and non-covalent. In a covalent approach, chemical bonds are formed with the surface carbon atoms, which often alters the graphitic characters of CNTs and compromises electrical conductivity and mechanical strengths. In contrast, a non-covalent approach utilizes adsorption of uniquely designed tie molecules, helping to improve the stability of CNTs without compromising the mechanical integrity.

Jana and Jie Feng, Ph.D., conducted computer simulations of tie molecule adsorption through the Ohio Supercomputer Center and obtained estimates of improvements of mechanical properties and thermal conductivity. They focused on gaining a fundamental understanding of physical adsorption mechanism of such tie molecules from solutions onto surfaces of multi-walled carbon nanotubes (MWCNTs). The tie molecules may include polymers, surfactants and biopolymers. The CNTs treated with the tie molecules may be used in the fabrication of sensors and devices or may be compounded with the host polymers to create bulk polymer composites.

"The methods we devised allow a large-scale quantitative investigation of MWCNT nanocomposites in solution," Feng said. *"The method can also be extended to the study of interfacial problems involving interactions between the polar and non-polar molecules with organic and inorganic fillers in solutions."*

Jana and Feng are collaborating with experimentalists at Zyvex Technologies and PolyOne Corporation to provide industry with guidance and theoretical explanations to aid in developing tie molecules and value-added composite materials for automotive, naval and aerospace industry applications. ■



left: With Ohio Supercomputer Center access, Sadhan Jana at the University of Akron simulated the equilibrium state of organization of 12 organic tie-molecules on the surface of MWCNT. The red dots represent oxygen, white represent hydrogen, and gray represent carbon atoms in tie molecules.

Project lead: Sadhan C. Jana, University of Akron
Research title: Hybrid modeling of functionalization of carbon nanotubes
Funding source: Ohio Third Frontier
Web site: www.poly-eng.uakron.edu/jana.php

Lacks increasing fundamental **understanding of disordered systems**

Over time, the properties of polymer materials slowly change through a process known as aging. Aging can cause changes in volume, which may lead to cracks in a material, and alter mechanical properties, making it more brittle. Thus, aging can seriously impact the performance of polymer products used in a wide range of applications. While the effects of aging are often laboratory-tested in "accelerated-aging environments" (e.g., higher temperatures), extrapolation of results from accelerated aging environments to ordinary environments is not straightforward.

Daniel J. Lacks, Ph.D., a professor of chemical engineering at Case Western Reserve University, is employing Ohio Supercomputer Center systems to better understand the aging process at the molecular level. His research team is focusing on the interplay between aging and mechanical deformation: how aging alters mechanical deformation and, in turn, how mechanical deformation alters the aging process.

"We are using molecular simulations to elucidate unresolved theoretical issues associated with the mechanical response of disordered systems," Lacks said. *"The project is motivated by a set of recent experimental results that are not fully understood; the simulations address the same systems studied in the experimental investigations, and are being carried out with realistic potential functions to allow meaningful comparison with experimental results."*

The project will have three thrusts: the interplay of physical aging and mechanical deformation; the effects of nanoscale structure on the mechanical properties of disordered materials; and the impact of disorder on the mechanical properties of crystalline materials.

"We are conducting molecular dynamics (MD) simulations that impose a step change in strain on a polystyrene material and then monitor the time dependence of the relevant stress," Lacks explained. *"Additionally, we are conducting MD simulations of polystyrene to elucidate the interplay between aging and mechanical deformation."*

Lacks and Greg Chung, a Case doctoral student on Lacks' team, plan to leverage the findings to advance the understanding of disordered systems in general. The results for the specific materials will be used to enhance theoretical frameworks – the unusual and unexplained nature of the motivating experimental observations suggests that there are interesting theoretical underpinnings that are likely to have implications beyond these particular materials.

"The project has the potential to benefit society by enhancing the understanding of fundamental scientific phenomena, which can lead to improved technology," Lacks said. *"The findings might help facilitate the design of materials with superior aging properties, the development of applications for nanoporous materials and the use of these materials in novel applications."* ■

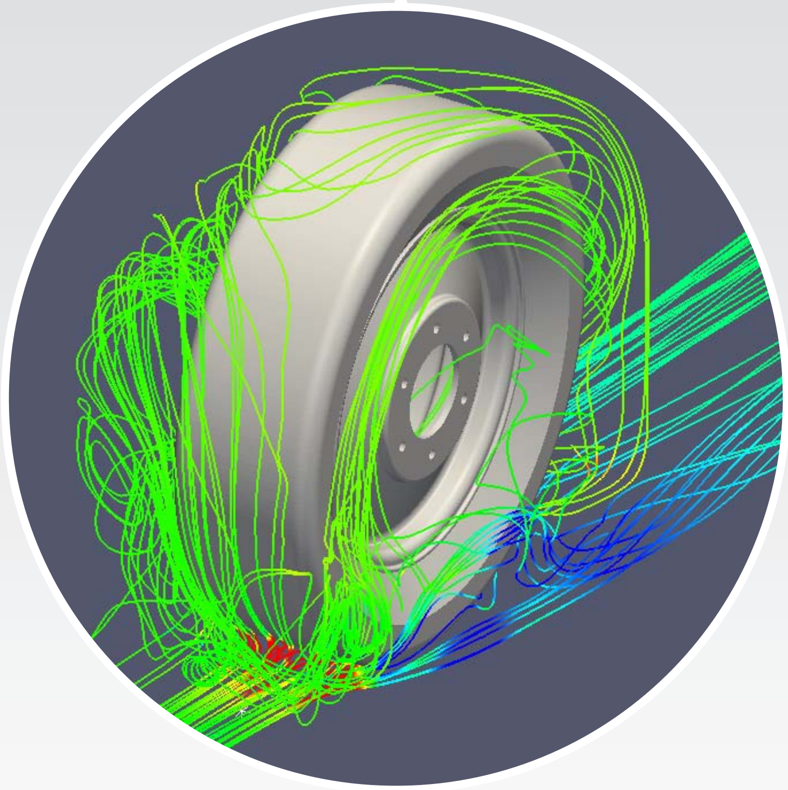
Project lead: Daniel J. Lacks, Case Western Reserve University

Research title: Molecular dynamics simulation of the aging and mechanical response of polymer materials

Funding source: National Science Foundation

Web site: www.case.edu/cse/eche/faculty_Lacks.html

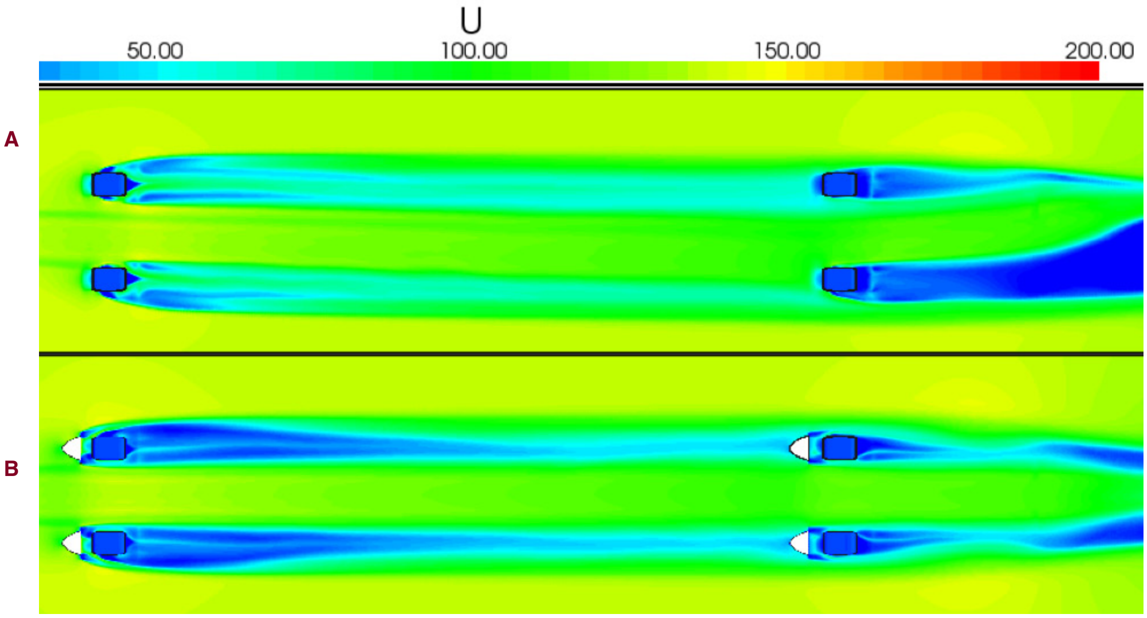
left: In comparison to a new polymethylmethacrylate wine glass (left), a six-month-old wineglass (right) demonstrates volume contraction associated with physical aging (Kotlewski and Picken, unpublished). Case Western Reserve's Daniel Lacks is using Ohio Supercomputer Center systems to focus on the interplay between aging and mechanical deformation: how aging alters mechanical deformation, and, in turn, how mechanical deformation alters the aging process.



Using Ohio Supercomputer Center systems, Ohio State's Cary Bork simulates airflow within the wheel well of the Buckeye Bullet land speed racer with the vehicle traveling at 300 mph.

Energy & the Environment

The solutions to significant, interrelated global energy and environmental sustainability issues will significantly increase the demand for computational modeling, simulation and analysis. The Ohio Supercomputer Center is supporting ambitious research addressing these complex challenges, such as finding innovative techniques to probe the efficiency of turbomachinery; augmenting satellite measurements of lake and river levels with algorithmic depth estimates; and creating new, virtual environments to increase educational access to remote environments. Scientists are developing alternative power systems for transportation by analyzing the mechanisms of proton transfer within fuel cells and by leveraging high-tech batteries to push the envelopes of speed. The Ohio Supercomputer Center provides powerful resources for researchers riding the crest of a worldwide Green Revolution, as seen throughout these pages.



left: In simulations Ohio State's Cary Bork conducted at the Ohio Supercomputer Center, airflow under the Buckeye Bullet traveling at 300 mph without wind deflectors installed in front of the wheel wells (A) is compared with the airflow under the vehicle with wind deflectors installed (B).

CAR's Rizzoni: Simulations help to **lift streamliner toward 400-mph goal**

A team of engineering students at The Ohio State University's (OSU) Center for Automotive Research (CAR) recently began running aerodynamics simulations, one of the first steps in the complex process of designing, building and racing the fourth iteration of their record-breaking, alternative-fuel streamliner.

"The third-generation electric land speed record vehicle to be designed and built by OSU students, the Buckeye Bullet 3, will be an entirely new car designed and built from the ground up," noted Giorgio Rizzoni, Ph.D., professor of mechanical and aerospace engineering and director of CAR. *"Driven by two custom-made electric motors designed and developed by Venturi, and powered by prismatic A123 batteries, the goal of the new vehicle will be to surpass all previous electric vehicle records."*

In 2004, the team achieved distinction at the Bonneville Salt Flats in Utah, by setting the U.S. electric land-speed record at just over 314 mph with the original Buckeye Bullet, a nickel-metal hydride battery-powered vehicle. Several years later, the team returned with the Buckeye Bullet 2, a new vehicle powered by hydrogen fuel cells, and set the international land speed record for that class at nearly 303 mph. The team then replaced the power source with a new generation of lithium-ion batteries and last year set an international electric vehicle record in partnership with Venturi Automobiles and A123 Systems at just over 307 mph.

This spring, the team, again in partnership with Venturi and A123 Systems, began the development process for a completely re-engineered vehicle designed to break the 400-mph mark. In consideration of that blistering speed, one of the first critical aspects the team had to consider was aerodynamic design.

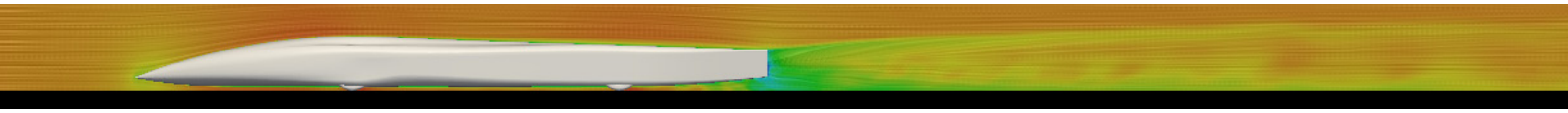
"What sets the new design apart from the previous vehicles is that at these higher speeds it is possible to produce shock waves under the vehicle," said Cary Bork, chief engineer for the team and an OSU graduate student. *"Minimizing or eliminating these shock waves is critical to ensuring the safety and stability of the vehicle."*

For both versions of the Buckeye Bullet 2, student engineers ran aerodynamics simulations on Ohio Supercomputer Center systems to compliment studies of physical models tested in wind tunnels. However, the current team quickly found that wind tunnels with a 'rolling-road' component required to test land-bound vehicles at the target speeds do not exist. Rizzoni and Bork, therefore, ran even more extensive simulations at OSC, giving shape to the lean, new streamliner.

After more than a year of preparation, the team hopes to unveil yet another record-setting Buckeye Bullet in 2012. ■

Project lead: Giorgio Rizzoni, The Ohio State University
Research title: Buckeye Bullet 3 aerodynamic simulation
Funding sources: The Ohio State University, Venturi Automotive, A123 Systems, TotalSim LLC
Web sites: www.buckeyebullet.com/ & http://car.osu.edu/node/46

below: A Buckeye Bullet simulation Bork developed at the Ohio Supercomputer Center illustrates the wake that follows the land speed racer as it accelerates past 300 mph.



Fried, Li model proton transfer to **improve fuel cell performance**

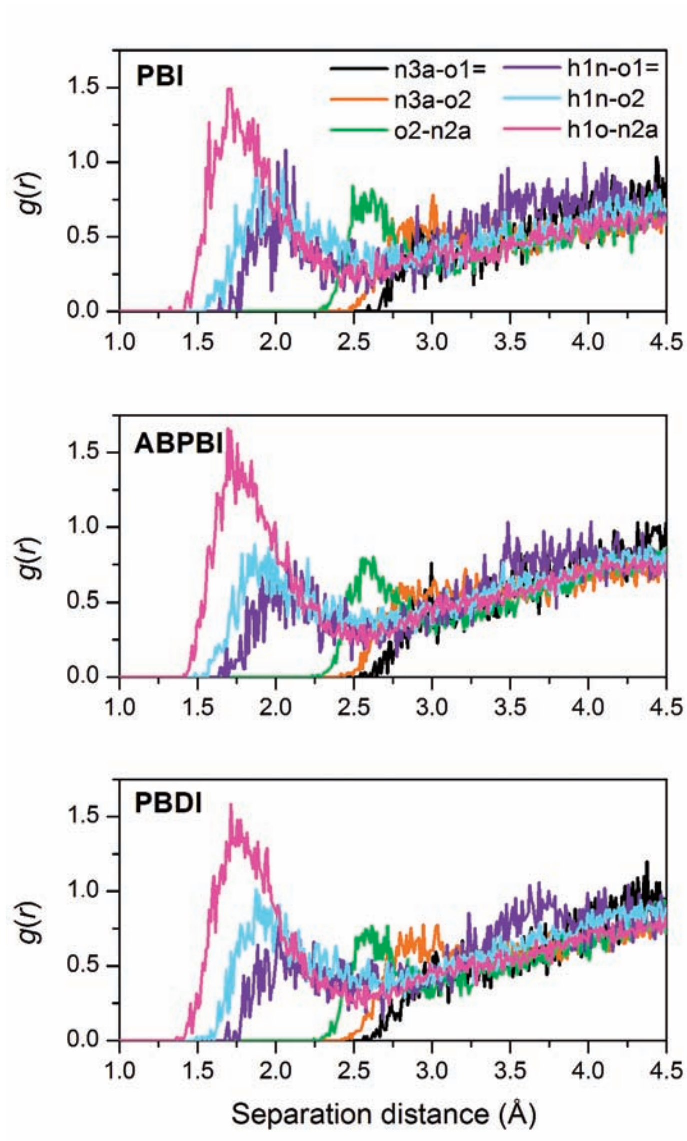
The overarching driver for the development of fuel-cell power is its potential to provide clean, highly efficient power generation. A fuel cell produces electricity from fuel (on the anode side) and an oxidant (on the cathode side), which react in the presence of electrolytes, substances containing free ions that make the substance electrically conductive.

In one basic design, proton exchange membrane (PEM) fuel cells operate with a polymer electrolyte in the form of a thin, permeable sheet. Research led by Joel Fried, Ph.D., professor emeritus at the University of Cincinnati and Wright Brothers Institute endowed chair in nanomaterials at the University of Dayton, leveraged Ohio Supercomputer Center resources to investigate the potential of PEMs that use phosphoric acid (PA) to dope polybenzimidazole (PBI) for improved performance. PBI is a polymer with an extremely high melting point used to fabricate protective apparel, such as firefighter coats, astronaut space suits and high-temperature protective gloves. Fuel cells using PA-doped PBI can operate in the range of 150-200 degrees Celsius.

"Compared with conventional PEM membranes (below 100 degrees Celsius), the high-temperature operation of a PA-doped PBI membrane allows increased catalyst activity at the electrodes and better carbon-monoxide tolerance in hydrogen fuel," said Shuo Li, a former Ph.D. candidate in chemical engineering advised by Fried at the University of Cincinnati. *"Ultimate success in the continuing development of these PEMs requires a fundamental understanding of the molecular structure of the membrane and the diffusional process of protons and small molecules."*

Proton transfer in fuel-cell membranes consists of proton-hopping along the hydrogen bond network (measured in picoseconds) and the diffusion of proton carriers between hops (measured in nanoseconds). Due to different time scales and difficult experimental techniques, Li explained, multi-scale simulation techniques are usually required to study these properties. Multi-scale modeling using quantum mechanics, molecular dynamics, and Atom-centered Density Matrix Propagation ab initio molecular dynamics were employed to study proton transfer and the hydrogen bond network structure in PA-doped PBI membranes.

Quantum mechanics calculations of gas-phase proton affinity, interaction energy and energy barriers for different proton transfer pathways indicated that proton transfer is prone to occur between the same molecules or between a molecule and its corresponding ion. The influences of different PBI structures, PA-doping levels, temperatures and water contents were evaluated through molecular dynamics simulations of hydrogen bond network structures and vehicular diffusion properties in neat, hydrated and PA-doped PBIs. Calculations were performed on the PA-doped PBI model to study the initial steps of proton transfer and the interfacial properties between PBI and PA. ■



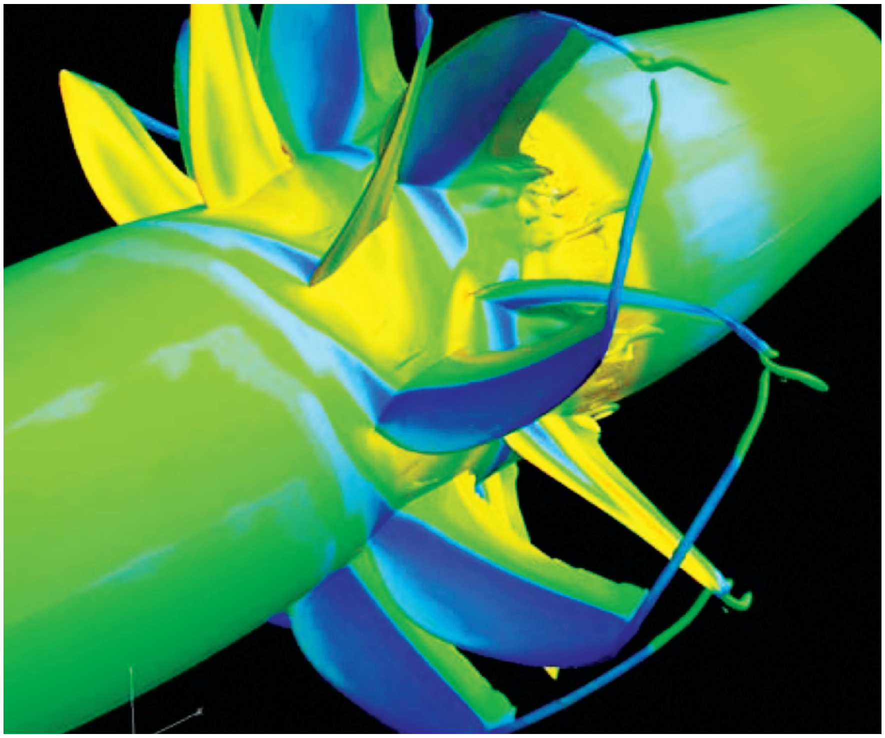
above: University of Cincinnati's Shuo Li used Ohio Supercomputer Center systems to create radial distribution function plots for various intermolecular atom pairs in three phosphoric acid-doped polybenzimidazoles: poly(2,2' -m-phenylene-5,5' -bibenzimidazole) (PBI), poly(2,5-benzimidazole) (ABPBI), and poly(p-phenylene benzobisimidazole) (PBDI).

Project lead: Joel Fried, University of Dayton

Research title: Computational chemistry and molecular simulations of phosphoric acid-doped polybenzimidazole

Funding source: American Chemical Society

Web site: www2.udayton.edu/engineering/profiles/fried_joel.php



left: Ohio State's Jen-Ping Chen used Ohio Supercomputer Center resources to create TURBO simulations for the flow field in an unducted counter-rotating fan.

Project lead: Jen-Ping Chen, The Ohio State University
Research title: Numerical investigations of rotating components in air-breathing propulsion systems
Funding sources: Air Force Office of Scientific Research, N&R Engineering
Web site: mae.osu.edu/people/chen.1210

Chen developing improved **turbomachinery simulation software**

Turbomachinery, such as that found in compressors and turbines, is instrumental in today's aeronautic, automotive, marine, space and industrial power generation. To achieve the most efficient propulsion and power systems, engine designers must understand the physics of very complex air-flow fields produced within multiple stages of constantly rotating rotors and stators.

While traditional wind-tunnel testing is the most straightforward approach, it also comes with high costs and severe constraints on placing the measurement probes. Numerical simulation, using computational fluid dynamics (CFD), has provided an alternative for studying such flows at a lower cost and with unconstrained probe placement. Yet, the accuracy of a simulation depends on the accuracy of the mathematical model behind the simulation.

"Our goal is to develop a reliable prediction technology to help improve turbomachinery component design," said Jen-Ping Chen, Ph.D., associate professor of mechanical and aerospace engineering at The Ohio State University. *"The successful combination of CFD simulation and experimentation can greatly supplement the understanding of fundamental fluid behavior of gas turbine systems, thus enhancing the ability of engineers to develop more advanced engine components."*

The focus of Chen's study is to develop improved simulation software and validate the flow field of engine components, specifically as applied to high-pressure compressors and low-pressure turbines. Each component has unique physical characteristics that present difficulties in design and operation, such as stall in a compressor and cooling in a high-pressure turbine. With a simulation tool that is validated and optimized to run efficiently on a parallel computer, engine designers will have more physical insight to the complex flow field, which will lead to reduced testing, reduced risk, faster time to market and lower costs.

Chen's team is investigating three specific areas of current industrial interest: coupled fluid-structure interaction, active flow control and turbine film cooling. Improved numerical simulation will allow engineers to analyze complex flow fields and aeroelastic phenomena, such as flutter, limit-cycle oscillations, forced response, nonsynchronous vibrations and separated-flow vibrations, which arise from fluid-structure interaction.

Application of a newly developed flow control simulation model for vortex-generating jets in low-pressure turbines will help improve engineers' understanding of how flow control can be used to increase the performance and operability of gas turbine engines. And, finally, simulations can help engineers accurately predict the effectiveness of film cooling on heat transfer in a three-dimensional, unsteady, rotating environment with actual engine geometry. ■

Durand **augmenting water depth readings** with data assimilation

Slated for launch in 2019-20, the Surface Water and Ocean Topography (SWOT) satellite mission is a collaborative project of NASA and the French space agency, Centre National d'Etudes Spatiales. SWOT features a swath-mapping radar interferometer that will provide data on inland bodies of water, as well as mapping ocean circulation at high spatial resolution.

The mission will measure rivers, lakes, wetlands and reservoirs for water elevation and the surface area inundated by water, data from which water slope and change-over-time are derived. From these fundamental measurements, scientists can calculate surface water-storage change and estimate river discharge, two principal components of the water cycle.

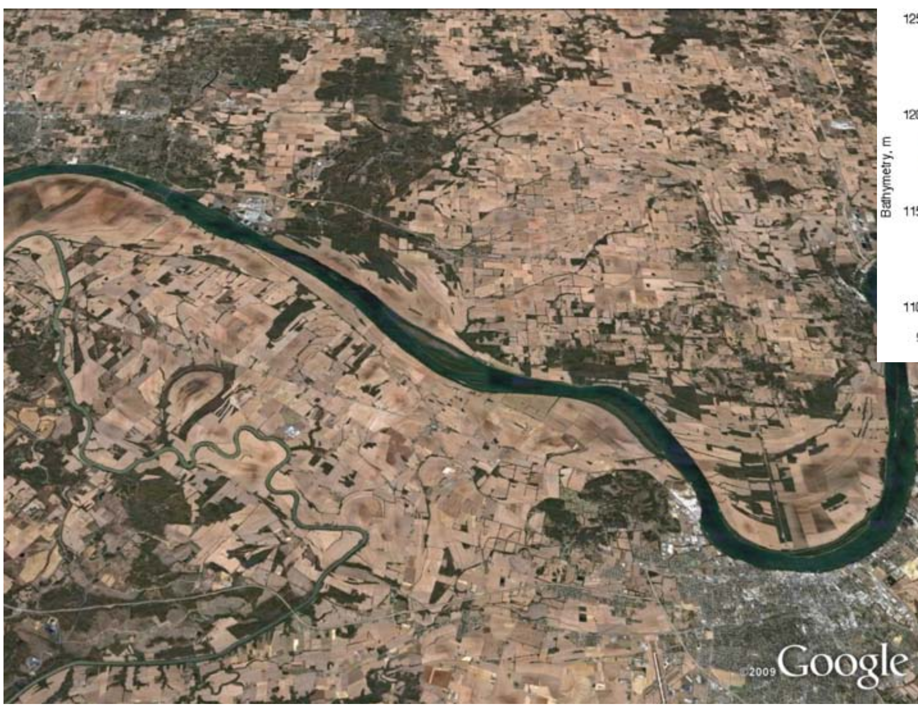
"SWOT represents a fundamentally new approach to characterizing fluvial processes, especially river discharge," said Michael Durand, Ph.D., assistant professor of earth sciences at The Ohio State University (OSU). *"However, because SWOT will observe water surface elevations, but not river bathymetric elevations, the cross-sectional flow area will be observed only above the lowest observed river depth. The remaining, unknown river depth must be estimated in order to produce river discharge estimates."*

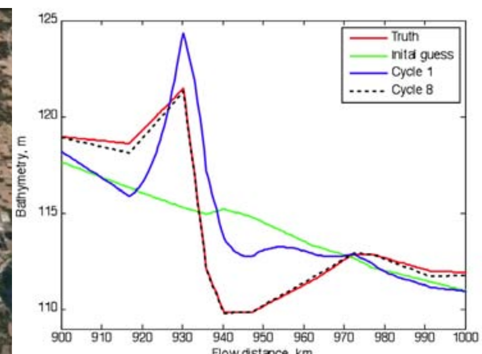
To address that issue, Durand is accessing Ohio Supercomputer Center computational resources to test strategies for estimating the unknown bathymetry of the Ohio River basin. Durand employed a numerical implementation of Saint Venant's Equation – used to describe the response of the free water surface to variations in river flowrate and river-channel bed forms – to numerically characterize the interactions between SWOT variables. With a data assimilation approach, he will solve an inverse problem to find river baseflow depth, given the measurements of slope and width.

"The data assimilation scheme used here essentially solves the inverse problem of classic open channel hydraulics," explained Yeosang Yoon, a doctoral student advised by Carolyn Merry, Ph.D., professor of civil and environmental engineering and geodetic sciences at OSU.

"While Saint Venant's equation describes the response of the free water surface to changes in bathymetry elevation and width, SWOT will measure the free water surface elevation, slope and width directly. The assimilation scheme will be used to estimate baseflow depth, given SWOT measurements of the free water surface."

For algorithm testing, a model of the Ohio River system was constructed using Corps of Engineers bathymetry data. Durand's colleague, Doug Alsdorf, Ph.D., OSU associate professor of earth sciences, serves as U.S. hydrology lead for the SWOT mission. ■





left: An aerial view of the Ohio River, near Evansville, Ind.

above: Accessing Ohio Supercomputer Center systems, Ohio State's Michael Durand obtained preliminary results for bathymetric estimates for a 100-kilometer section of the Ohio River. While the first guess does not closely match true bathymetry, accuracy increases significantly between the first and eighth cycles.

Project lead: Michael Durand, The Ohio State University

Research title: Estimating river bathymetry using water elevation measurements

Funding source: National Aeronautics and Space Administration

Web site: www.geology.ohio-state.edu/faculty_bios.php?id=166

Stredney team **simulating cave** to increase field experience access

College geoscience students with mobility impairments soon will be able to explore a computer simulation of a large cave system to meet degree requirements of field-based learning experiences.

A research team led by visualization experts at the Ohio Supercomputer Center (OSC) and a geoscience researcher at Georgia State University (GSU) seeks to develop an interactive, virtual field trip through a portion of Kentucky's famous Mammoth Cave – the world's longest known cave, with nearly 400 miles of interconnected chambers and passages. The two-year National Science Foundation project will develop an alternative to the physically demanding conditions normally encountered during field study, conditions that have led to an underrepresentation of geoscience graduates with mobility impairments.

"Although there are many sub-disciplines within the geosciences that create different opportunities, this science does not lend itself well to those who are physically unable to venture past the controlled laboratory setting," said Christopher Atchison, Ph.D., recently a graduate research assistant at OSC and now an assistant professor of geoscience education at GSU.

In addition to structural data previously obtained, the team will gather high-precision data through laser remote-sensing technology, called LIDAR (Light Detection And Ranging), and high-resolution digital photography of specific geological formations.

The data will be integrated into a virtual environment that can be explored and evaluated for usability by a representative group of students with mobility impairments.

"Through this experience, students will better inform the creation and development of a synthetic environment tailored to emulate a geological field study," explained Don Stredney, OSC senior research scientist for biomedical applications and director of the center's Interface Laboratory. *"Additionally, the students' experiences will assist the developers in creating an environment that is tailored to their abilities, as well as in establishing a sense of realism based on their experiences within the actual field site."*

The interdisciplinary effort includes individuals with expertise in modeling and simulation, virtual environments, human factors, geosciences and testing. The team is collaborating with members of the Mammoth Cave International Center for Science and Learning, the Advanced Computing Center for the Arts and Design at The Ohio State University (OSU), the School of Teaching and Learning in OSU's Collge of Education, the National Cave and Karst Research Institute, the Cave Research Foundation, Ohio's STEM Ability Alliance and the International Advisory for Geoscience Diversity. The team seeks to prove the vast potential for a simulated field experience and lead to an even broader study of a virtual field education module that can be used by all students. ■

Project lead: Don Stredney, Ohio Supercomputer Center

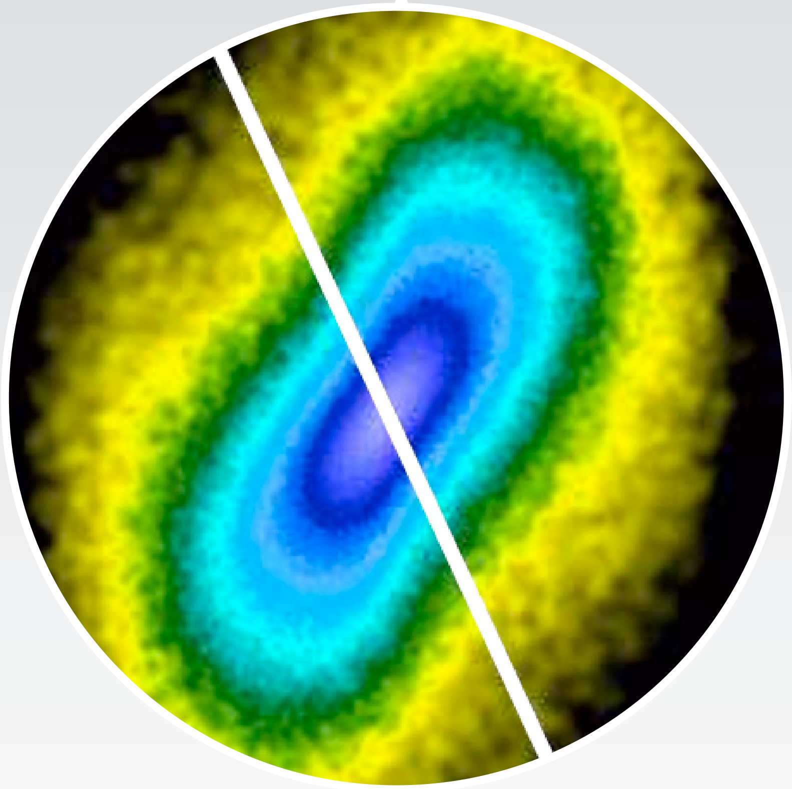
Research title: Expanding geoscience diversity through simulated field environments for students with physical disabilities

Funding source: National Science Foundation

Web site: www.osc.edu/research/Biomed/people/index.shtml

above: Students with mobility impairments are led through Mammoth Cave by Georgia State's Christopher Atchison. An OSC study aims to further develop a virtual cave system to increase career opportunities in the geosciences.

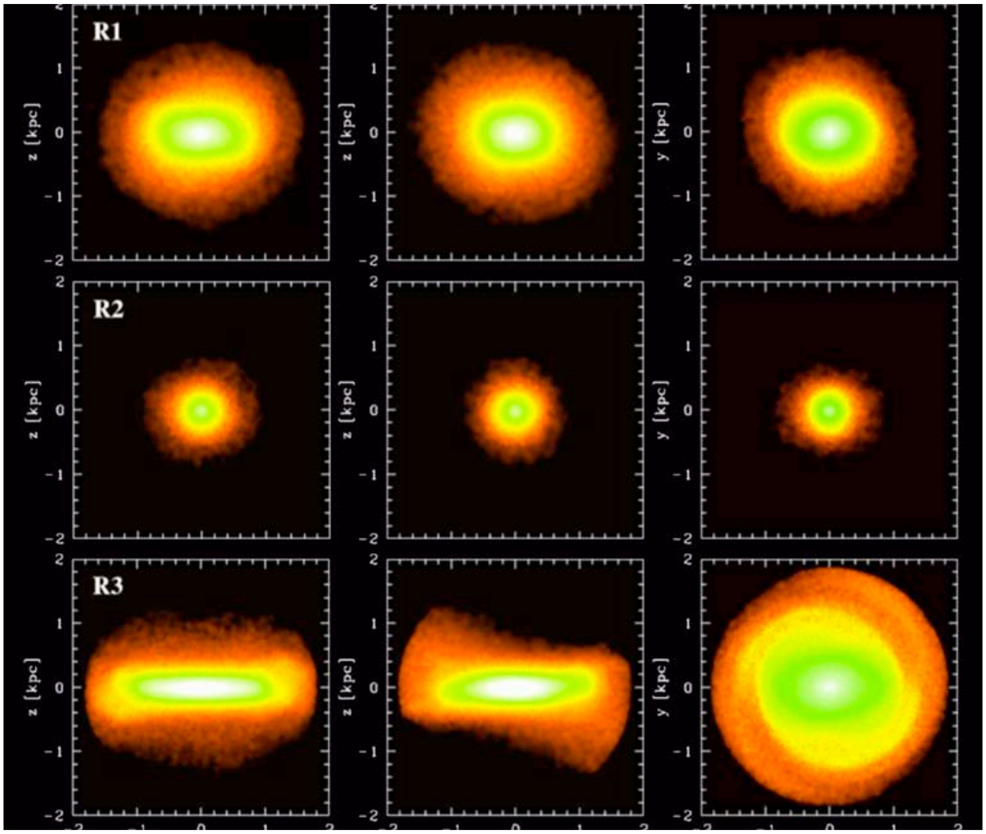
below: A screenshot shows a preliminary simulation of a portion of Mammoth Cave. The simulation was developed at the Ohio Supercomputer Center as part of a National Science Foundation planning study that resulted in additional funding to further develop the virtual cave system.



Ohio State's Stelios Kazantzidis employed Ohio Supercomputer Center systems to create a surface density map of the stellar distribution of a dwarf galaxy, with a line indicating the center of the host galaxy.

Research Landscape

Ohio's strengths in basic and applied research are broad and deep, spanning a multitude of academic, business and industrial interests. Likewise, the wide spectrum of clients served by the Ohio Supercomputer Center encompasses many fields of study. This diversity attracts eminent scholars and innovative entrepreneurs, as well as a wealth of regional, national and global research funding. Their research includes an astronomer who simulates the collisions of galaxies and black holes, researchers investigating techniques to provide more effective national security and a physicist who leverages supercolliders, supercomputers and a super-sized data network to unlock mysteries of the universe. 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.



left: Kazantzidis used Ohio Supercomputer Center systems to compile these three-panel surface density maps from three different simulations of the final stellar configurations of dwarf galaxies.

Kazantzidis **simulates effects of star formation**, black hole growth

Supercomputing centers allow astronomers to create extremely sophisticated models that are not feasible to build on desktop systems. However, simulating the multitude of elements involved in these galactic processes remains an enormous challenge.

"Our models can follow only a small subset of, say, the stars in a galaxy," explained Stelios Kazantzidis, Ph.D., a long-term fellow at Ohio State's Center for Cosmology and Astro-Particle Physics. *"For example, a galaxy like our Milky Way contains hundreds of billions of stars, and even the most sophisticated numerical simulations to date can simulate only a tiny fraction of this number. The situation becomes increasingly more difficult in simulations that involve dark matter. This is because the dark-matter particle is an elementary particle and, therefore, it is much less massive than a star."*

Leveraging Ohio Supercomputer Center resources, Kazantzidis' research teams simulated disk galaxies merging with supermassive black holes (SMBH). They found the mass ratios of SMBH pairs in merged-galaxy centers do not necessarily relate directly to the ratios they had to their original host galaxies, but are *"a consequence of the complex interplay between accretion of matter onto them and the dynamics of the merger process."* As a result, one of the two SMBHs can grow in mass much faster than the other.

Kazantzidis believes simulations of the formation of binary SMBHs have the potential to open a new window into astrophysical and physical phenomena that cannot be studied in other ways and might help to verify general relativity, one of the most fundamental theories of physics.

Kazantzidis and his colleagues also developed sophisticated computer models to simulate the formation of dwarf spheroidal galaxies, which are satellites of the Milky Way. The study concluded that, in a majority of cases, disk-like dwarf galaxies – known in the field as disky dwarfs – experience significant loss of mass as they orbit inside their massive hosts, and their stellar distributions undergo a dramatic morphological, as well as dynamical, transformation: from disks to spheroidal systems.

"These galaxies are very important for astrophysics, because they are the most dark-matter dominated galaxies in the universe," Kazantzidis said. *"Understanding their formation can shed light into the very nature of dark matter. Environmental processes, like the interactions between dwarf galaxies and their massive hosts, which we've been investigating, should be included as ingredients in future models of dwarf galaxy formation and evolution."* ■

Project lead: Stelios Kazantzidis, The Ohio State University

Research title: Simulating structure formation in the universe: From dwarf galaxies to supermassive black holes

Funding sources: The Ohio State University, Swiss National Science Foundation, Polish Ministry of Science and Higher Education

Web site: www.physics.ohio-state.edu/~stelios/

Panda team designing library to **raise HPC efficiency, performance**

Scientific computing is credited for many of the technological breakthroughs of our generation and is used in many fields, ranging from drug discovery and aerospace to weather prediction and seismic analysis. Scientific computation often deals with very large amounts of data, and its algorithms need to compute results from mathematical models. Due to their compute- and data-intensive nature, these applications are often parallel, i.e., they perform calculations simultaneously on multiple computers – from a handful of processors to thousands interconnected by a high-speed communications network.

Message Passing Interface (MPI), the lingua franca of scientific parallel computing, is a library of communications standards that control how software programs communicate with each other and is available on a variety of parallel computer platforms. On the hardware side, InfiniBand is a widely used processor interconnect favored for its open standards and high performance. MVAPICH2 is a popular implementation of the MPI-2 standard prevalent on InfiniBand-based systems.

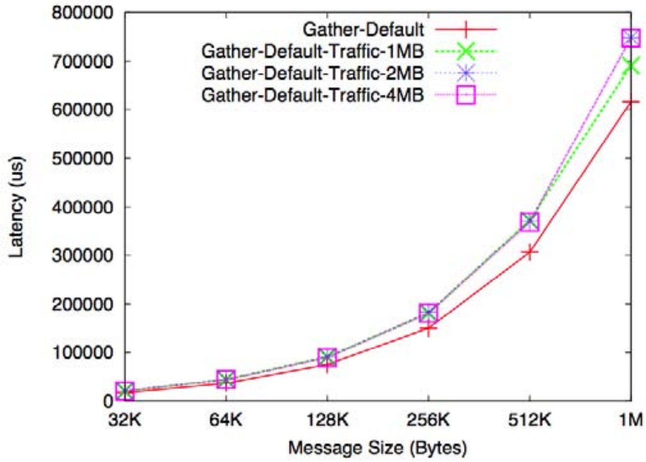
"It is anticipated that the first exaflop machines (calculating one quintillion floating point operations per second) will be available before the turn of the decade," said Dhabaleswar K. Panda, Ph.D., an Ohio State University professor of computer science. *"As the rates of computation increase further, it is crucial to design processor architectures, networks and applications in a 'co-designed' manner, so as to extract the best performance out of the system."*

To that end, Panda leads a team (including researchers Karen Tomko and Sayantan Sur) that is co-designing the MVAPICH2 MPI library with the underlying InfiniBand communication network and end applications to significantly improve the efficiency and performance of a system. The team is designing MPI-2 and the proposed MPI-3 one-sided communications using InfiniBand's Remote Direct Memory Access feature. Additionally, they have developed a design for the upcoming MPI-3 non-blocking collective communication for Ialltoall and Ibcast operations on state-of-the-art network offload technology.

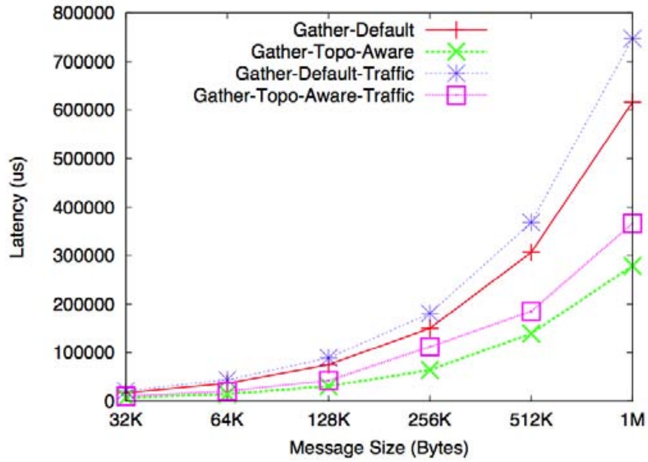
"An underlying design principle in HPC is to expose, not hide, system features that lead to better performance," Panda said. *"However, as system complexity grows, this must be done in a manner that does not overwhelm application developers with detail."*

Tomko, an Ohio Supercomputer Center senior researcher, works with students and postdoctoral researchers in the Network-Based Computing Laboratory, sharing insights culled from her expertise in science applications. She also assists the team in securing computer resource allocations and short-term reservations on OSC's IBM 1350 Opteron cluster.

"Using our techniques, a seismic simulation application (AWP-ODC), can be sped up by 15 percent on 8,000 processor cores," Tomko explained. *"And, three-dimensional Fourier transforms can be improved up to 23 percent on 128 cores."* ■



above: Ohio State's Dhabaleswar Panda accessed Ohio Supercomputer Center resources to measure the effect of background traffic on the MPI Gather operation for various message sizes.



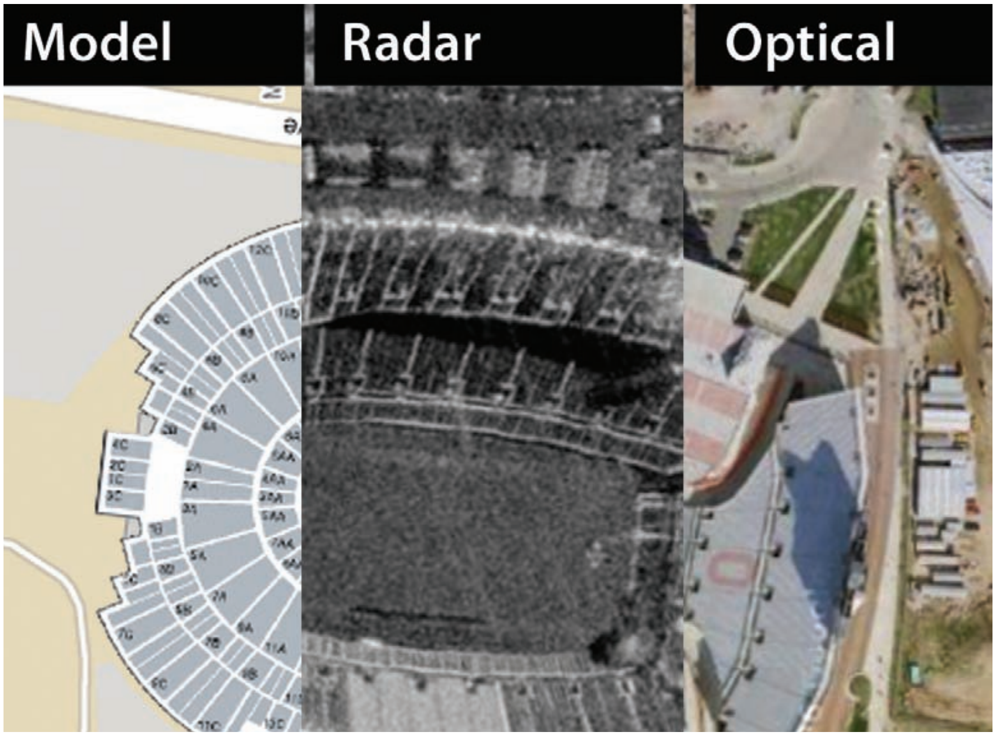
above: Panda demonstrated that his proposed topology-aware algorithms perform almost 50 percent better than the default algorithms under quiet conditions and are also resilient to the background traffic in the network.

Project lead: Dhabaleswar K. Panda, The Ohio State University

Research title: Design of advanced MPI features in MVAPICH2 and applications-level case studies

Funding sources: National Science Foundation, Department of Energy

Web site: nowlab.cse.ohio-state.edu/



left: Illustrating various examples of surveillance mediums, Ohio Stadium is depicted here as a line drawing, a radar image and an optical image. The Ohio Supercomputer Center's Alan Chalker serves as the program manager for the Center for Surveillance Research, a collaborative effort of academia, government and industry to conduct pre-competitive research and student training.

Project lead: Alan Chalker, Ohio Supercomputer Center
Research title: Center for Surveillance Research
Funding source: National Science Foundation
Web site: csr.osu.edu/index.html

Chalker: OSC provides foundation for **surveillance system research**

The Center for Surveillance Research (CSR), a National Science Foundation Industry/ University Cooperative Research Center, is a collaborative effort by academia, government and industry to conduct pre-competitive research and student training. Surveillance and situational awareness are critical technologies needed to address societal needs of safety and security, providing international and homeland security, situational awareness for disaster mitigation/management and environmental monitoring.

The key to addressing these crucial issues lies in the effective use of sensors and sensor systems. While individual sensor technology is advancing, there is a compelling need to understand composite surveillance systems. The challenge is to design quantitative tools that aid in designing surveillance systems to achieve particular inference goals and to develop a theory for predicting surveillance performance.

CSR's scientific research program addresses the breadth and depth of surveillance science. The core disciplines include sensor exploitation, signature prediction, computation and functional baseline descriptions. Performance prediction and uncertainty characterization accompany every level (signal, feature, detection, localization, tracking, targeting and intent).

The Ohio Supercomputer Center (OSC) supports the center in several ways, including through its management of an online repository of information for all members. This information is made available through a secure site hosted by the Air Force Research Laboratory at Wright-Patterson Air Force Base.

"We archive data, code and other vital information generated by researchers working on CSR projects," said Alan Chalker, Ph.D., program manager for CSR and for computer science engineering research applications at OSC. *"A staff member catalogues scientific papers on related topics, annotates complex algorithms and adds commentary to various sections of code so that students and researchers new to a project can pick up where someone else left off. OSC also provides industry members with easy access to center materials."*

CSR operates at two university sites: The Ohio State University (under center director Lee Potter, Ph.D., associate professor of electrical and computer engineering) and Wright State University (under site director Brian Rigling, Ph.D., associate professor of electrical engineering). OSU has strengths in video surveillance, machine learning, distributed sensor networks, hyper-spectral imaging, radar image exploitation, human factors and multi-sensor integration. Wright State University brings expertise in information theory for automated threat recognition, terahertz imaging and radar system design — including waveform diversity and bistatic/multistatic systems. ■

Bonakdarian shows **evolutionary computation** provides flexibility

A recently developed, evolutionary computation approach offers researchers an alternative approach to search for models that can best explain experimental data derived from applications such as economics. Esmail Bonakdarian, Ph.D., a Franklin University assistant professor of computing sciences and mathematics, leveraged Ohio Supercomputer Center resources to test the underlying algorithm.

"Every day, researchers are confronted by large sets of survey or experimental data and faced with the challenge of 'making sense' of this collection and turning it into useful knowledge," Bonakdarian said. *"This data usually consists of a series of observations over a number of dimensions, and the objective is to establish a relationship between the variable of interest and other variables, for purposes of prediction or exploration."*

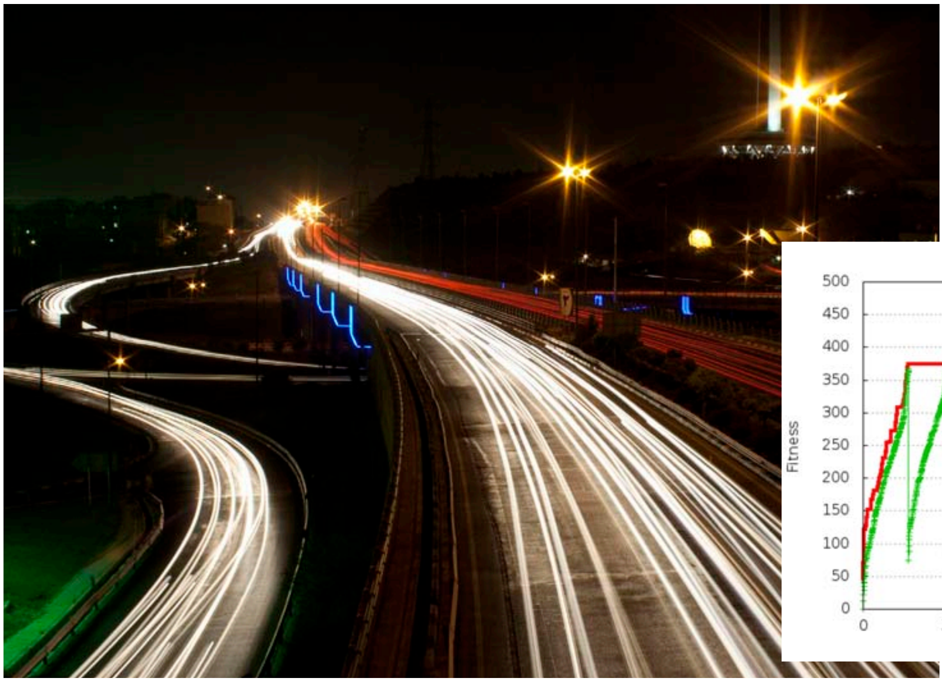
Bonakdarian applied the approach to two classical 'public goods' problems from economics: When goods are provided to a larger community without required individual contributions, it often results in 'free-riding,' while people also tend to show a willingness to cooperate and sacrifice for the good of the group.

"Evolutionary algorithms are inherently suitable for parallel or distributed execution," Bonakdarian said. *"Given the right platform, this would allow for the simultaneous evaluation of many candidate solutions in parallel, greatly speeding up the work."*

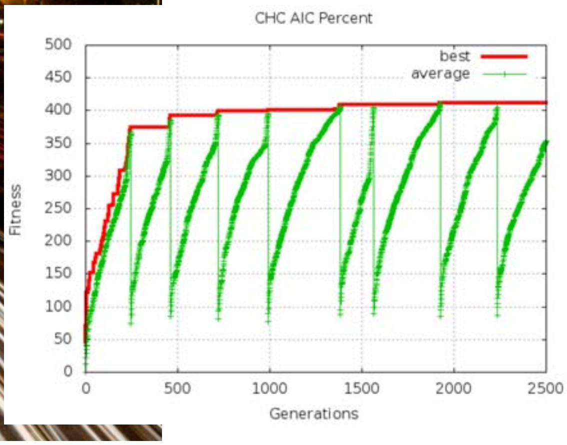
Regression analysis has been the traditional tool for finding and establishing relationships in research projects, such as for the economics examples Bonakdarian chose. When the number of independent variables is relatively small, or the experimenter has a fairly clear idea of the possible underlying relationship, it is feasible to derive the best model using standard software packages and methodologies.

However, Bonakdarian cautioned, if the number of independent variables is large, and there is no intuitive sense about the possible relationship between these variables and the dependent variable, *"the experimenter may have to go on a 'fishing expedition' to discover the important and relevant independent variables."* Using an evolutionary algorithm to "evolve" the best minimal subset with the largest explanatory value offers the analyst one more data analysis tool in addition to the standard automated approaches.

"This approach offers more flexibility, as the user can specify the exact search criteria on which to optimize the model," he said. *"The user can then examine a ranking of the top models found by the system. In addition, the algorithm can also be tuned to the number of variables in the final model. This ability to direct the search provides flexibility to the analyst and results in models that provide additional insights."* ■



below: A chart shows that optimization of the search over subsets of the maximum model proceeds initially at a quick rate and then slowly continues to improve over time until it converges.



above: Based on two classic public goods problems from economics, Franklin's Esmail Bonakdarian developed an evolutionary computation approach using Ohio Supercomputer Center systems. Public goods include such things as public roads, bridges and lighting.

Project lead: Esmail Bonakdarian, Franklin University

Research title: The use of evolutionary algorithms in the analysis of economics experiments

Funding source: Franklin University

Web site: faculty.franklin.edu/esmail-bonakdarian/

Humanic leverages OSC cycles, storage to study supercollider data

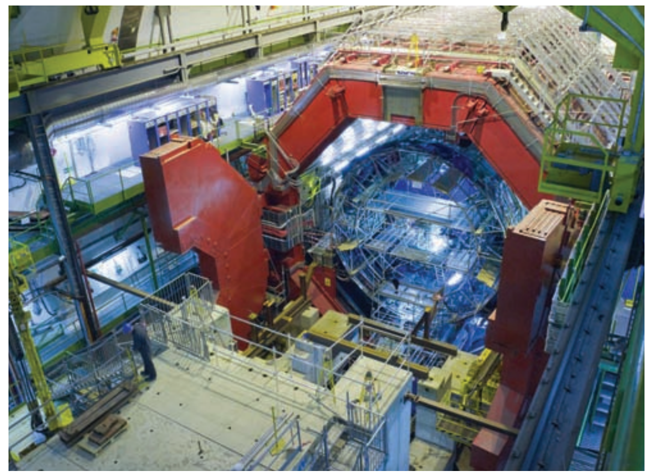
In huge tunnels below the Swiss-Franco border, the European Organization for Nuclear Research's Large Hadron Collider (LHC) is operating at half of its peak energy goal of 14 TeV or 'teraelectronvolts.' With the assistance of detectors built into the collider, physicists are searching for answers to questions about the birth of the universe, the existence of alternate dimensions and other key facets underlying the "Standard Model" of the fundamental forces of nature.

At the LHC, the 52-foot tall ALICE (A Large Ion Collider Experiment) detector is tracking the fleeting trails of infinitesimal particles (quarks and gluons) ejected from violent collisions of subatomic lead particles known as hadrons: protons in some experiments and nucleons (protons and neutrons) in others. Upon impact, the quarks and gluons are released from their connecting bonds for an instant, producing a miniature expanding cloud of plasma – visible to the sensitive detectors – before quickly reassembling.

During these experiments, the detectors are producing terabytes of data – at up to five gigabytes of data per second, or enough to fill 100,000 dual-layer DVDs every year. The information is quickly distributed to computers in 33 different countries through the Worldwide LHC Computing Grid. In preparation, Thomas Humanic, Ph.D., professor of physics at The Ohio State University, leads a team that has been working since 2002 to help install and test the grid software at the Ohio Supercomputer Center (OSC), a Tier-2 ALICE data storage, retrieval and computation site. In fact, while Europe is home to dozens of such ALICE sites, OSC is one of only four in the United States.

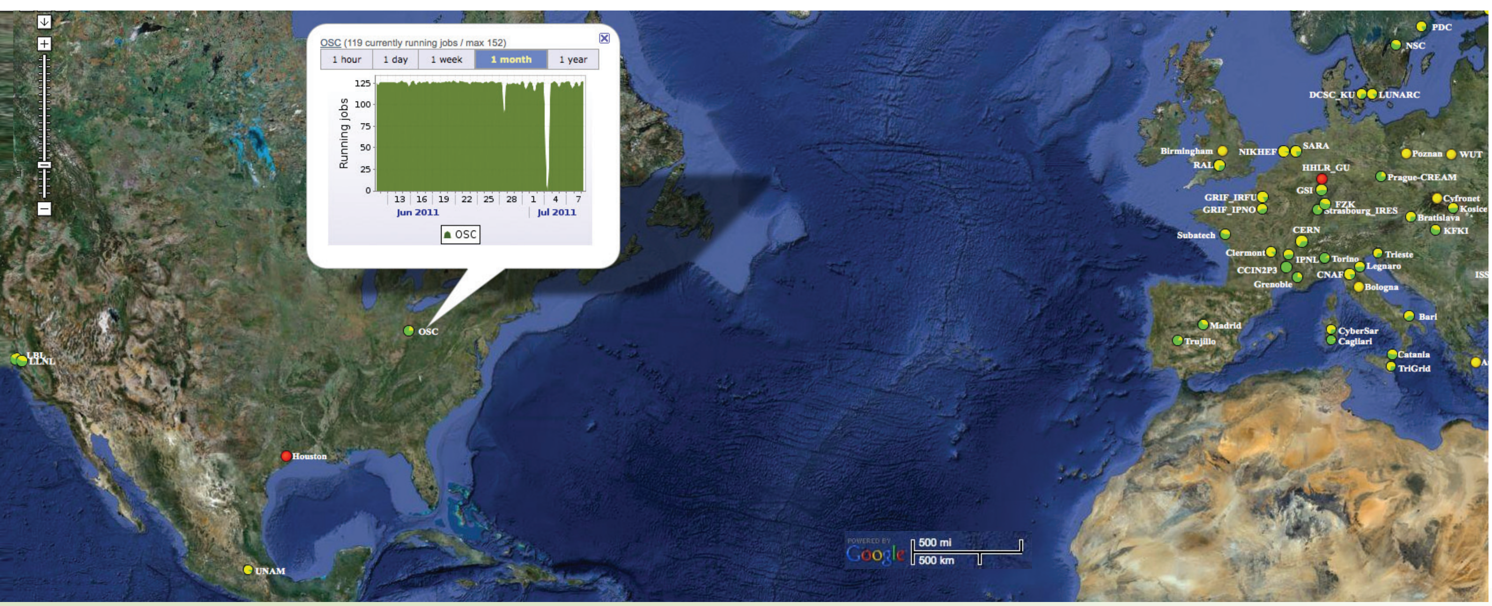
"Simulated data via ALICE Physics Data Challenges have been used to test the ALICE GRID computing environment at computing centers in Europe and at OSC," Humanic said. *"The real test of this system is happening now with real LHC data."*

Humanic also is developing and running physics Monte Carlo codes at OSC to measure the response of the ALICE detector to specific types of events and signals, as well as signatures for miniature black hole production. At the international conference Quark Matter 2011 in May, Humanic presented preliminary findings of ALICE proton+proton data. He found that some of the features expected from the heavy ion collisions are, somewhat unexpectedly, being observed in the smaller proton+proton collisions at half-energy. LHC is expected to run at full energy by 2014. ■



above: The LHC's ALICE experiment leverages a 52-foot tall detector to track sub-atomic particles that may reveal secrets about the birth of the universe.

below: Researchers can view the status of data being analyzed at ALICE GRID locations through a monitoring site called MonALISA. The Ohio Supercomputer Center is one of only four such sites in the United States.



Project lead: Thomas Humanic, The Ohio State University

Research title: $K^0_S K^0_S$ correlations in 7 TeV pp collisions from the ALICE experiment at the LHC

Funding source: National Science Foundation

Web site: www.physics.ohio-state.edu/~humanic/

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

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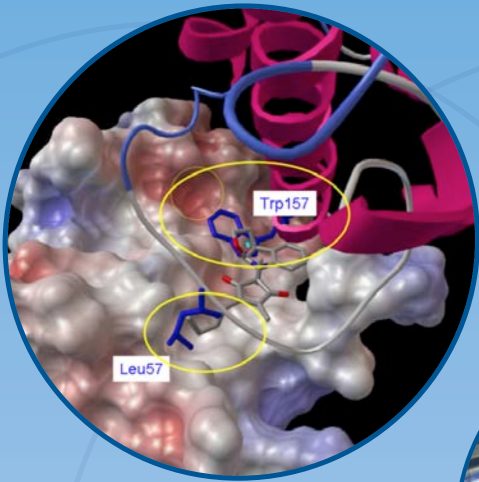

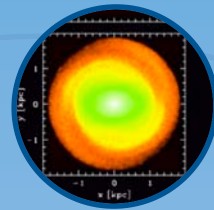

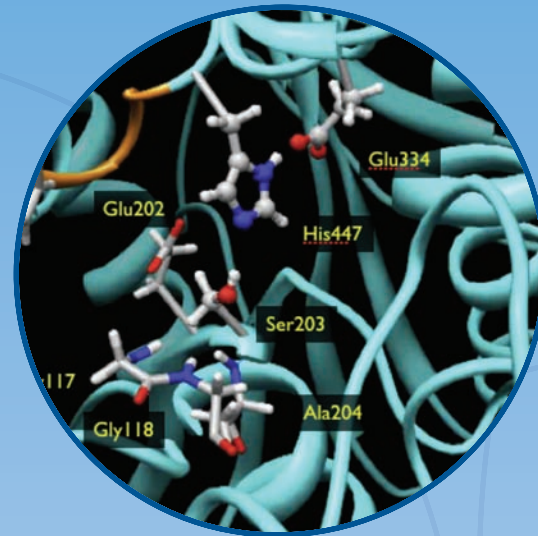

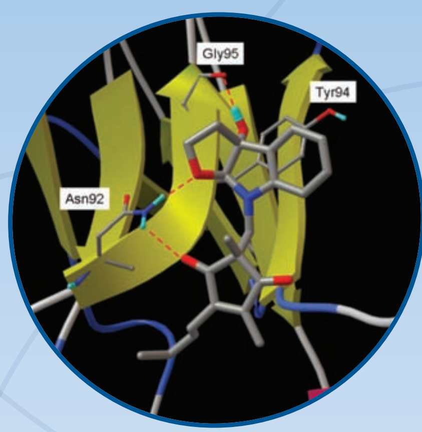

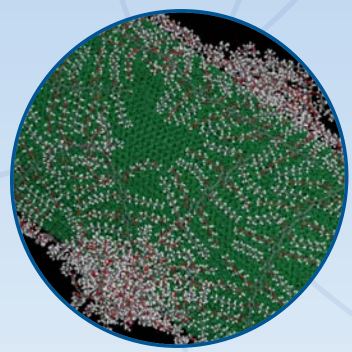

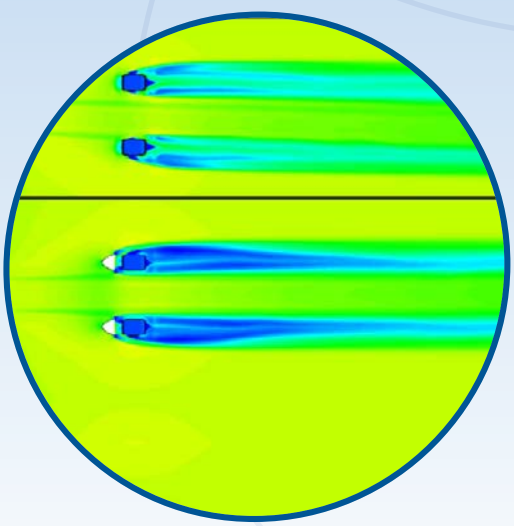

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