25

2012

OHIO SUPERCOMPUTER CENTER ANNUAL RESEARCH REPORT

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Researchers, *follow the purple line throughout this report to discover the powerful technologies available to you and the successes of fellow Ohio researchers.*

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STUDENTS

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INTRODUCTION

A MESSAGE FROM THE CHANCELLOR, JIM PETRO

I am pleased to join my colleagues statewide as we applaud the Ohio Supercomputer Center for addressing the computational, storage and analysis needs of Ohio's research, innovation and education communities. The professionals at OSC have laid the groundwork for the center to be highly regarded by researchers across the state and around the world. This level of recognition has been achieved across a challenging span of time that has seen great leaps in technology and approach.

I also want to recognize the outstanding vision of the policymakers and other leaders who created the Center in 1987, and the commitment of those who have continued to support the organization for two and a half decades. Through their wisdom, Ohio students, professors, doctors, patients, police officers, rescue personnel and all citizens benefit from a steady, reliable resource for generating knowledge, information and opportunity.

The Center continues to be responsive to emerging trends and realities, providing the superior quality of services for which the organization is known. With continued support and excellent leadership, we, and those who follow us, will surely have good reason to gather together to congratulate OSC on the organization's golden anniversary 25 years from now.

A MESSAGE FROM THE EXECUTIVE DIRECTOR, PANKAJ SHAH

Since 1987, the Ohio Supercomputer Center has provided its users with a powerful and vital resource for accelerating discovery and innovation. In many cases – such as in industrial outreach and computational science education – the Center has gained widespread recognition as a leader in the field. That pioneering spirit continues today, as we expand into exciting initiatives such as innovative visualization laboratories and advanced web portals for industry and education.

Our services, though, are but one part of OSC's success.

Our stakeholders, especially those serving with the Supercomputer Users Group, have always played a central role in managing the assets of the organization, providing long-term assistance in awarding resources, determining job priorities and advising on equipment upgrades. Our success on a national and international scale as a state-funded member of the Ohio Technology Consortium is due, in part, to our users' active participation in our governance structure.

We appreciate the constant drive for increased computational speed and storage space from our academic researchers, as well as from our business and industry partners. We also are very grateful to the long history of state and university leaders whose support has empowered the Center and its mission.

Above all, OSC's greatest asset is our resident human capital – dedicated and talented staff members who accept nothing short of excellence, as they have for the past 25 years as well as the next 25.

Left: Ohio Supercomputer Center officials and users gather around the new Cray X-MP system, which was installed at OSC in 1987. Pictured (from rear and left to right) are Charles "Charlie" Bender, executive director of OSC; Alison Brown, director of OSC's Ohio Academic Resources Network (OARnet); Comer Duncan, Ph.D., professor of physics at Bowling Green State University; Michael Lee, Ph.D., professor of physics at Kent State University; and Charles "Chuck" Csuri, director of the Computer Graphics Research Group.

25 years of innovation

TWENTY FIVE YEARS OF INNOVATION

Forward-looking foundation delivers big returns

"I am very grateful for OSC – without you all, my job would be much more difficult. I am really pleased to have such a wonderful computing facility to use, and I am confident that we will bring significant research achievements."

– Jack J. McNamara, Mechanical & Aerospace Engineering Assistant Professor, The Ohio State University upon receiving acceptance of his Discovery Level allocation request for OSC resources.

Although 2012 signaled the 25th anniversary of the Ohio Supercomputer Center, the genesis of the organization began much earlier than 1987.

The Genesis Years (1963-86)

In 1967, Ohio State University art professor Chuck Csuri helped to ignite the field of digital art when he began creating his pieces using a mainframe computer and a plotter. By the early 1970s, OSU professors, primarily in chemistry, had been attempting to increase the computing power in their research and eventually gained access to NASA Lewis supercomputer facilities in Cleveland and a Boeing Computer Services system in Seattle.

In 1984, the National Science Foundation (NSF) proposed to establish three national supercomputer centers, and OSU officials submitted a pair of unsuccessful bids. In 1985, Csuri revised and resubmitted the computer graphics section, which was funded and created the foundation for what would become the Advanced Computing Center for Art and Design (ACCAD) at Ohio State.

The Foundation Years (1986-94)

In July 1986, state and university officials met to organize a state-supported center at Ohio State. That fall, a proposal for a $10 million center was included in the Ohio Board of Regents biennial budget for 1987-88. The first official meeting of the statewide Supercomputer Users Group was held at OSU in November.

In 1987, the Regents funded the first staff at the center, and OSU leased a Cray X-MP, the center's first real supercomputer. The machine arrived June 1, and the first segments of a network, now known as the Ohio Academic Resources Network (OARnet), to connect university researchers to the Cray were installed, piggybacking on the state's telecom network. On the last day of June, the Ohio General Assembly passed the state operating biennium budget bill, providing $7.5 million to fund operations. In December, a resolution officially established OSC stating:

"WHEREAS, the State of Ohio has established an Ohio Supercomputer Center as a statewide resource designed to place Ohio's research universities and private industry in the forefront of computational research … the Ohio Board of Regents hereby establishes the Ohio Supercomputer Governing Board … that the Center will be a unit within and operated for the State of Ohio users of the Supercomputer, by The Ohio State University …that a network established by the Center will provide communications links from the Center at Ohio State to the campuses of member Ohio academic institutions … that a supercomputer training program will be conducted by the Center."

1986 Fall | OSU taps McCurdy, Pitzer as acting, associate directors.

1987 June | State operating budget bill creates OSC.

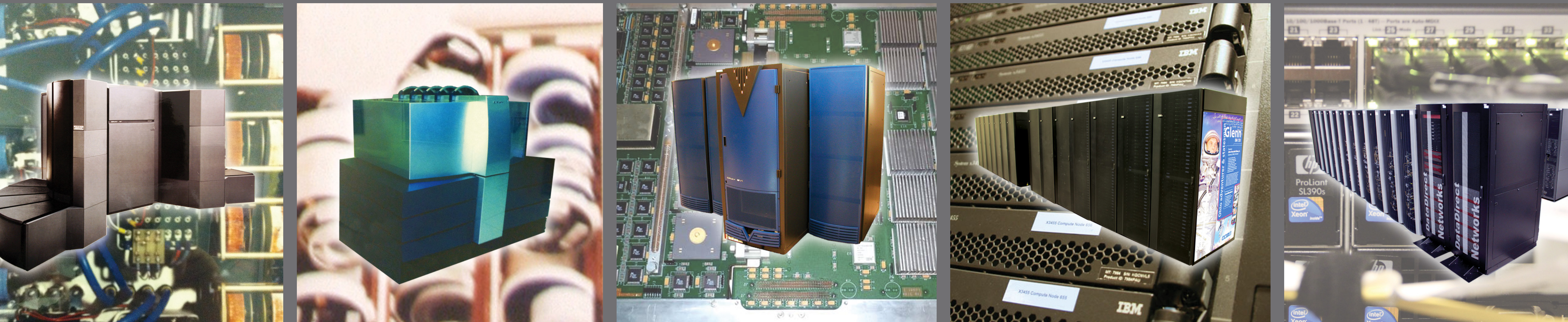
1987 December | Regents resolution establishes OSC, board.

1988 April | Bender named first OSC director.

1989 Summer | OSC holds first high school Summer Institute.

1989 August | OSC installs world's fastest supercomputer, Cray Y-MP.

1992 June | OSC installs first mass storage system.



Above: A retrospective of OSC hardware over the years. Pictured (from top left to right) are the Cray Y-MP 8D; Cray T94; Cray SV1; (next row) Glenn IBM 1350 Cluster; Oakley HP-built Intel Xeon Cluster; SGI Itanium Linux Cluster; (bottom row) IBM Mass Storage System; Cray X1; Itanium2 Linux Cluster

1997 November | OSC installs CRAY T94, CRAY T3E systems.

1998 September | OSC installs SGI Origin 2000 system.

1998 November | OSC erects SGI system at SC99 conference.

1999 September | OSC leads ECom-Ohio to assess electronic commerce.

1999 October | OSC installs Cray SV1 supercomputer system.

2000 June | OSC creates YWSI – STEM program for girls.

2001 April | First round of Cluster Ohio Project announced.

2001 April | OSC selected Sun Center of Excellence.

2001 August | OSC installs SGI 750 Itanium Linux Cluster.

2001 May | OSC, partners awarded large Defense PETT contract.

2001 Summer | State grant creates Platform Lab at OSC.

2002 March | OSC installs AMD Linux Cluster.

2002 Spring | Systems moved to State of Ohio Computing Center.

2002 July | OSC opens Blueprint for Advanced Learning Environment.

In 1988, Ohio Governor Richard Celeste committed his administration to funding a newer Cray supercomputer for OSC, and in March, the General Assembly authorized the purchase of a $22-million Cray Y-MP.

Also in 1988, the center named Charlie Bender executive director, launched its Industrial Interface Program to serve business and industry and created the Ohio Visualization Laboratory. The first Governor's Summer Institute, which marked the beginning of OSC's legacy of educational outreach, was launched in 1989, and the center became a founding member of the Coalition of Academic Supercomputer Centers (CASC). That year, OSC also deployed the Ohio Library Information System, a consortium of 88 Ohio college and university libraries and the State Library of Ohio that would become known as the Ohio Library and Information Network (OhioLINK).

In 1989, OSC engineers completed the installation of the $22 million Cray Y-MP8/864 system, which was deemed the largest and fastest supercomputer in the world. In 1992, OSC installed the center's first mass storage system, a whopping 1 TB of storage. In 1993, OSC established the Biomedical Applications Research group, a group of faculty, scientists and clinicians who apply high performance computing and advanced interface technology to the virtual exploration of complex computational biomedical information.

OSC and OSU collaborated in 1993 to deploy the Greater Columbus Free-Net, an outreach project that provided dial-up Internet connection, email, Usenet news and web hosting for more than 40,000 students, staff and non-profit agencies. Also that year, OSC officials signed a contract to help the Department of Defense (DoD) train scientists and engineers at Wright-Patterson Air Force Base near Dayton in the latest ways computers were being used to help solve scientific problems.

The Expansion Years (1994-2000)

In 1998, OSC's Electronic Commerce, Law, and Information Policy Strategies (ECLIPS) program was named a think tank for its research on privacy and the legal, policy and technological issues related to new computing and information technology applications.

In 1999, OSC purchased a cluster of 33 systems from SGI that was shipped to the Supercomputing '99 conference in Portland, Ore., where it was assembled and run on the conference floor before being dismantled and shipped to OSC's offices, where it was installed and put into production.

In 1999, state, business and academic leaders kicked off ECom-Ohio, a project that assessed Ohio's readiness for global electronic commerce.

At an Internet2 meeting in Seattle, Wash., OSC Networking (OARnet) staff members organized the first Megaconference, the world's largest H.323 Internet videoconference. In November 1999, OSC participated in a meeting to create InfraGard, a national program to address cyber and physical threats to security.

In 2000, OSC announced the creation of YWSI – a program for middle-school girls in Ohio designed in response to the documented lack of interest in math, science and engineering among girls and women's low participation in the science, engineering and technology fields.

The Movement Years (2001-05)

In 2001, OSC announced the Cluster Ohio Project, the first of three hardware, software, training and maintenance grants to encourage Ohio faculty to build local computing clusters from components of retired OSC systems. Also in 2000, OSC was selected as a Sun Center of Excellence in High Performance Computing Environments, and was awarded part of a DoD User Productivity Enhancement and Technology Transfer (PETT) contract to support the High Performance Computing Modernization Program.

That same year, the center partnered to operate and manage the Maui Supercomputing Center, and OSC and the Business Technology Center created the Platform Lab, now a leading-edge, shared-software testing and development facility.

"We think we should let you know our sincere appreciation for the help we received from OSC – without it we could not have increased the amount of statistics by a factor of 10 within just 2 weeks."

– Dr. Ulrich Heinz, Physics Professor, The Ohio State University & Dr. Zhi Qiu, Graduate Student, The Ohio State University

"The impact of having OSC established as a combined center for the state of Ohio was phenomenally intelligent. One significant advantage of OSC is that we can get a tremendous amount of work done with the least amount of effort. While I have used other centers in the past, most of my students who have left my group and gone elsewhere have been begging to know how they can come back and use the OSC because it is just very well optimized for function and for production"

– Christopher Hadad, Ph.D., Chemistry Professor, *"This process would take way too long if we had to rely on a single desktop, but by farming out the work to many OSC nodes, we can condense many CPU months' worth of work into just a few hours or days. This has allowed us to achieve a much more comprehensive characterization of how our algorithms perform under many different settings than would otherwise be possible."*

– **Justin Ziniel**, Doctoral Student in Electrical and Computer Engineering, The Ohio State University, on OSC's role in his compressed sensing research.

In 2002, OSC officials put the finishing touches on a facility expansion called the Blueprint for Advanced Learning Environment, or BALE, providing an environment for testing and validating the effectiveness of new tools, technologies and systems in a workplace setting.

That spring, OSC engineers moved the center's HPC systems to the fourth floor of the State of Ohio Computing Center, providing OSC with a secure and reliable facility with security, climate control and redundant electrical and mechanical support systems. In June, Stanley Ahalt, OSU professor of electrical engineering, was named OSC's executive director.

In 2003, OSC Networking announced efforts to build the Third Frontier Network, the nation's most advanced statewide fiber-optic service for education and research, and a little more than a year later, federal and state officials, industry leaders and university researchers launched the high-speed network. In December, OSC established a supercomputing center in Springfield, Ohio, to focus on data management and mining, as well as remote data mirroring across high performance networks. OSC and several partner organizations also released the Parallel Virtual File System (PVFS), an open-source parallel file system.

In 2004, OSC engineers installed the IBM Mass Storage System, increasing OSC's data storage capacity five-fold over its previous system. In November, at SC04 in Pittsburgh, Ahalt delivered the conference keynote speech, "Toward a Blue Collar Computing Economy." As more than 1,000 international audience members listened, Ahalt argued that a fundamental shift in the HPC market – the addition of Blue Collar Computing – needs to take place to revitalize the country's leadership in computational science, engineering and product design.

The Program Years (2005-07)

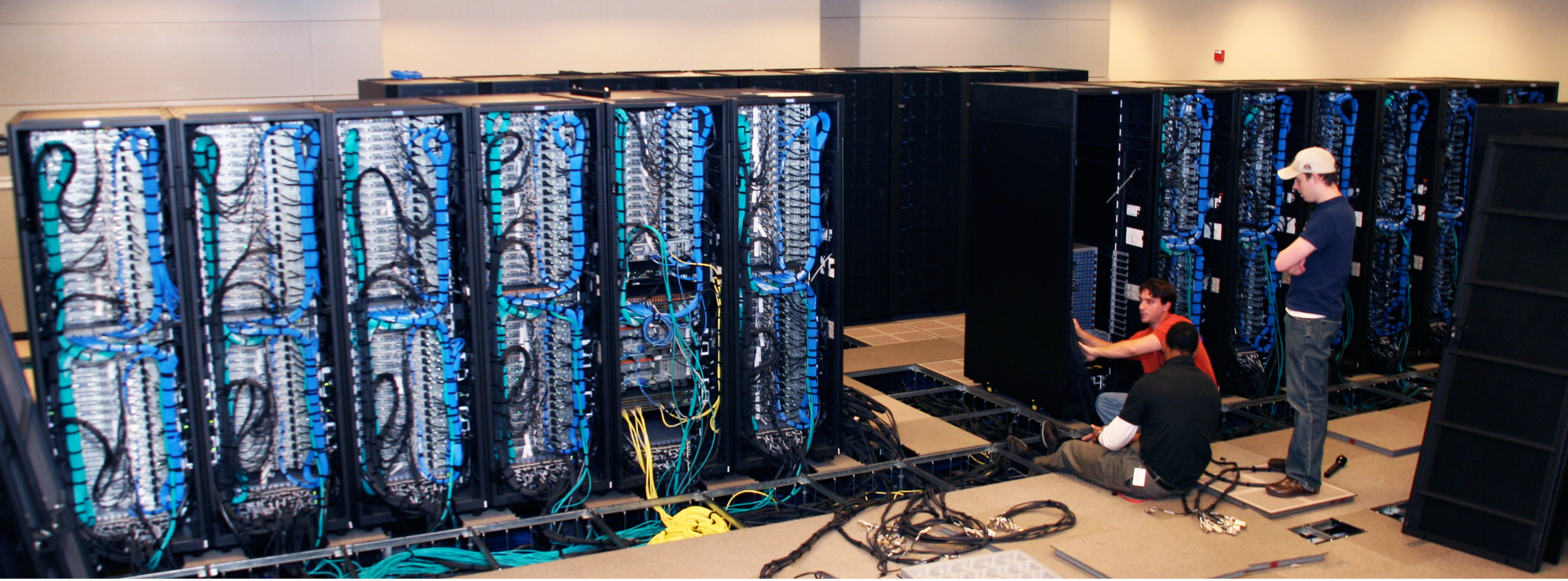
In 2005, OSC dedicated the statewide virtual Ralph Regula School of Computational Science, a collaborative creation of OSC, BOR, the Ohio Learning Network and Ohio colleges and universities and focused on the new field of computational science.

The Ohio Department of Development commissioned OSC in 2006 to conduct another ECom-Ohio Study to examine the availability and cost of high bandwidth network services for business and government use. Later in June, OSC helped organize the Inaugural Ohio Collaborative Conference on Bioinformatics (OCCBIO). Also in 2006, OSC won a significant NSF grant to help develop faster and smarter storage systems to improve and increase the processing power of high performance computing.

In November 2006, OSC and Edison Welding Institute began providing remote portal access of HPC systems and software to engineers, who could input product dimensions, welding process parameters and other specifications to conduct complete online simulations of prototype welding procedures. In December, researchers remotely accessed and operated electron microscopes at OSU over the Internet, expanding the potential for making new discoveries about the structure-property relationships of wide spectrum materials.

In 2007, the NSF awarded funding to the Ralph Regula School to develop an associate degree concentration program in computational science. That summer, OSC purchased an IBM Opteron Cluster (named after former astronaut and statesman John Glenn), which was ten times as powerful as any of OSC's existing systems with a peak performance of more than 22 trillion floating point operations per second.

In the fall of 2007, under an agreement with PolymerOhio, OSC pledged to develop web-based applications that would allow polymer companies to transparently access the center's



Above: Engineers complete the 2007 installation of the IBM Cluster 1350 system for the Ohio Supercomputer Center. The system was named the Glenn Cluster in honor of the former astronaut and statesman from Ohio, John Glenn.

supercomputing systems and software. In October, BOR funded a “shared instrumentation” pilot research project to gain a greater return on large investments by universities in extraordinary instruments, such as electron microscopes, nuclear magnetic resonance spectrometers, Raman spectrometers and ion accelerators.

The Collaboration Years (2008-12)

In 2008, the NSF funded the development of computational science certificate courses for Ohio’s workforce and advanced Internet portals for businesses. Yet another NSF project allowed for expanded programs in computational science at the associate degree level. A directive that sprang from Chancellor Eric Fingerhut separated OARnet from OSC and created a governing body for the networking operation. In September, OSC entered into an agreement with Nimbis Services Inc. to connect regional industry supply chains to OSC’s computational and expertise resources.

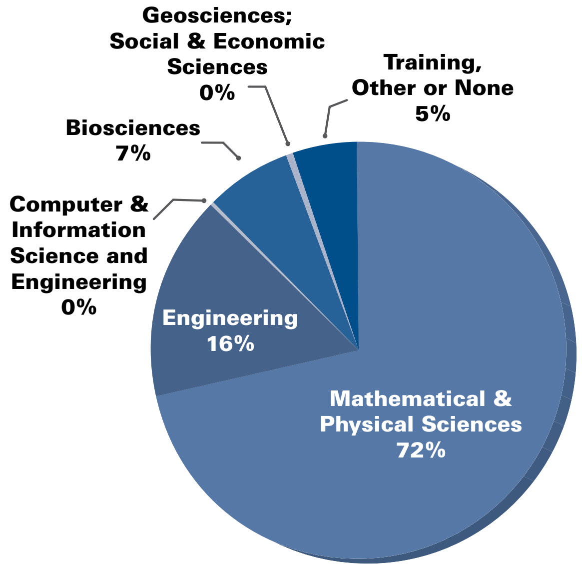
The following fall, OSC expanded the Glenn Cluster, and the combined system provided 75 teraflops of computing power. Six months later, OSC would add the “Csuri” Advanced GPU Environment, increasing OSC’s capabilities for remote visualization and batch-rendering applications, as well as GPGPU applications.

With the departure of Stan Ahalt in September 2009, OSC senior director of education and client support Steven Gordon and senior director of research Ashok Krishnamurthy were named interim co-directors of the center. In November, Korea Institute of Science and Technology Information (KISTI) officials signed an agreement with OSC leaders to enhance the center’s Blue Collar Computing program and the institute’s Small and Medium Business Supercomputing initiatives.

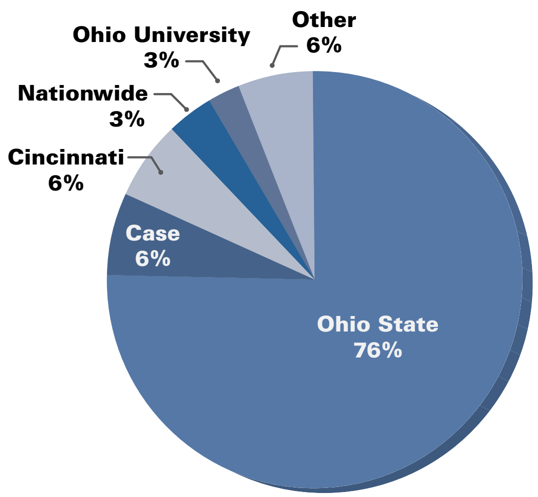
OSC signed a collaboration agreement with the Procter & Gamble Company in 2011, enabling the two to work together on modeling and simulation projects aimed at accelerating innovation collaboration between industry and academia. In March, the federal Economic Development Administration awarded a substantial National Digital Engineering and Manufacturing Consortium (NDEMC) grant to OSC and several partner organizations to support the advanced manufacturing efforts of Midwestern manufacturers.

That fall, Chancellor Jim Petro reorganized Ohio’s statewide higher education technology consortia under an umbrella organization known as the Ohio Technology Consortium (OH-TECH), merging OARnet, OSC and OhioLINK, as well as reorganizing the Ohio Learning Network and other initiatives into eStudent Services and creating the Research and Innovation Center. Pankaj Shah was named executive director of OSC and OARnet.

OSC officials in 2012 unveiled the center’s new HP-built, Intel Xeon processor-based super-computer, named after legendary Ohio sharpshooter Annie Oakley, which can achieve 88 teraflops, and, with acceleration, a total peak performance of 154 teraflops.



above: OSC system usage by field of science



above: OSC system usage by institution

HARDWARE & SOFTWARE

OSC offers clients critical computational resources

The Ohio Supercomputer Center offers invaluable supercomputing and storage resources to nearly 1,000 active users across the state, providing support for major research endeavors and saving significant campus resources as a state-of-the-art, shared facility.

This past year, OSC delivered nearly 43.3 million CPU hours to academic and healthcare researchers and offered nearly ten percent of the center's computing resources to industrial clients. The Oakley Cluster, named for legendary Ohio sharpshooter Annie Oakley, is an HP-Intel Xeon processor-based cluster system that delivers a theoretical system peak performance of more than 88 trillion floating-point operations per second (88 teraflops or TFs). The integration of 128 NVIDIA Tesla GPU accelerators provides an additional 65.5 TFs of double-precision performance, for a total of 154 TFs of total system peak performance.

Named for pioneering Ohio astronaut and statesman John Glenn, OSC's IBM 1350 Glenn Cluster's 650 nodes of AMD Shanghai quad-core hardware provide clients with 53 TFs of computing power, augmented by another 6 teraflops of double-precision performance from 36 NVIDIA GPU nodes.

Storage services represent a critical resource, and the center's Mass Storage Environment (MSE) provides those through its servers, data storage systems and networks and offers a single, centralized point of control for managing storage devices and data. The MSE features more than 2 petabytes of disk storage and provides common home directories for users across all OSC HPC systems.

Named for an Ohio State graduate and professor known as the "father of digital art," Charles 'Chuck' Csuri, OSC offers users the power of the Csuri Advanced GPU Environment. The Csuri environment offers researchers 128 NVIDIA Tesla M2070 units in the Oakley Cluster and 18 NVIDIA Quadro Plex 2200 S4 units in the Glenn Cluster, as well as the capabilities of the CUDA toolkit.

Additionally, OSC remains on the cutting-edge of high performance computing by preparing to deploy a research cluster in early 2013 for HPC software development and testing on new technology. The innovative components of the cluster include an Intel Xeon Phi accelerator and 200 GB solid-state storage drive per node. The cluster features eight HP SL250 nodes, each with two Intel E5 2670 processors for a total of sixteen cores, 128 gigabytes of RAM and a 1-terabyte disk drive. A group of OSC and OSU researchers has been working with Intel on pre-release Xeon Phi processors (SE10P cards) since mid-2011 (see story, pg. 35). The research cluster will allow the team to expand these efforts and assist users in the design and use of the next large system at OSC.

Finally, OSC continues to provide a variety of software applications, including GPU-capable packages, to support all aspects of scientific research. The center offers more than 30 software applications and access to more than 70 different software packages, including OpenFOAM for computational fluid dynamics, LS-DYNA for structural mechanics and Parallel MATLAB for numeric computation and visualization.

HPC ACCESS VIA THE WEB

For the past year, OSC OnDemand v1 has provided users with remote visualization services through their web browser.

Based upon the positive response from users, an expanded version, known as OSC OnDemand v2, or "OD2," is being developed and is scheduled for release in early 2013. In order to improve the user experience, OD2 provides a single point-of-entry for all OSC functions, adding web-based file access, job management, system monitoring and login access. OSC web applications provide job and system functions via a unique web architecture. A version tailored for tablet computers and smartphones is planned for a subsequent release.

VISUALIZATION & INTERFACE

Technology allows researchers to see, hear, feel data

As virtual environments become increasingly sophisticated, their use in evaluating human behavior and cognition in a wide variety of situations has dramatically increased. Virtual environments are particularly useful in the study of behavior involving dangerous conditions, especially where traumatic injuries are likely. Quantifying how these environments affect the subject is essential to validate the simulation's efficacy as a correlate to reality.

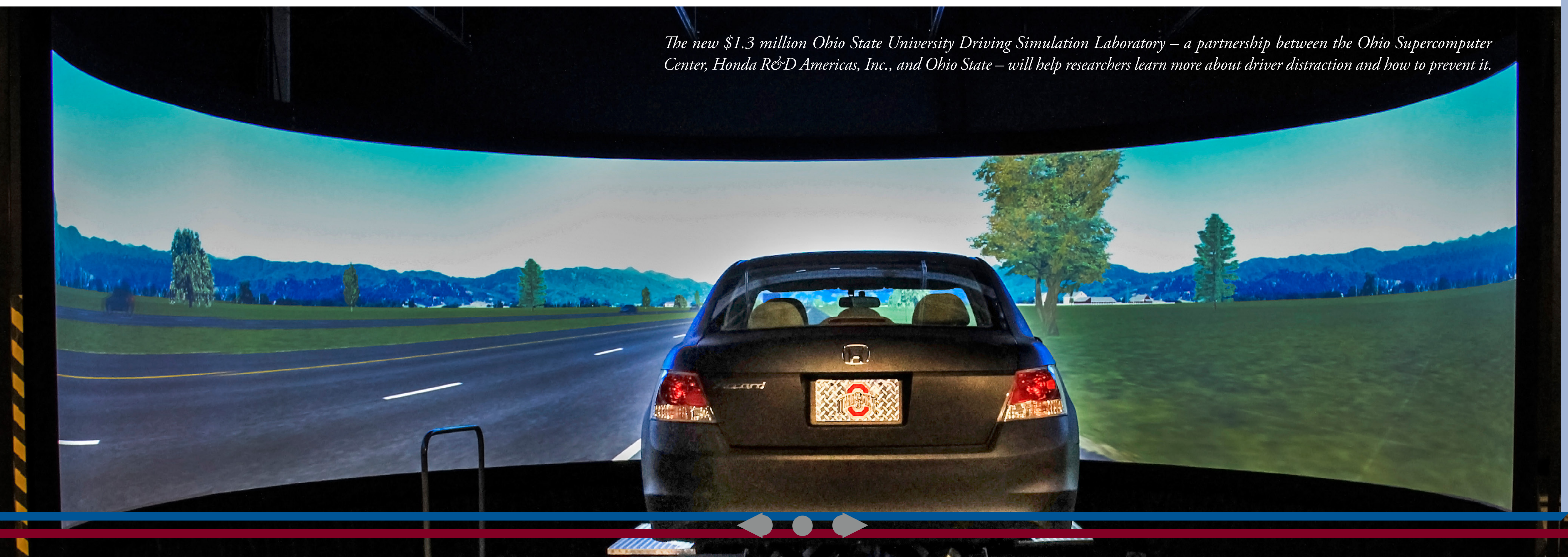
By validating user-response to dangerous situations via simulations, we can further trust these environments to portray a realistic assessment for equipment and procedure modification and testing, as well as evaluate the training methods in situations hazardous for human exposure or difficult to access.

The latest tool added to the visualization services available through the Ohio Supercomputer Center is a 5,800 square-foot Ohio State University Driving Simulation Laboratory (DSL), which supports the design and implementation of vehicle instrument panels and in-vehicle information systems that can be used safely by the driver. A unique university and industrial partnership, the DSL receives significant funding from Honda R&D Americas, oversight from The Ohio State University's Office of Research and management by OSC. The lab features three unique simulator environments, each running Realtime Technologies' SimCreator software. A desktop system allows for rapid prototyping and building of scenarios. The second allows for testing of production vehicles using a "drive-on" turntable system and a single, forward-projected display. The largest environment features a full-size vehicle situated within a 260-degree panoramic screen for maximum visual, sound and motion representations.

The following examples illustrate the array of funded simulation projects underway at OSC:

A research team led by simulation 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.

Developed in partnership with Nationwide Children's Hospital and OSU's Department of Otolaryngology, OSC's Virtual Temporal Bone Project allows future surgeons to practice delicate drilling techniques on a computer-based teaching system. The use of force-feedback technology in the simulator allows residents to "feel" the surgery they are practicing, as well as see and hear it. The simulator is presently being assessed through a multi-institutional study that includes ten sites around the U.S. in addition to The Ohio State University.



The new $1.3 million Ohio State University Driving Simulation Laboratory – a partnership between the Ohio Supercomputer Center, Honda R&D Americas, Inc., and Ohio State – will help researchers learn more about driver distraction and how to prevent it.

TECHNOLOGY INNOVATION

Portals, programs give business easy access to HPC

As a key resource supporting the Technology Innovation Services initiative of the Ohio Technology Consortium (OH-TECH), the Ohio Supercomputer Center provides hardware, software, expertise, training and customized portal access to provide business and industry with modeling, simulation and analytics tools to boost research and deliver success. OSC has long contributed to the economic competitiveness of the state, introducing the concept of Blue Collar Computing to a large audience of technology industry heavyweights at an international supercomputing conference in 2004.

In 2011, industry researchers consumed almost 3.5 million CPU hours, about 8 percent of the total usage of OSC flagship systems. This percentage is expected to continue to grow alongside OSC's role in the National Digital Engineering and Manufacturing Consortium (NDEMC). NDEMC is the first large-scale, public-private partnership of the federal government, original equipment manufacturers, state and university computing centers, the State of Ohio, and other non-governmental organizations to provide education, training and access to computing resources to small- and medium-sized enterprises. With the program initially focusing on the Midwest, OSC has been actively supporting 13 of 23 approved projects, nine of which have some physical presence in Ohio. Several of the companies involved in NDEMC projects at OSC have already have seen tangible benefits:

- Greenlight Optics, an optical systems product design company seeking to enter the Lockheed Martin supply chain, modeled thermal properties involved in producing an injection-molded lens used for collimating LED light (see story, pg. 34). With the modeling software, the company's engineers were able reduce the manufacturing cycle time by 64 percent.
- Applied Sciences, a carbon nanofiber manufacturer based in Cedarville, Ohio, is part of the Lockheed Martin supply chain. OSC helped them use extrusion modeling simulation software to better understand how carbon nanofibers are distributed when mixed with polymers, and has cut in half the company's time-to-market for CNF-reinforced plastics.
- Jeco Plastics, a plastic pallet and shipping container manufacturer simulated changes to the design of a large plastic pallet in support of a large customer request. As a result of the project, Jeco was awarded a large contract by the automobile manufacturer.

This national program follows on the heels of several successful portal development projects spearheaded by the Center.

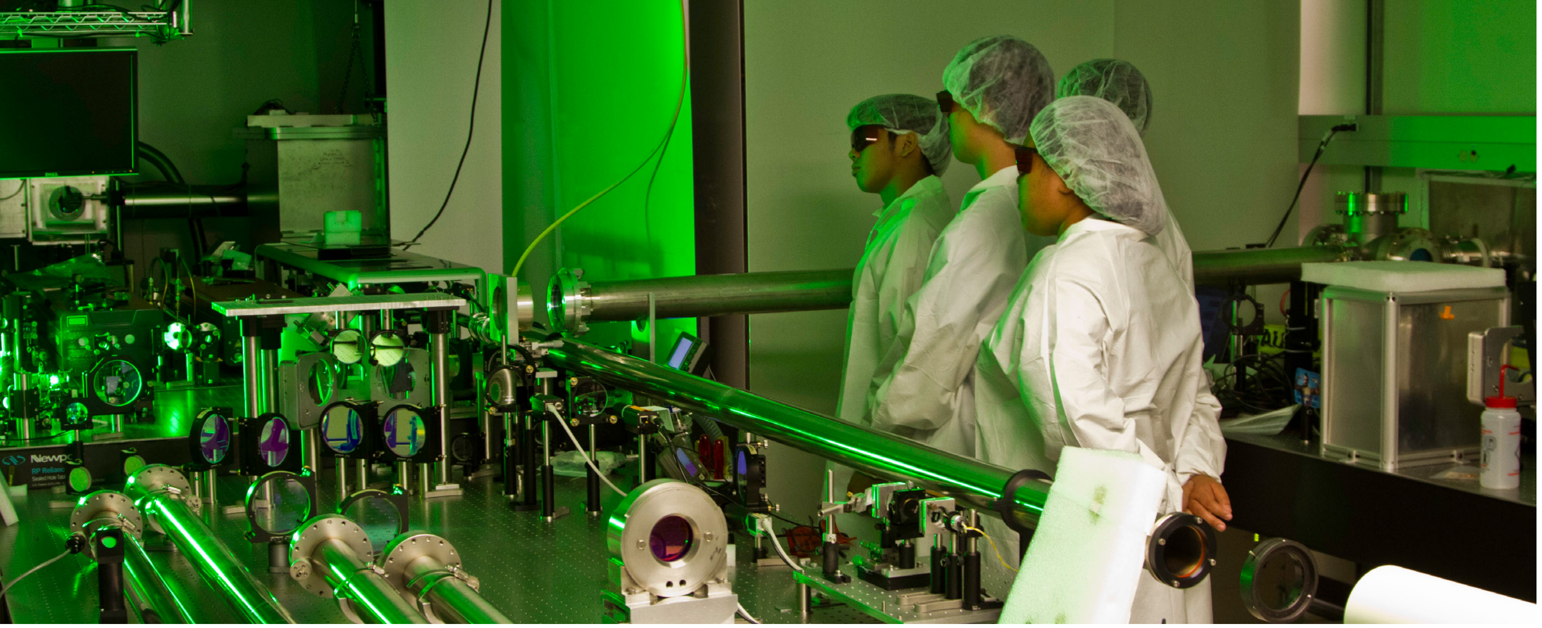
- This year, OSC, Procter & Gamble and TotalSim, Inc. have deployed an application called the Manifold Flow Predictor (MFP) as part of an effort by NDEMC to extend computational fluid dynamics capabilities to smaller manufacturers. Large manufacturers require advanced modeling and simulation to predict 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. Today, an engineer enters a computer-aided design file describing the manifold into the MFP portal, selects the fluid (e.g., water, air, glue, hydraulic fluid) and

> *"We started a U.S. sister company to a British engineering firm that specializes in automotive fluid dynamics and were deciding whether North Carolina or car racing mecca Indianapolis was a better fit than Central Ohio. But the proximity of auto manufacturers, support from TechColumbus and, perhaps most important, the ability to tap into the state-run Ohio Supercomputer Center for complex simulations drew our firm to the Dublin Entrepreneurial Center in 2009. To have a resource like OSC … it was kind of the key part of putting the company together."*
>
> – Ray Leto, President
> TotalSim

Computational science is impacting nearly every segment of industry, such as modeling new approaches to fuel efficiency. Through a Department of Energy program, the National Center for Manufacturing Sciences, Ohio Supercomputer Center, TotalSim, SimaFore and Nimbis Services have collaborated to create a computational fluid dynamics tool with which automotive suppliers can model aerodynamic forces over a joint vehicle/trailer body.

- enters an input pressure. The CFD and visualizations are calculated using OSC resources and displayed to the user.
- In 2011, the National Center for Manufacturing Sciences (NCMS), OSC and other partners launched the Truck Add-on Portal to allow suppliers to model the airflow over a tractor/trailer and the corresponding aerodynamic forces generated on them. By understanding the forces on the various surfaces, trailer designers and part suppliers can reduce the weight of key structural components, replace them with other materials or utilize novel shapes while potentially increasing the aerodynamic efficiency of the trailer. The project is funded in part by the Department of Energy's Lightweight Automotive Materials Program, or LAMP.
- A year earlier, PolymerOhio Inc. launched the Polymer Portal, an initiative developed in collaboration with OSC to enhance productivity for small- and mid-sized polymer companies by providing affordable access to advanced modeling and simulation capabilities. The National Institute of Standards and Technology's Hollings Manufacturing Extension Partnership (NIST MEP) funds the innovative portal. PolymerOhio is an Ohio Edison Technology Center that focuses on enhancing the global competitiveness of Ohio's polymer industry, including companies from the plastics, rubber, bioproducts and advanced materials segments.
- In 2007, Edison Welding Institute (EWI) and OSC launched WeldPredictor, an online weld simulation tool that offers improved productivity and profitability to EWI's thousands of member-companies. This on-demand product allows engineers to evaluate changes in temperature profiles, material microstructures, residual stresses and welding distortion to reduce the extent of experimental trials during the design of welded joints. Since its establishment as an Ohio Edison Center in 1984, EWI has helped manufacturers in the aerospace, automotive, government/defense, heavy manufacturing, consumer products, energy and rail industry sectors.

In addition to the vital computational resources of OSC, the OH-TECH Technology Innovation Services initiative also enhances the economic prospects of companies by tapping the many potent capabilities of the consortium's other member-organizations, such as high-speed network connectivity through OARnet, vast library resources through OhioLINK, workforce development programs through eStudent Services and, in the near future, a discovery pipeline through the Research & Innovation Center.



EDUCATION & TRAINING

OSC programs promote computational science skills

Supercomputing is the technological foundation for large-scale, data-intensive science and engineering, while 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 and computational science can accomplish holds the potential to improve the lives of everyone.

The Ohio Supercomputer Center's virtual Ralph Regula School of Computational Science coordinates classroom and online computational science education programs at the baccalaureate minor, associate concentration and workforce certificate levels, further cementing OSC's reputation as a national leader in the field.

Based on the school's strong reputation, Steven Gordon, Ph.D., OSC senior director of education and client support and executive director of the Ralph Regula School, has been leading the National Science Foundation's Extreme Science and Engineering Discovery Environment (XSEDE) project. The program's education and outreach efforts attempt 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.

Also, Karen Tomko, a senior researcher in computer science at OSC, was designated a XSEDE Campus Champion; she is charged with empowering researchers and educators to advance scientific discovery by serving as their local source of knowledge about national high performance computing opportunities and resources.

National leaders 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. And OSC staff members associated with the National Digital Engineering and Manufacturing Consortium (NDEMC) helped industrial clients with the required training needed to develop advanced manufacturing production.

Over the summer OSC's Summer Institute provided educational programming to high-school students for the 23rd year, and Young Women's Summer Institute provided the same to middle-school girls for the 13th year. Also, OSC once again hosted 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.

Cure cancer. Prevent future strokes. Treat night blindness. Ohio's bioscience researchers are using the Ohio Supercomputer Center to analyze vast amounts of genetic, molecular and environmental data to better understand human physiology and diagnose and treat diseases. The research on the following pages illustrates a sampling of these efforts.

BIOLOGICAL **SCIENCES**

Research Building III houses the Battelle Center for Mathematical Medicine, a new, $93 million facility that nearly doubled the dedicated research space at Nationwide Children's Hospital.

GENETIC ARCHITECTURE

Vieland develops PPL framework for data analysis

Genetic data analysis uses statistical methodology to map disease genes on the genome; statistical genetic research has long shifted from looking at a single gene disorder to complex diseases.

"When two genes interact to cause a clinically important phenotype, we can leverage genotypic information at one of the loci in order to improve our ability to detect the other," said Veronica Vieland, Ph.D., vice president for computational research and director, Battelle Center for Mathematical Medicine.

Vieland and researchers at the Center, which is part of the Research Institute at Nationwide Children's Hospital, have developed a class of linkage statistics, called the posterior probability of linkage (PPL), that allow for gene × gene interaction, parent of origin and many other genetic architectures. Implemented in KELVIN, a statistical genetic data analysis software package, the PPL framework treats trait model parameters as nuisance parameters and integrates them out of the likelihood rather than fixing them at arbitrary values.

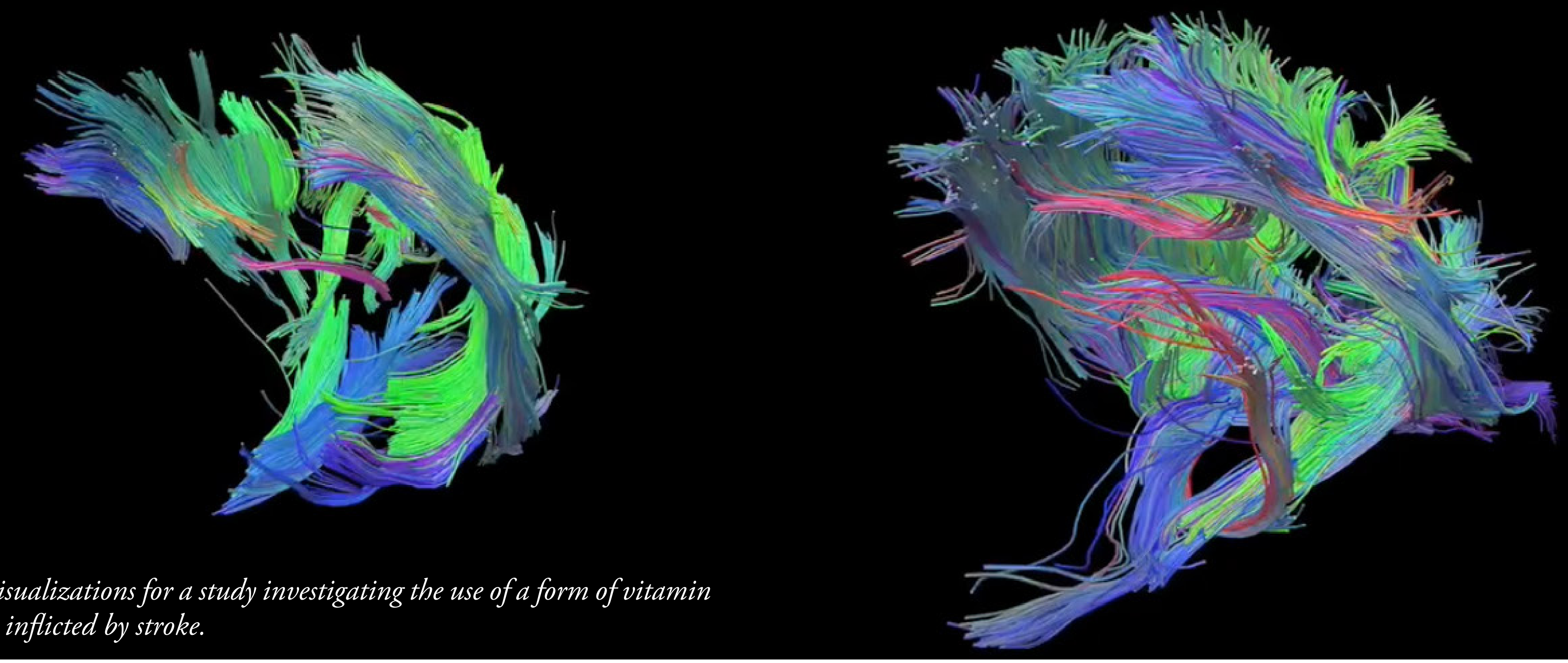
Using KELVIN to model genetic architecture is computationally intensive and requires continuous software development. Ongoing software engineering focuses on extending the complexity of the calculations that KELVIN can perform in order to address emerging data analysis needs, including such things as multipoint likelihood calculations in large and complex pedigrees based on dense SNP maps and genetic analyses involving multiple interacting loci.

"We are expanding KELVIN and further developing the PPL framework, as well as implementing a web-based infrastructure to make the package more user-friendly to other investigators," Vieland said. "The considerable resources we have access to through the Ohio Supercomputer Center are an important component of what we need for this computationally intensive work."

PPL framework and its variants have been successfully applied to genetic data analysis for various genetic diseases, such as schizophrenia, autism and autoimmune thyroid disease. As Vieland works to refine KELVIN and the PPL framework, she also is more fully modeling the genetic architecture of schizophrenia, autism and bipolar disorder by evaluating the methods using simulations and applying them to public domain data sets that have been deposited by various research groups.

"By enhancing the power of our statistical and computational methods, we expect to shed new light on the genetic architecture of schizophrenia, autism and bipolar disorder," Vieland said.

Project lead: Veronica Vieland, The Research Institute at Nationwide Children's Hospital
Research title: Modeling genetic architecture with extended PPL framework
Funding source: National Institute of Mental Health
Web site: http://bit.ly/OSC-RR-Vieland



Streamline tractography visualizations for a study investigating the use of a form of vitamin E to reduce tissue damage inflicted by stroke.

BIOMEDICAL VISUALIZATION

Machiraju, Rink combine imaging and tractography

Researchers at The Ohio State University's Center for Clinical and Translational Science (CCTS) are using sophisticated scanners and powerful supercomputers to study how vitamin E can be used to reduce the extent of brain injury suffered by stroke patients.

Cameron Rink, Ph.D., assistant professor of surgery in the College of Medicine at Ohio State's Wexner Medical Center, is part of a research team that has been investigating stroke treatments for more than a decade. He teamed up with a pair of computer scientists who leveraged Ohio Supercomputer Center resources to create detailed visualizations of brain activity during a stroke, providing researchers with an extraordinary window into treatments for ischemia, the loss of blood flow and resulting tissue damage.

Supported by CCTS funding, Rink discovered that the preventive use of a form of vitamin E called tocotrienol reduces stroke-induced brain damage in small animals in multiple ways. Tocotrienol appears to enhance the body's natural ability to use other blood vessels in the brain to bypass a clot and may reduce the chances of a repeat stroke.

"The study involved combining MR diffusion tensor imaging with streamline tractography techniques," explained Raghu Machiraju, Ph.D., an associate professor in both computer science and engineering and biomedical informatics at Ohio State University. "Originally, Dr. Rink was doing this himself on a laptop. We were able to apply some sophisticated preprocessing tools to the data and access OSC's 'big iron' to do the analysis. It's computationally very expensive."

In neuroscience, streamline tractography is a procedure that illustrates an implied flow along neural pathways, or 'tracts,' using special magnetic resonance imaging (MRI) techniques and computer-based image analysis to produce two- and three-dimensional visualizations. This study used diffusion tensor MRI (DTI) imaging of an animal's brain both during and after a stroke. This allowed researchers to glean tracts of white matter to determine the damage to the surrounding tissue.

Machiraju and Okan Irfanoglu, Ph.D., then an OSU research assistant, ran more than 60,000 jobs to apply a complex set of algorithms to large data files from seven MRI scans to create the visualizations. Irfanoglu now works at the National Institute of Child Health and Human Development of the National Institutes of Health in the lab of Peter Basser, Ph.D., and Carlo Pierpaol, M.D., Ph.D., the inventors of DTI.

Project lead: Raghu Machiraju, The Ohio State University
Research title: Tocotrienol vitamin E protects against preclinical canine ischemic stroke by inducing arteriogenesis
Funding source: The Ohio State University Center for Clinical and Translational Science
Website: http://bit.ly/OSC-RR-Machiraju

DNA SEQUENCE ANALYSIS

Yan converts sequencing data into useful information

At The Ohio State University Comprehensive Cancer Center – Arthur G. James Cancer Hospital and Richard J. Solove Research Institute (OSUCCC), cancer researchers turn to the multifunctional Nucleic Acid Shared Resource (NASR) Illumina Core to analyze genomic and epigenomic influences on the disease – and indirectly, the Ohio Supercomputer Center.

"We provide reliable, high-quality, affordable, computation support for researchers who sequence epigenomics libraries in our Core, whether they are from The James, The Ohio State University, The Ohio State University Wexner Medical Center, or another university," said Pearlly Yan, technical director, NASR Illumina Core.

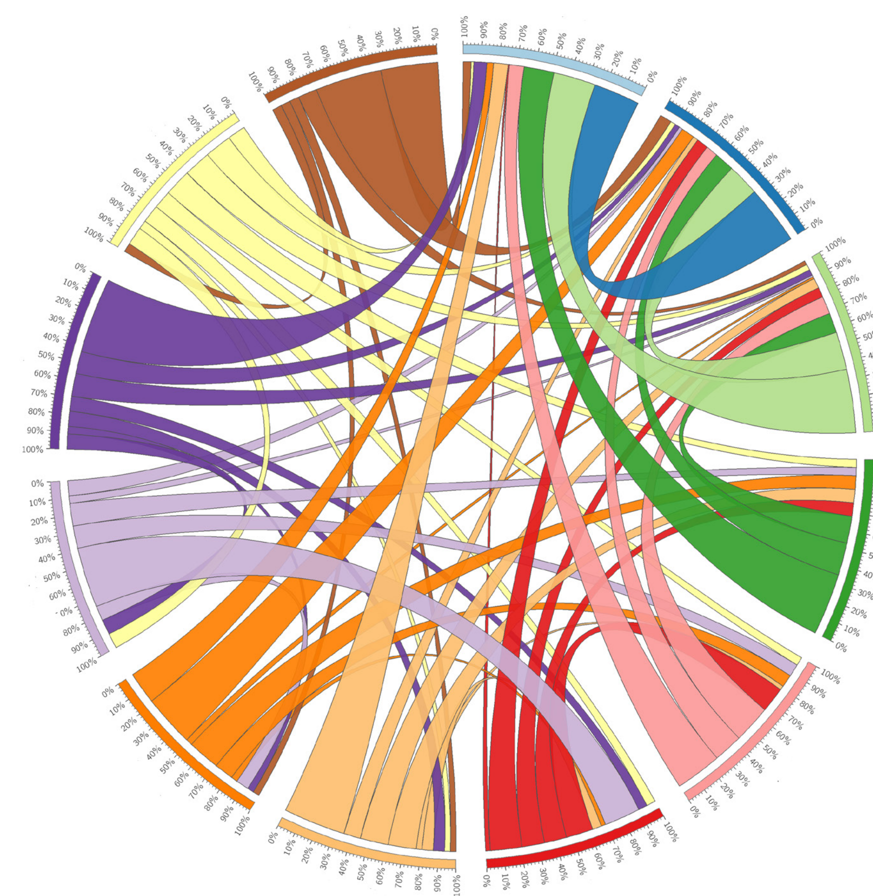
Specifically, NASR provides the research community with centralized instrumentation and expertise for Sanger-based and non-Sanger-based DNA sequencing, genotyping, DNA methylation analysis and gene expression analysis. It also offers accessory equipment for quantitative measurement and quality control of nucleic acids, and nucleic acid imaging.

"Next-generation sequencing files typically generate several Gigabits of data per sample and datasets often exceed 100 samples," Yan said. "Analyzing such large datasets requires computationally intensive, complex calculations for such processes as quality control after sequencing, genomic alignment, and custom downstream analyses."

The primary vehicle for this analysis is the Illumina HiSeq 2000, a machine specifically designed for sequencing genomes, methylomes and transcriptomes that allows researchers to quickly sequence large volumes of samples. For example, with the current data output, up to 192 indexed samples can be sequenced per run (two concurrent HiSeq flow cells generating 20 million reads per sample) for high-throughput gene expression profiling study. If the intent is to perform high-resolution transcriptome analysis, more than 50 samples can be analyzed per run at about 100 million reads per sample.

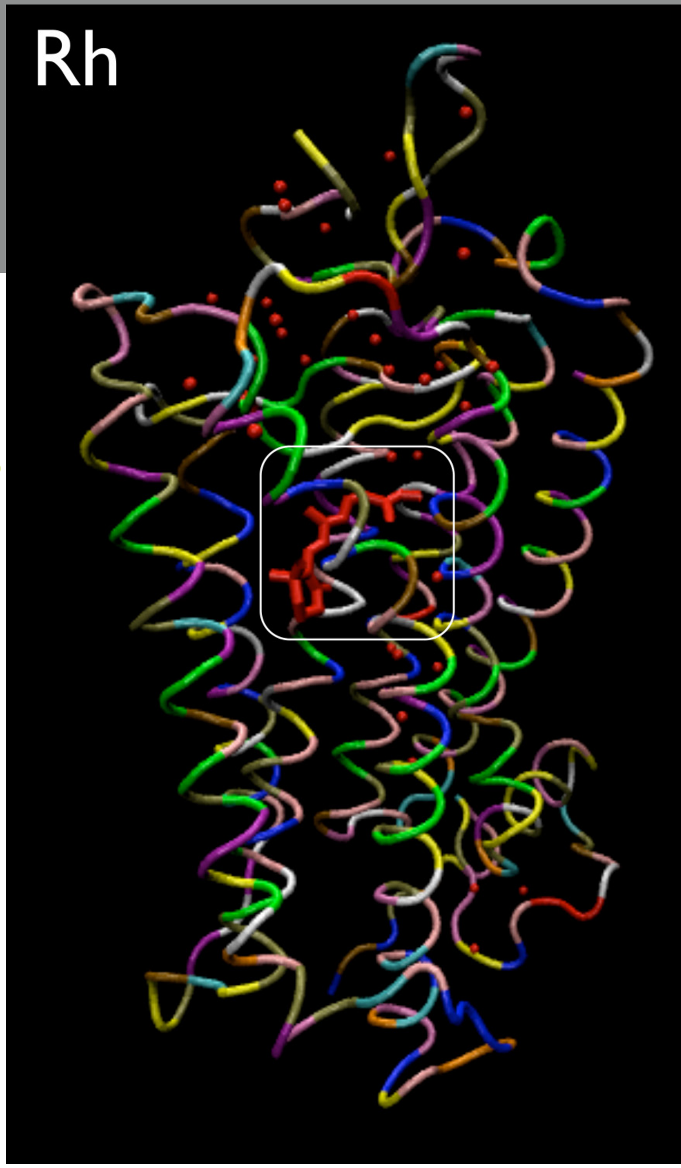
"The collaboration between the Ohio Supercomputer Center and our Core is invaluable in turning large amounts of sequencing data into information that drives clinical and translational research in OSUCCC and Ohio State's Wexner Medical Center. This type of collaboration has allowed us to provide better services to our users and timely custom analyses of sequencing data," Yan said. "Also, a good portion of our computation staff members are undergraduate assistants. Their ability to perform data analysis in the OSC environment offers them the unique education experience of learning about both cutting edge genomic data and the supercomputer environment."

The shared resources at Ohio State's Comprehensive Cancer Center – James Cancer Hospital and Solove Research Institute are an NCI-recognized network of specialized service facilities, or core facilities, which facilitate an investigator's ability to conduct cancer research by reaching across medical disciplines.



Distilled from a 134-patient study, this Circos plot links differentially methylated regions shared between mutation subgroups.

Project lead: Pearlly Yan, The Ohio State University
Research title: OSU Comprehensive Cancer Center NASR-Illumina core epigenetics projects
Funding source: The Ohio State University
Web site: http://bit.ly/OSC-RR-Yan



LOW-LIGHT DETECTION

Olivucci studies thermal noise effects on night vision

Human sight depends on an organized choreography of the retina with its cone and rods cells, the optic nerve, the brain's visual cortex and light – be it a sunny day or a dark, star-studded night.

Remarkably, in extremely poor illumination conditions, the retina can still perceive intensities corresponding to only a few photons. Rod rhodopsins enable this high sensitivity.

"Night vision represents the last frontier of light detection," said Massimo Olivucci, Ph.D., director of the Laboratory for Computational Photochemistry and Photobiology (LCPP) at the Center for Photochemical Sciences, Bowling Green State University. "If we can understand the mechanism for low-light detection, we will open new pathways that could shed light on the molecular basis of currently incurable diseases such as night blindness or tell us how to build extremely efficient light detectors approaching the sensitivity of a single-photon."

For this reason, the research group at LCPP has been investigating thermal noise, one of the main factors reducing the sensitivity of dim-light vision. Thermal noise is due to a thermal, rather than photochemical, activation of rod rhodopsins; it can be thought of as the number of activation events triggered by ambient body heat in the absence of light.

The highly sensitive rods depend on extremely low levels of thermal noise. British neuroscientist Horace Barlow first proposed in 1957 that the ubiquitous bluish color perceived during night vision – the Purkinje effect – is determined by the need to minimize thermal noise in dim light.

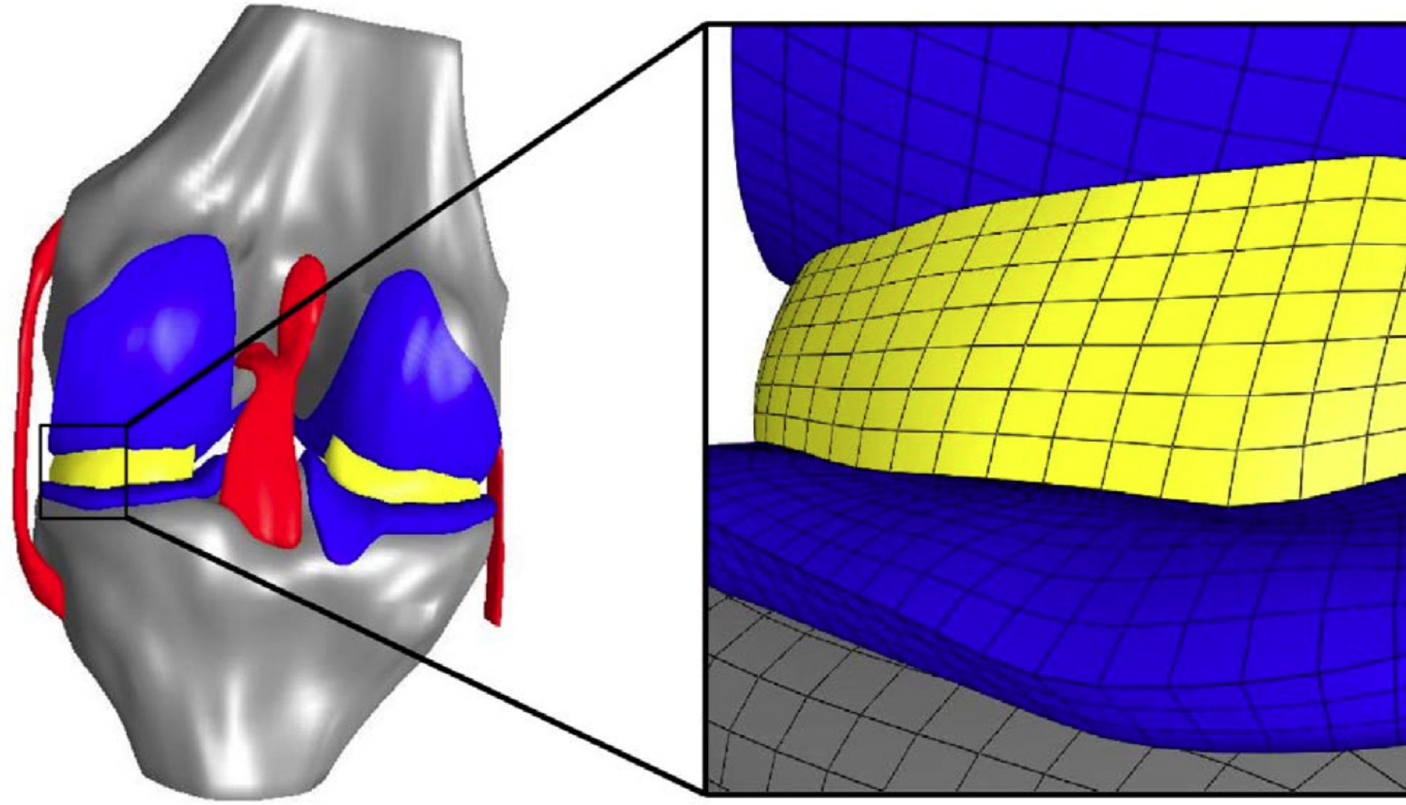
Through a series of sophisticated computer simulations of the thermal activation of a set of rod rhodopsins, the LCPP research group has provided a first-principle explanation for the Purkinje effect and a molecular level understanding of thermal noise. Their results appeared in the September 7 issue of *Science Magazine*. The simulations successfully explain the existence of a link between the color of light perceived by the sensor and its thermal noise and establishes that the minimum possible noise is achieved when the absorbing light has a wavelength that corresponds to blue light.

Using the powerful computation and storage resources of the Ohio Supercomputer Center, the work was directed by Olivucci, and completed by Nicolas Ferré, Ph.D., at the Université d'Aix-Marseille, France, BGSU graduate student Samer Gozem and BGSU research assistant Igor Schapiro, Ph.D.

(top) Photographic reconstruction of the Purkinje effect, a blue-shift of perceived color under diminishing levels of illumination.

(bottom) Tube representation of the molecular structure of the dim-light visual receptor rhodopsin. The frame shows the location of the molecular fragment capable of absorbing light (in red).

Project lead: Massimo Olivucci, Bowling Green State University
Research title: The molecular mechanism of thermal noise in rod photoreceptors
Funding source: Bowling Green State University
Web site: http://bit.ly/OSC-RR-Olivucci



A finite element model of the knee joint with representation of the cartilage, menisci and the associated bone structures. The enlarged model region to the right illustrates the mesh resolution of the simulation.

MULTI-SCALE LOADING

Erdemir simulates knee at micro and macro scales

A Cleveland Clinic research team is developing virtual models of human knee joints to better understand how tissues and their individual cells react to heavy loads – virtual models that someday can be used to understand damage caused by the aging process or by debilitating diseases, such as osteoarthritis.

Led by Ahmet Erdemir, Ph.D., the team is leveraging the powerful computing systems of the Ohio Supercomputer Center to develop state-of-the-art computational representations of the human body to understand how movement patterns and loads on the joints deform the surrounding tissues and cells. Erdemir is the director of the Computational Biomodeling Core at the Lerner Research Institute (LRI) in Cleveland, Ohio.

"The aging process and debilitating diseases affect many aspects of the mechanical function of the human body, from the way we move to how our muscles, joints, tissues and cells accommodate the loading exerted on the body during daily activities," Erdemir explained. "Computational modeling techniques provide an avenue to obtain additional insights about mechanics at various spatial scales."

Many macro-scale studies have looked at how the various components of a knee joint – cartilage, menisci, ligaments and bone – respond to weight and other external loads. However, Erdemir and colleague Scott C. Sibole, a research engineer at LRI, wanted to better understand how those large mechanical forces correspond to the related deformation of individual cartilage cells – or chondrocytes – within the knee. Previous micro-scale studies of cartilage have not commonly been based on data from body-level scales or, in particular, on musculo-skeletal mechanics of the knee joint.

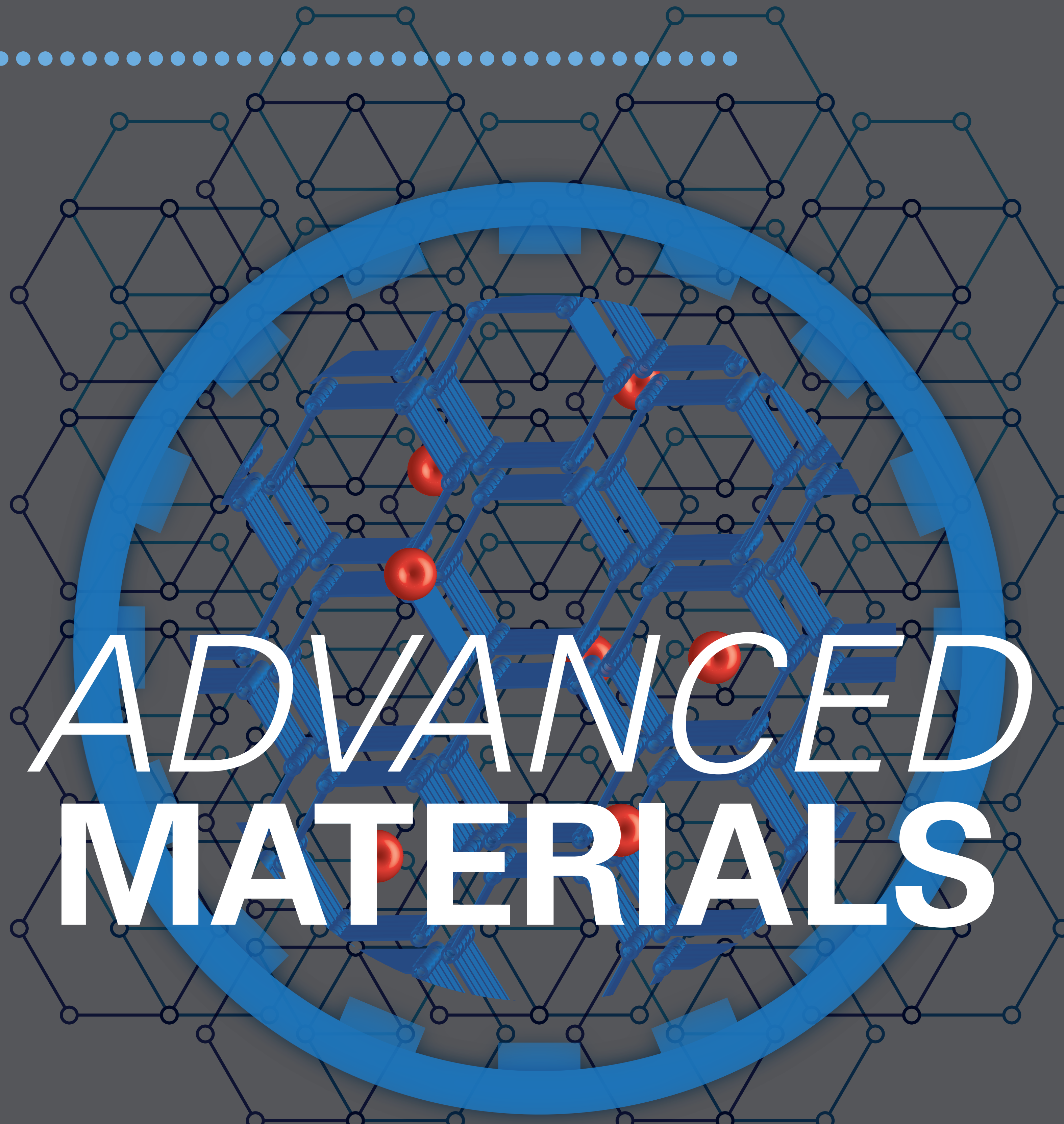
In addition, calculated deformations typically have been for a single cell at the center of a 100-cubic-micrometer block of simulated tissue; Erdemir used an anatomically based representation that calculated deformations for 11 cells distributed within the same volume.

"In both micro-scale approaches, the cartilage cells experienced amplified deformations compared to those at the macro-scale, predicted by simulating the compression of tissues in the knee joint under the weight of the body," Erdemir found. "In the 11-cell case, all cells experienced less deformation than the single cell case, and also exhibited a larger variance in deformation compared to other cells residing in the same block."

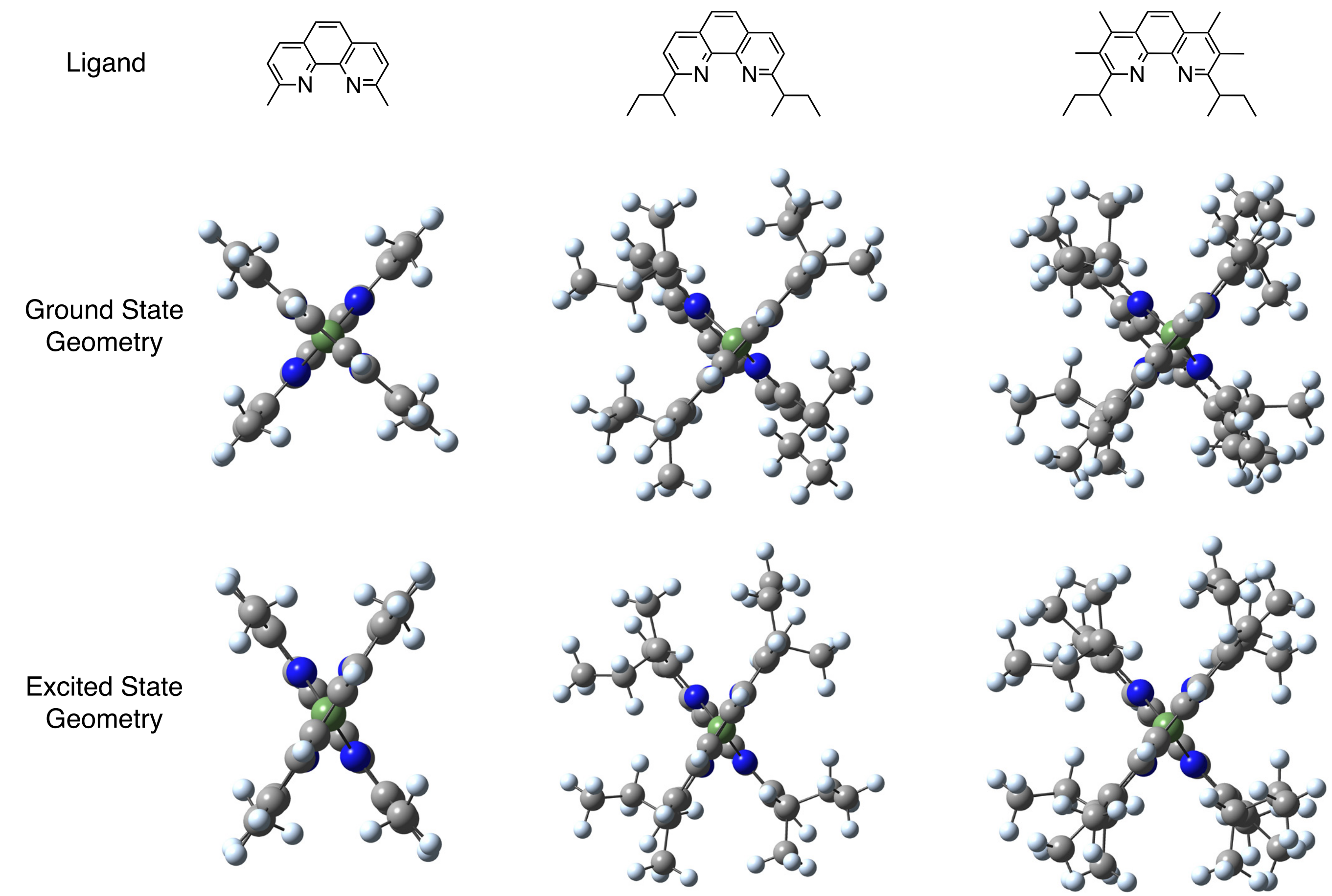
Erdemir's method proved to be highly scalable because of micro-scale model independence that allowed exploitation of distributed memory computing architecture.

Project lead: Ahmet Erdemir, The Cleveland Clinic
Research title: Chondrocyte deformations as a function of tibiofemoral joint loading predicted by a generalized high-throughput pipeline of multi-scale simulations
Funding source: National Institute of Biomedical Imaging and Bioengineering, National Institutes of Health
Web site: http://bit.ly/OSC-RR-Erdemir

ADVANCED MATERIALS



Computational modeling often lies at the crux of advanced materials research. For example, the Ohio Supercomputer Center is powering studies to develop a material for soft, artificial muscles, improve optical recording devices and create better docking seals for the International Space Station. These projects, described on the following pages, are just a few of the advance materials research projects supported by OSC.



(top) Optimized geometries of the ground state (bottom) and lowest energy triplet state of a series of substituted copper bis-phenanthroline complexes.

PHOTOPHYSICAL PROCESSES

Castellano eyes copper's photosensitizing potential

A Bowling Green State University research team led by Felix N. Castellano, Ph.D., is studying the photochemistry and photophysics of metal-organic chromophores. Currently, Castellano's team is studying the photophysical properties of coordination and organometallic complexes of copper, platinum, ruthenium and iridium along with their potential application as photosensitizers for a variety of photochemical reactions.

"From the fundamental perspective, we are interested in the interplay of closely-lying excited states and the influence these interactions have on the resulting photophysics," said Castellano, a professor of chemistry. "These processes are investigated with a battery of static and time-resolved spectroscopic techniques, the latter revealing excited state dynamics evolving from the femtosecond regime to milliseconds."

Castellano's group uses the resources of the Ohio Supercomputer Center to better understand the nature of the static and time-resolved spectroscopic data measured for these molecules in the visible and infrared portions of the spectrum.

"The application of density functional theory (DFT) and time-dependent-DFT methods to the analysis of complex electronic structures of metal complexes has emerged as a powerful complement to optical spectroscopic measurements," said Castellano. "These computational results are used in conjunction with experimental spectra to gain a deeper understanding of the electronic structure of the studied metal complexes than is possible with experimental data alone."

One focus of research in the Castellano group is the development of inexpensive copper containing dyes to replace more costly platinum, iridium and ruthenium sensitizers traditionally used in bimolecular photochemical reactions. The group currently is investigating a series of substituted copper bis-phenanthroline complexes for potential use as photosensitizers for photon upconversion. These types of copper complexes are known to undergo a large geometry change in the excited state leading to very short lifetimes. These short lifetimes limit their usefulness as photosensitizers in chemically relevant bimolecular reactions.

The researchers use DFT methods to compare the geometries of the complexes in their ground and lowest-energy excited state to predict which substituents will form complexes with the least amount of distortion in the excited state and, therefore, exhibit lengthened lifetimes. Calculations clearly demonstrate that increasing the size and number of aliphatic groups on the phenanthroline ligand decreases the amount of distortion observed in the lowest energy excited state.

Project lead: Felix N. Castellano, Bowling Green State University
Research title: DFT and TD-DFT on transition metal complexes
Funding source: Department of Energy, National Science Foundation
Web site: http://bit.ly/OSC-RR-Castellano

LIQUID CRYSTAL ELASTOMERS

Selinger leads team evaluating new class of polymers

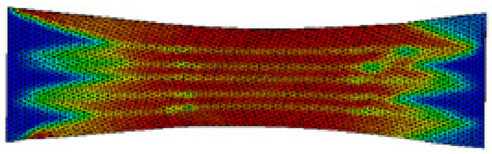
The emerging field of soft robotics requires mechanical components that grasp objects with the same delicacy as human hands. At present, most soft robots are powered by hard, sometimes bulky, actuators such as a servo motor, air compressor or hydraulic pump. However a new class of polymers, called "liquid crystal elastomers," may eventually find use as soft artificial muscles. A Kent State University research team led by Robin Selinger, Ph.D., leveraged Ohio Supercomputer Center's resources to analyze how these exciting new materials stretch, contract, curl or fold when heated, illuminated or exposed to an electric field.

"By modeling the co-evolution of a sample's microstructure and its strain field, we can predict its overall mechanical response and the sample's shape change," said Selinger, a professor of chemical physics. "My students and I wrote a finite element elastodynamics code from scratch and adapted it to model a variety of liquid crystal elastomers with different types of internal structure." The team collaborates with experimenters in Japan and the Netherlands.

A liquid crystal elastomer with uniform molecular alignment simply contracts and stretches when heated or cooled, but more complex types of actuation are also possible. Graduate student Vianney Gimenez-Pinto studied the way a liquid crystal elastomer with more complex internal microstructure behaves. She showed that a narrow liquid crystal elastomer ribbon can spontaneously twist and contract into a shape reminiscent of a rotini noodle when heated, while wider ribbons curl into the shape of a hollow cylinder. In both cases, she demonstrated that the twist direction reverses with change of temperature, in close agreement with experimental data.

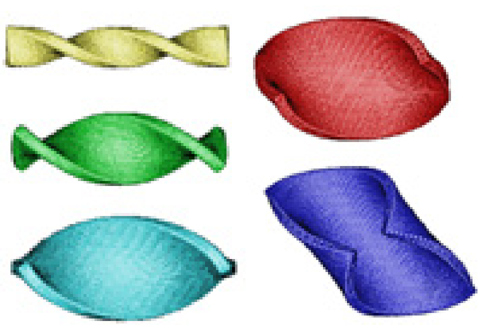
Even more complex structures produce contraction like a pleated window shade on heating. "In fact, by imposing a particular microstructure in a sample," Selinger suggested, "we can design a material that will spontaneously fold itself into any desired shape, a process known as auto-origami. The challenge here is to determine what internal microstructure will produce a particular desired shape or actuation behavior." Just for fun, Selinger also modeled how a liquid crystal elastomer "worm" could be actuated to crawl over hilly terrain.

Former graduate student Badel Mbanga, now a post-doctoral student at Tufts University, modeled how a liquid crystal elastomer's internal structure evolves when a sample is stretched. The resulting soft elastic response suggests that these materials may also find application as directional acoustic dampers.

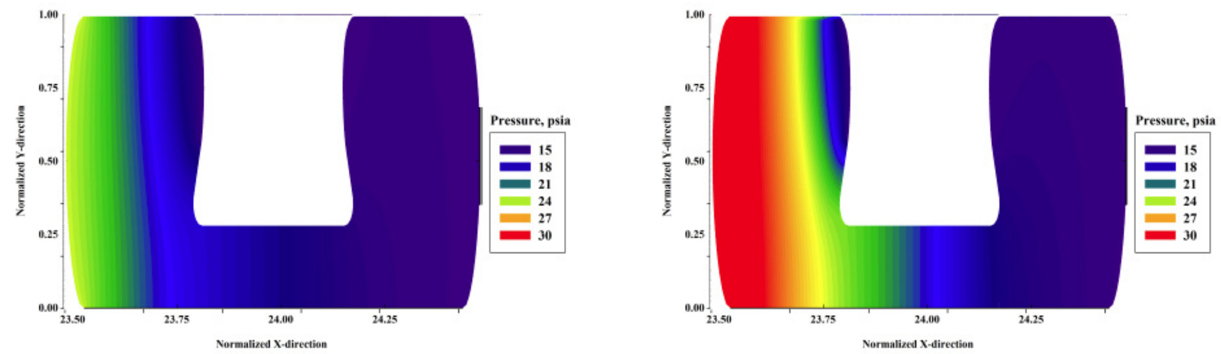


(above) When a sample with uniform microstructure is stretched laterally, the microstructure evolves to form a pattern of stripes, giving rise to a remarkably soft elastic response.

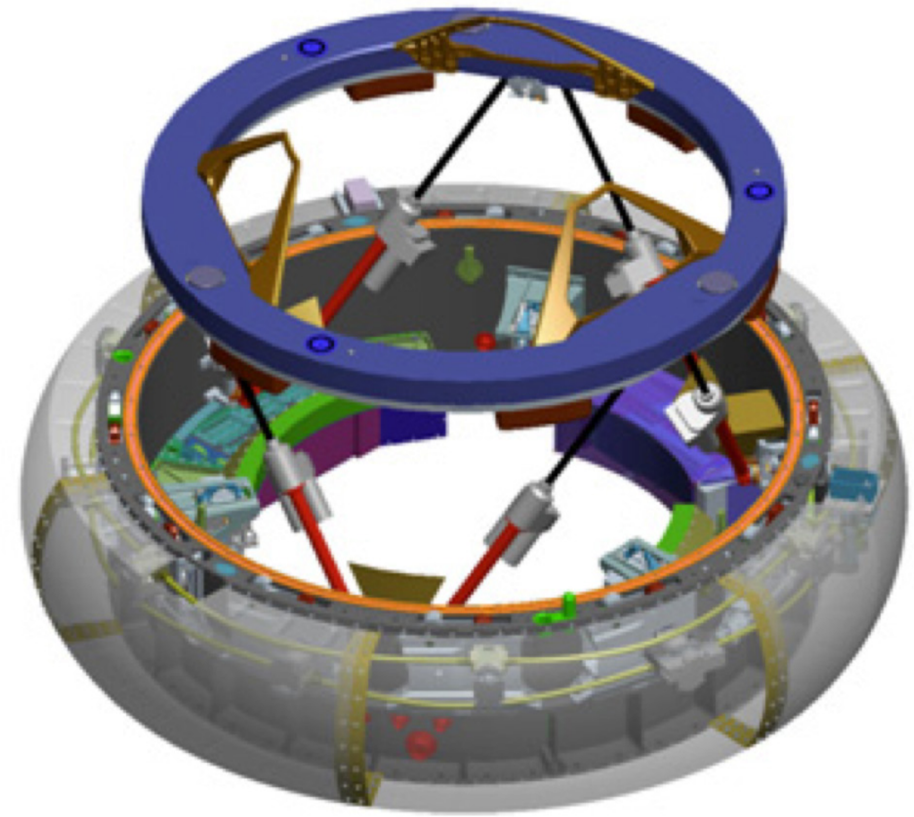
(below) When heated, liquid crystal elastomer ribbons with twisted internal microstructure spontaneously deform from a flat initial state into a variety of curved shapes. The final shape depends on the ribbon's width-to-thickness ratio.



Project lead: Robin Selinger, Kent State University
Research title: Modeling rubber that moves: Liquid crystal elastomers
Funding source: National Science Foundation, Ohio Board of Regents
Web site: http://bit.ly/OSC-RR-Selinger



(a) 10 psid (b) 20 psid



(Right) An analysis of air leakage of main interface seals – shown here as an orange ring – used in NASA's International Low Impact Docking System (iLIDS). (above) Characterization of computational pressure profiles of a potential main interface seal for docking at the International Space Station and other new spacecraft.

ELASTOMERIC SPACE SEALS

Garafolo studies approaches to test docking systems

A University of Akron researcher is designing computer prediction models to test potential new docking seals that will better preserve breathable cabin air for astronauts living aboard the International Space Station and other NASA spacecraft.

Nicholas Garafolo, Ph.D., a research assistant professor in Akron's College of Engineering analyzed a two-piece elastic silicone – or elastomer – seal, using systems at the Ohio Supercomputer Center. His model simulated air leakage through the elastomer, taking into account the effects of gas compressibility and variable permeability.

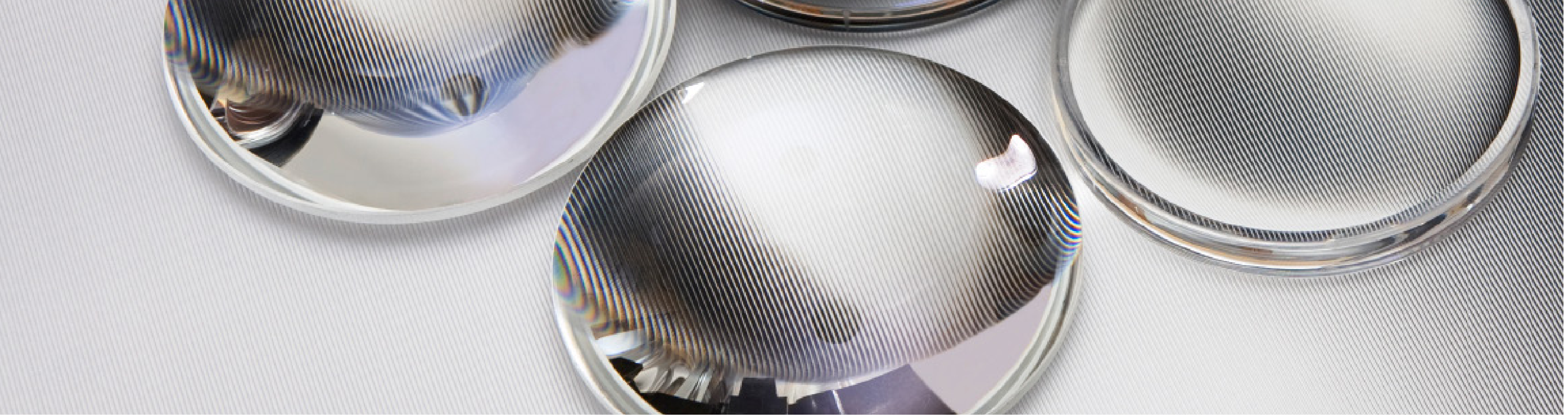
"Recent advances in both analytical and computational permeation evaluations in elastomer space seals offer the ability to predict the leakage of space seals," said Garafolo. "Up until recently, the design of state-of-the-art space seals has relied heavily on intuition and costly experimental evaluations. My research evaluated the performance of the compressible permeation approach on a space seal candidate."

Garafolo serves on a research team tasked with testing polymer/metal seals being considered for future advanced docking and berthing systems. The university researchers work with partners in Cleveland, Ohio, at NASA's Glenn Research Center, which is responsible for developing the main interface seals for the new International Low Impact Docking System. NASA has been developing low-impact docking seals for manned missions to the International Space Station, as well as for future exploratory missions. Common to all docking systems, a main interface seal is mated to a metallic flange to provide the gas pressure seal.

To establish an analytical understanding of space seal leakage and construct their computational prediction tool, Garafolo and his colleagues modeled how air leaked into and through the elastomer seal, while taking into account the effects of gas compressibility and the variability of permeation on air pressure. The research team's first evaluations showed significant correlations between the experimental values and the computer modeled results.

For pressure differentials near operating conditions, the leak rates determined by the model accurately reflected the experimental results, within the bounds of uncertainty. For pressure differentials exceeding normal operating conditions, the differences between the experimental results and computational numbers were not quite as close as expected. The larger differences in the leak rates, however, were attributed to extrapolation errors of the model parameters.

Project lead: Nicholas Garafolo, University of Akron
Research title: An evaluation of the compressible permeation approach for elastomeric space seals
Funding source: National Aeronautics and Space Administration
Web site: http://bit.ly/OSC-RR-Garafolo



CHALCOGENIDE GLASSES

Drabold models candidates for computer memory

Chalcogenide glasses, compounds based upon the elements sulphur, selenium and tellurium, have been studied extensively for the last few decades. Scientists have examined these compounds both for basic scientific interest in the compounds and because they are preferred materials for technology applications, such as optical recording devices and two novel forms of non-volatile computer memory: "phase change" (PCM) and "conducting bridge" (CBRAM).

"Since the properties of chalcogenide glasses are derived from their structure, knowledge of the structure of these glasses is an essential precursor for further study," said David Drabold, Ph.D., a distinguished professor of physics at Ohio University.

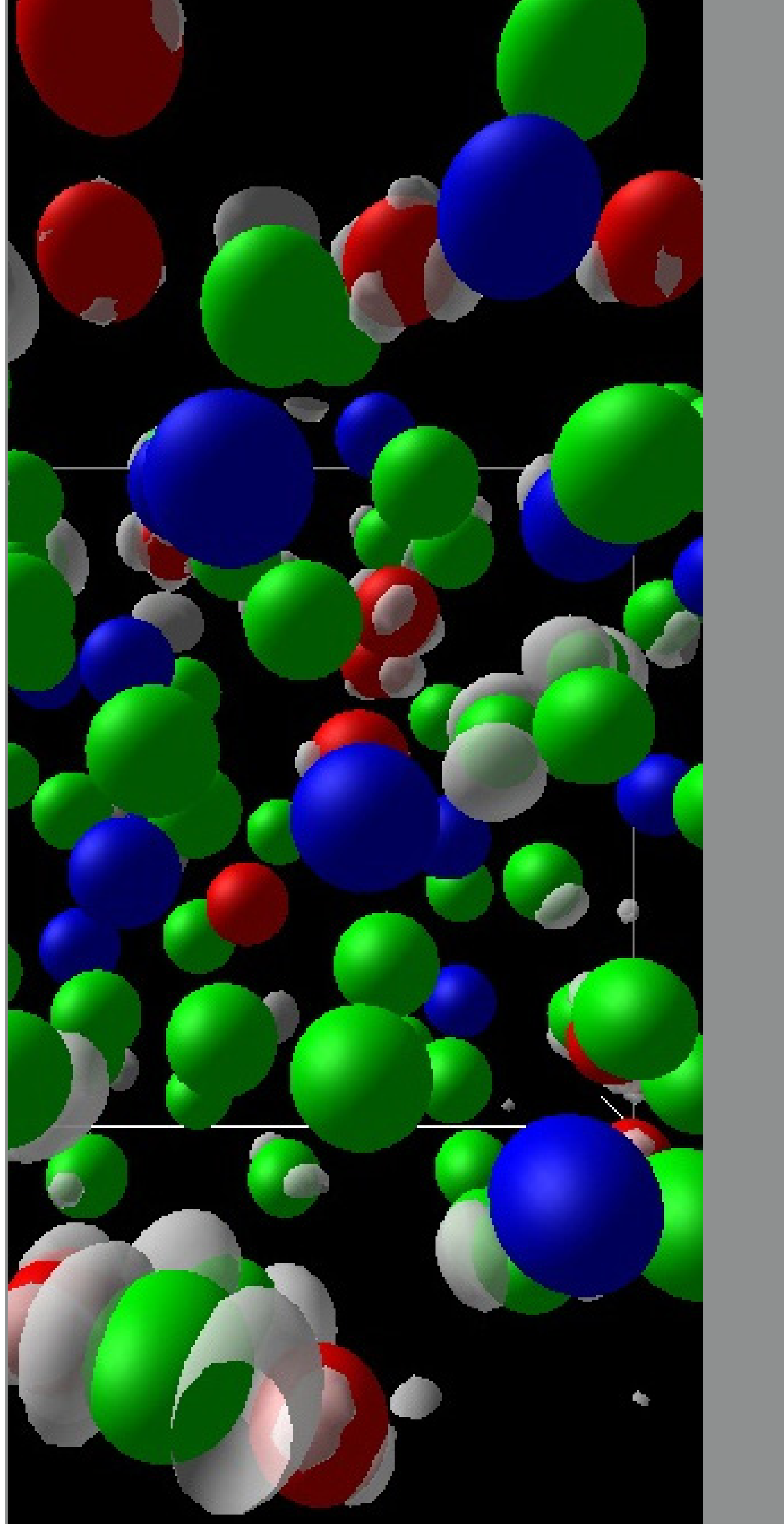
"We use density functional methods to model both PCM and CBRAM materials and work out the key dynamical processes. It's known somewhat empirically that these devices perform very well, but there are many mysteries as to how the devices rapidly switch, such as at the atomistic level. We hope to offer information on how to optimize the materials."

The CBRAM materials are based upon glasses composed of germanium and selenium. When doped with metals like silver or copper, germanium-selenium glasses become solid electrolytes with high ionic conductivities. Under different bias conditions, they possess two stable phases with different electrical conductivities, a contrast that enables their use for information storage.

For PCM materials (also used in DVDs) the contrast is found between the amorphous and crystal phases. Drabold and his research team have directly simulated amorphization and crystallization on extremely fast time scales of ~500 picoseconds (500 trillionths of a second).

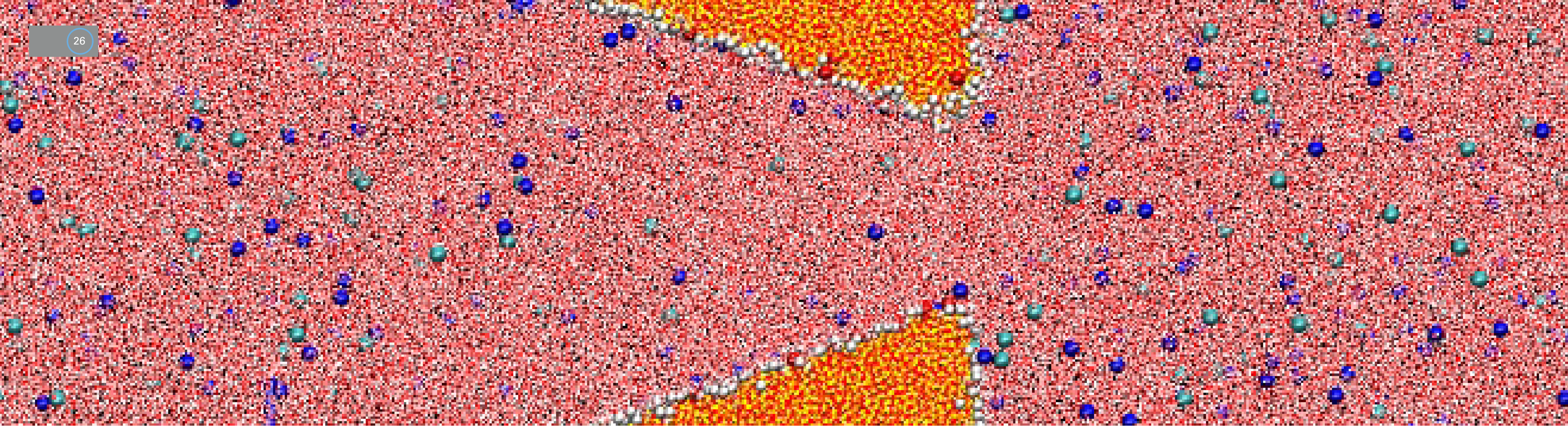
"We have employed Ohio Supercomputer Center facilities to explore new materials, previously terra incognita experimentally and theoretically," said Drabold. "It is most unusual to be able to directly simulate phase transitions or ionic diffusion using standard ab initio molecular dynamics. We have a unique opportunity to work out important physical processes of basic interest, and also to provide information of value to applied scientists hoping to optimize their electronic devices."

The chalcogenide glasses work has been carried out in collaboration with Gang Chen, Ph.D., Ohio University assistant professor of physics, and graduate student Binay Prasai. The Vienna Ab Initio Simulation Package (VASP) has been a key tool used for creating the simulations.



Representation of a fully crystallized germanium, selenium, tellurium and silver structure.

Project lead: David Drabold, Ohio University
Research title: Structure and dynamics of chalcogenide glasses
Funding source: National Science Foundation
Web site: http://bit.ly/OSC-RR-Drabold



Fully atomistic simulations of electroosmotic flow in a "nano-nozzle" device.

ELECTRICAL DOUBLE LAYERS

Singer performs simulations of electroosmotic flow

Many biological molecules and common surfaces carry an electrical charge. For example, DNA has a strong negative charge, and so does an amorphous form of silicon dioxide known as silica, the material most people recognize as "glass." A charged molecule or surface, along with the electrically compensating layer of ions in the adjacent solution, is known as the electrical double layer (EDL).

"Interest in the EDL has never waned for roughly a century, and today that interest is especially intense because of the importance of EDL dynamics in nanoscale devices, especially for biomedical applications," said Sherwin Singer, Ph.D., professor of chemistry at The Ohio State University.

In these devices, electric fields are used to manipulate biological fluids in tiny channels. A voltage applied parallel to the surface forces the ions to move with the field. This, in turn, causes electroosmotic flow (EOF), fluid flow induced by the moving ions. EOF can be harnessed to control the transport biological fluids in micro- and nano-scale lab-on-a-chip devices. The goal is rapid, point-of-care screening of patients for biomarkers identifying heart disease or cancer.

Singer's group uses the computational resources at the Ohio Supercomputer Center to perform detailed atomistic studies in complex device configurations that have not been explored to this point.

"Departure from the slit pore leads to a complex interplay between non-uniform charge density and pressure gradients," Singer explained. For example, the Singer group has been able to perform fully atomistic simulations of EOF in a "nano-nozzle" device.

The work also has bearing on fundamental scientific issues. Before such atomistically detailed work was possible, scientists who study substances that are microscopically dispersed evenly throughout another substance, or colloids, could rely only on "effective" continuum models. These continuum models have to be invoked with contradictory assumptions to explain different experiments.

For example, to account for electroosmotic fluid flow, continuum theories give sensible predictions only if water adjacent to the surface is assumed to be immobile. At the same time, the ion current would disagree with experiment, unless ions in that same layer flowed virtually unimpeded. Realistic, atomistic modeling of that surface layer at OSC reveals that water and ions are mobile right up to the surface and explains why different and contradictory "effective" models were needed to fit the data.

Project lead: Sherwin Singer, The Ohio State University
Research title: Statics and dynamics of the electrical double layer near silica
Funding source: National Science Foundation, The Ohio State University
Web site: http://bit.ly/OSC-RR-Singer

ENERGY & ENVIRONMENT

Manage wildlife habitat. Design efficient engines. Improve air quality. The solutions to significant, interrelated global energy and environment sustainability issues such as these significantly increase demand for computational modeling, simulation and analysis. The Ohio Supercomputer Center supplies the researchers working towards these important outcomes – sampled on the following pages – with the resources they need to power their data-rich projects.

ANIMAL MOVEMENT

Bohrer studies climatic impacts for habitat management

Animals are in constant movement across the surface of the earth, and climate affects their movements, especially for migrating and flying animals. Understanding animal movement is pivotal to predicting and ensuring the survival of populations in the face of rapid global changes to climate, land-use and habitats. Understanding the mechanisms of animal movement can improve forecasting for the future needs of endangered species and can allow more effective planning for habitat management in national wildlife refuges.

As part of a NASA-funded project, an Ohio State University research team led by Gil Bohrer, Ph.D., assistant professor of civil, environmental and geodetic engineering, has been working with Ohio Supercomputer Center staff to develop an online portal to effectively tie animal tracking data to a variety of weather and land surface data. To ensure relevance and effectiveness, the portal and its toolboxes are being designed in collaboration with wildlife biologists from the U.S. Fish and Wildlife Service, National Parks Service and Geological Survey.

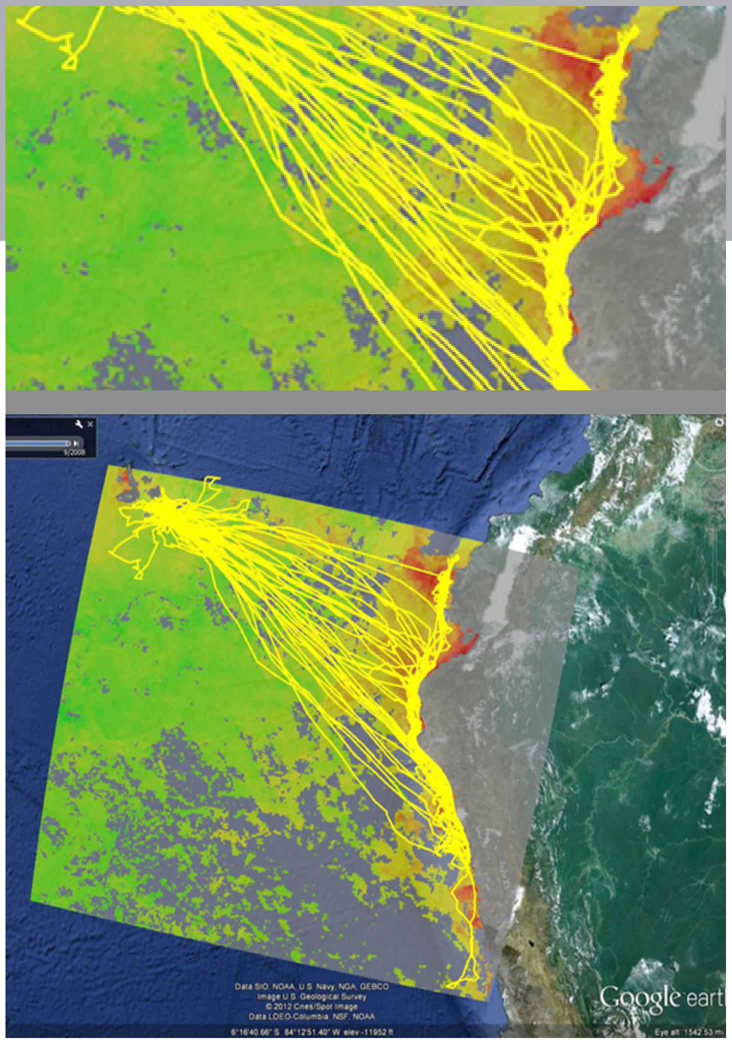
The infrastructure developments will improve and expand Movebank.org, an existing free and sustainable online portal, run by the Max Planck Institute of Ornithology in Germany, which currently houses more than 51 million data points from 185 species archived by hundreds of registered users.

The environmental data will be obtained from satellite remote sensing products, as well as from high-resolution weather reanalysis projects. Wildlife migrations are presently tracked using satellite-based systems such as GPS.

"The size and format of several of the datasets form a particular challenge," Bohrer said. "Processing all the data over the network would be unsustainably slow. Additionally, users must figure out the format and processing of each dataset."

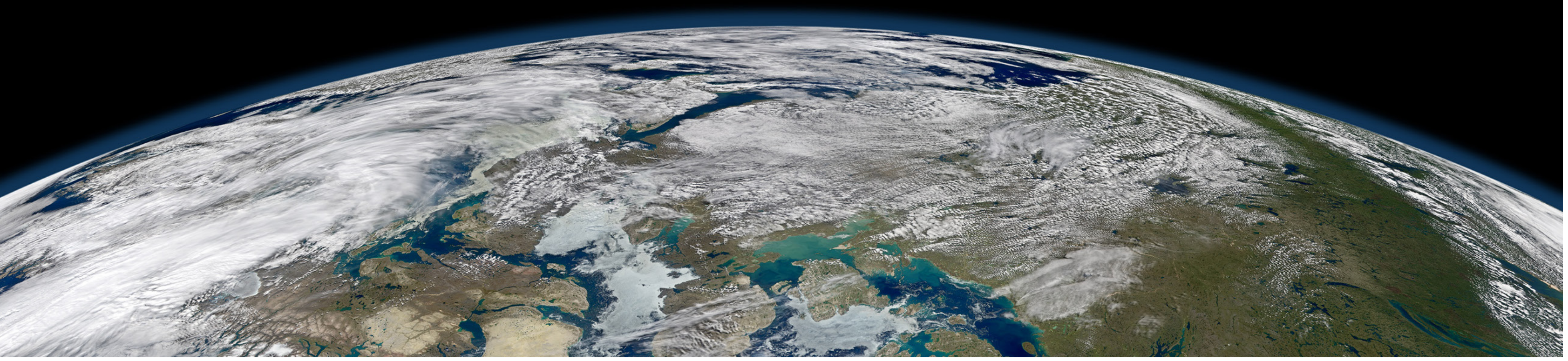
An efficient server process that analyzes and standardizes the data will need to either download high-resolution global snap-shots for the periods of the processed study or use locally stored data. Mirroring all of NASA's earth-surface moderate-resolution data so that processing can be done locally would require up to 100 terabytes of storage. Adding other datasets would double that requirement.

Bohrer is mirroring subsets of environmental data limited only to the variables and time periods most commonly needed, with an expected total storage size of 25 terabytes. He is collaborating with OSC staff to develop a server process that will receive requests from Movebank.org and process the environmental data locally, returning the compact, processed results over the network.



Albatross tracks from their nesting site in the Galapagos Islands to feeding grounds near the coast of Peru. The map is overlaid with satellite data of Ocean Net Primary Productivity (NPP), which can be derived from the ocean color (greener means more productive).

Project lead: Gil Bohrer, The Ohio State University
Research title: Discovering relationships between climate and animal movement with new tools for linking movement tracks with remote-sensing land-surface data
Funding source: National Aeronautics and Space Administration
Web site: http://bit.ly/OSC-RR-Bohrer



ARCTIC SYSTEM REANALYSIS

Bromwich synthesizes datasets for climate reconstruction

The Arctic is in the midst of rapidly escalating change with pronounced increases in surface air temperature over subarctic land areas, as well as over the Arctic Ocean. Sea ice cover in the Arctic has declined substantially in summer, rendering both the Northwest Passage around Arctic Canada and the Northeast Passage above Russia ice-free in the summer months, probably for the first time in centuries.

Even more disconcerting, the warming of the Arctic region has occurred at a much faster rate than scientists and traditional computer models have been predicting.

“In 2012, the Arctic sea ice smashed the low-extent record of 2007 by about 20 percent,” noted David Bromwich, Ph.D., a senior research scientist for the Byrd Polar Research Center at The Ohio State University and professor of atmospheric sciences in the geography department. “And, over a few days in July this summer, almost the entire ice sheet of Greenland experienced surface melt, a very anomalous event.”

To help better gauge the changes taking place there, Bromwich and his research team have been awarded National Science Foundation funding to develop the Arctic System Reanalysis (ASR). Bromwich is feeding 11 years of historical atmosphere/sea ice/land surface observations into the Polar Weather Research and Forecasting model (Polar WRF). Polar WRF was created by the Polar Meteorology Group of the Byrd Polar Research Center at Ohio State and is a modification of the Weather Research and Forecasting model widely used by researchers and most federal agencies.

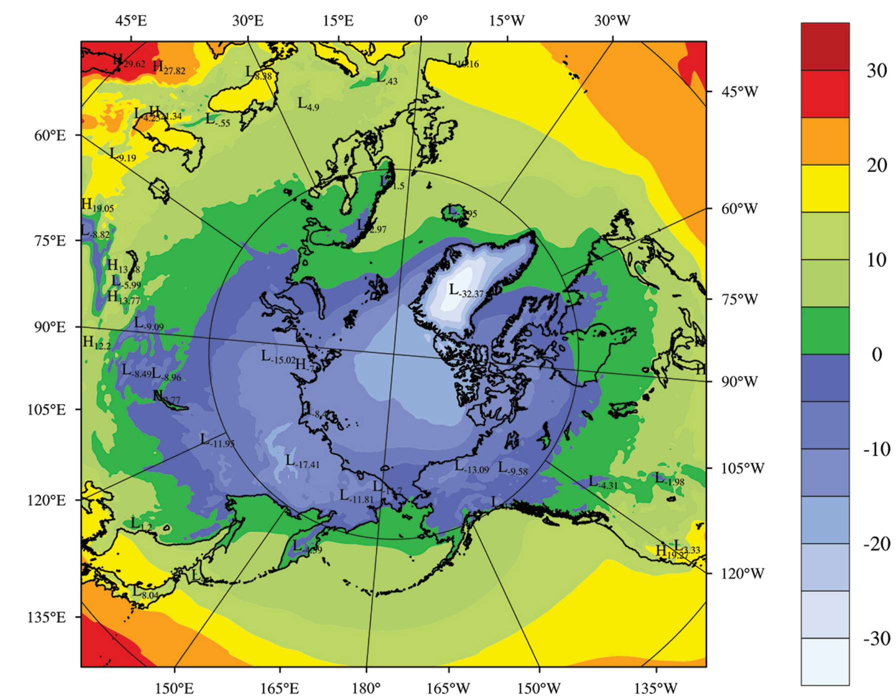
For ASR, the complex Polar WRF system analyzes 17 surface variables, 71 forecast surface variables, 13 forecast upper air variables and 3 soil variables. The goal of ASR is to provide researchers with high-resolution information against which researchers can validate climate prediction tools.

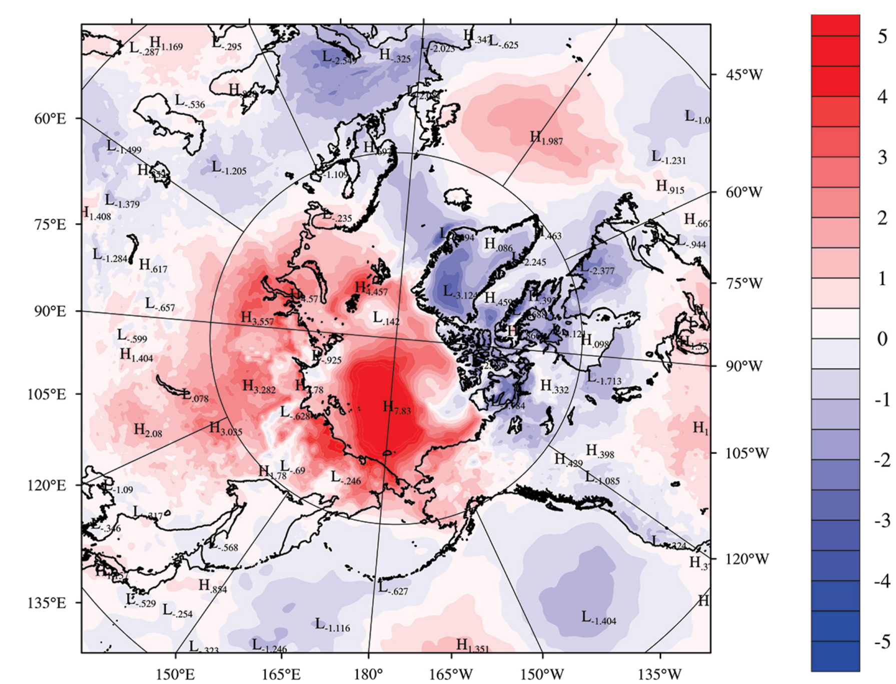
“The ASR will permit reconstructions of the Arctic system’s state, thereby serving as a state-of-the-art synthesis tool for assessing Arctic climate variability and monitoring Arctic change,” Bromwich noted. “Appropriately, Arctic enhancements developed for this project by Ohio State are being funneled through the National Center for Atmospheric Research for release to the scientific community.”

To synthesize the vast troves of data, Bromwich has leveraged the computational and storage resources of the Ohio Supercomputer Center. A low-resolution interim version of the ASR, covering 2000-2010, is currently available to the scientific community.

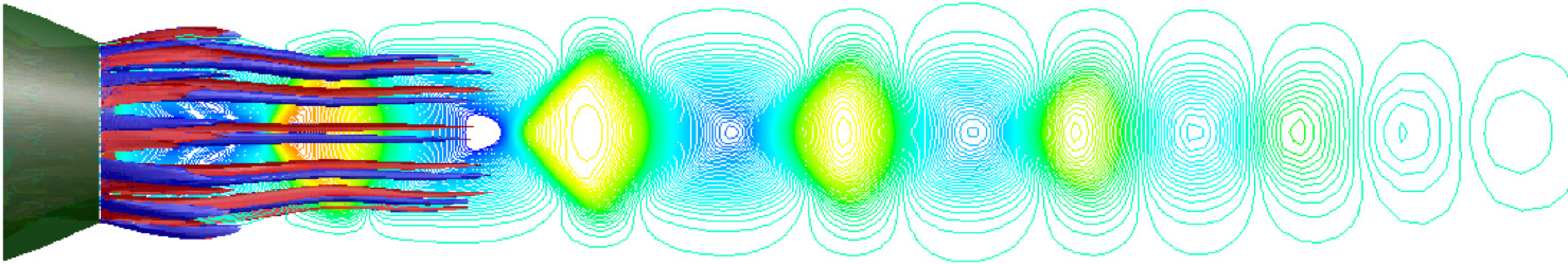
(top) Average near-surface air temperature distribution from ASR-Interim in degrees Celcius (colors) for fall (Sept.-Nov., 2000-2010 average).

(bottom) Departure from the average shown in figure above of the temperature during Fall 2007, when the summer sea ice extent was lowest prior to the all-time record minimum in 2012. The warm center in the Arctic Ocean (+7.8°C) is located where the sea ice was prevented from reforming by heat stored in the water during summer.

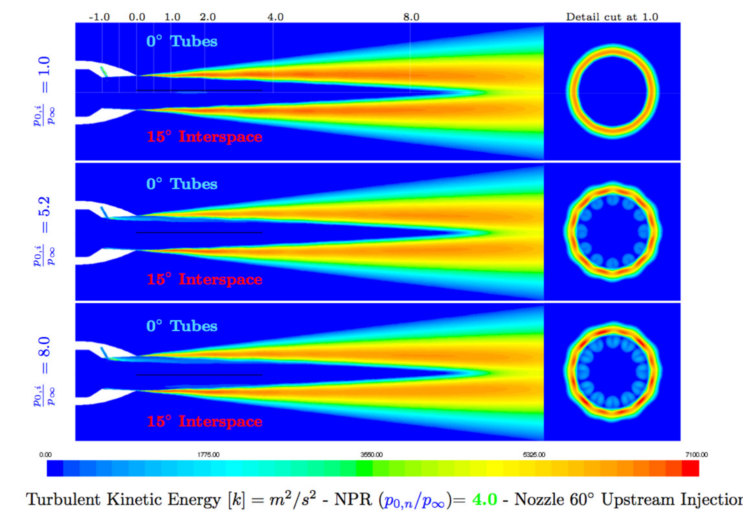




Project lead: David Bromwich, The Ohio State University
Research title: Arctic System Reanalysis
Funding source: National Science Foundation
Web site: http://bit.ly/OSC-RR-Bromwich



A qualitative image of the supersonic flow field exhausting the convergent-divergent nozzle with fluidics on.



The effect of injection on the turbulent kinetic energy levels for an upstream injection (near-by the nozzle throat) at 60 degrees angle.

OPTIMIZED FLUIDIC CONTROL

Gutmark analyzes aircraft noise suppression techniques

The roar of jet engines is the major source of noise created by commercial and military aircraft, which are bound by numerous stringent noise regulations. A research team led by Ephraim Gutmark, Ph.D., D.Sc., at the University of Cincinnati, is leveraging both experimental and computational tools to optimize existing aircraft noise suppression techniques and to develop new ones.

One method for decreasing noise levels is to enhance the turbulent mixing in the shear layer of the jet just downstream of the nozzle exit. This is accomplished by using fluidic injection ports or flow mixing enhancement devices called chevrons. The positioning, number, geometry of the device, inclination angles and injection-pressure (for fluidics) of the applied system affect the efficiency of noise suppression. Gutmark's team is working to identify the best combination of these parameters to achieve optimal results.

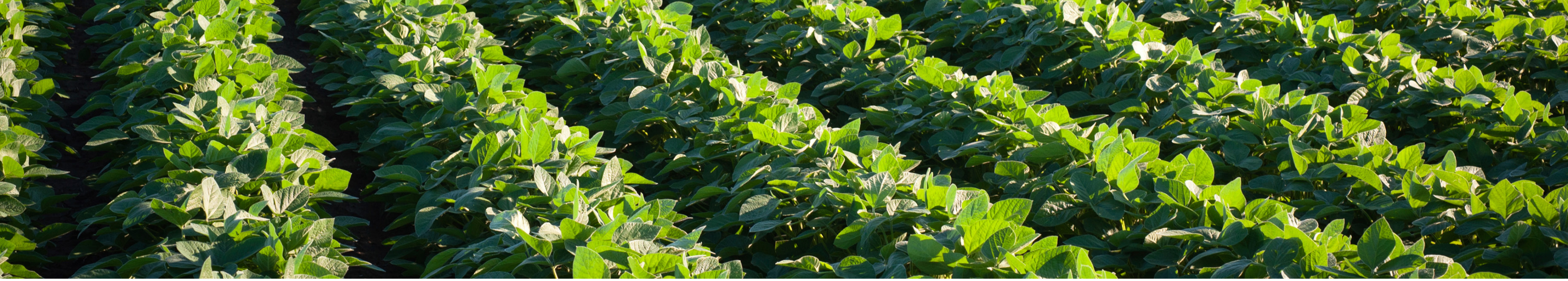
Gutmark has employed detailed flow analyses of factors, such as flow variables gradients, turbulent quantities and stream-wise vorticity, to expose information about the location and strength of the acoustic sources. The analyses also inform Gutmark's team on how the selected noise suppression methodology affects flow behavior. With this data, correlations between flow and acoustic data can be performed.

"Since running physical flow and acoustic experiments for all possible configurations is time consuming and very expensive, we use compressible steady-state Reynolds averaged Navier-Stokes (RANS) models with correspondent turbulence closures as a fast-screening procedure," explained Gutmark, an Ohio Eminent Scholar and professor of aerospace engineering and engineering mechanics at the University of Cincinnati.

"For each configuration, we quantify flow variables, such as turbulent kinetic energy, stream-wise vorticity, pressure and density gradients," he said. "Using computational fluid dynamics software on Ohio Supercomputer Center systems, we obtain 3-D flow data in regions or at locations where experiments cannot be performed (e.g., inside the nozzle) or other parameters that are difficult to measure."

Aware of drawbacks of steady-state RANS models, Gutmark uses them in this parameter study to identify trends in the flow behavior. Identified cases that have shown a potential for reducing the jet noise without significant thrust penalties are considered for transient flow calculations using the more expensive, but more accurate, Large Eddy Simulation (LES) approach. Information about the near-field acoustics is computed directly from the compressible LES solution, while far-field noise predictions are obtained using acoustic analogies.

Project lead: Ephraim Gutmark, University of Cincinnati
Research title: Fluidic control on high velocity jets; optimization by CFD
Funding source: Swedish Defence Materiel Administration
Web site: http://bit.ly/OSC-RR-Gutmark



PARTICULATE DISPERSION

Kumar leads investigations of air pollution problems

For generations, farmers have applied biosolids to their fields to improve soil fertility, leading scientists to examine its effects on human health. A University of Toledo research team led by Ashok Kumar, Ph.D., has leveraged resources at the Ohio Supercomputer Center to study air quality issues such as these in outdoor and indoor environments.

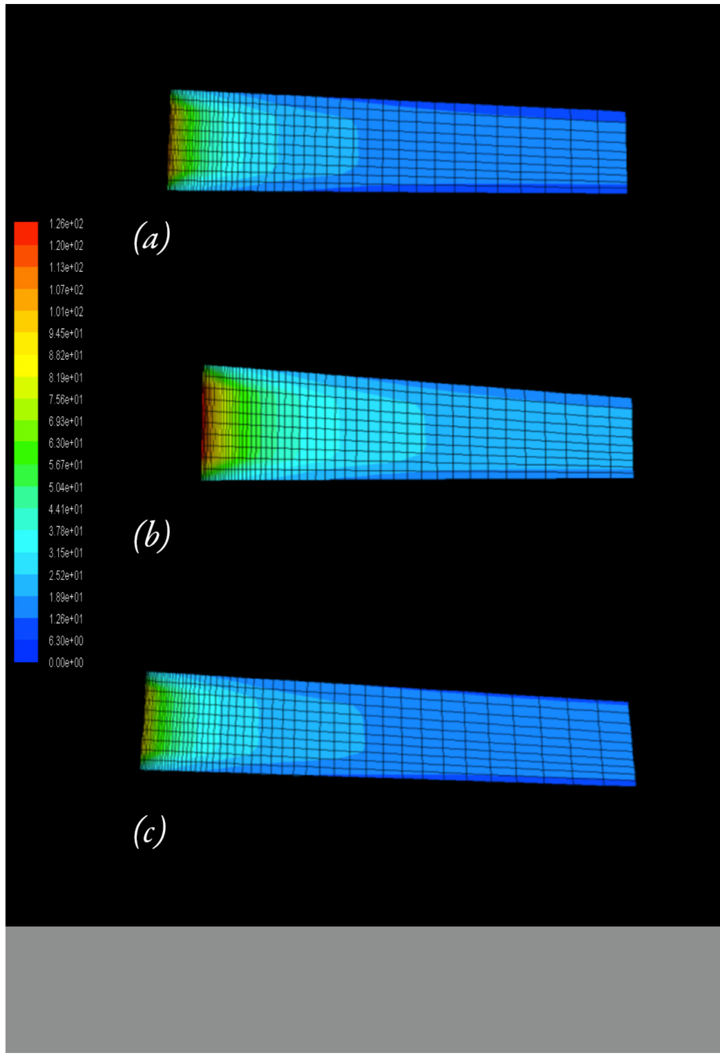
"The use of computational fluid dynamics (CFD) to simulate environmental problems has increased significantly over the last two decades, with more emphasis on solving new and complex air dispersion problems," Kumar explained. "The dispersion of particulate matter and gases emitted from indoor and outdoor sources can be simulated using mathematical models with varying degree of accuracy. The models can predict the contaminant concentrations at different downwind distances from the source under diverse atmospheric conditions."

Graduate student Abhishek Bhat developed a numerical model that simulated particulate dispersion outside the biosolids application field under real-world conditions and validated the model with field data collected earlier using statistical indicators. Meanwhile, graduate student Praneeth Nimmatoori conducted an extension of the work, predicting the ground-level concentrations at various downwind distances of an Ohio agricultural field to which biosolids were injected. The study focused on near-field dispersion problems, which has received little attention in atmospheric dispersion literature.

"Several research studies have developed empirical and analytical models to predict the contaminant concentrations from the application of biosolids," Kumar said. "Empirical methods and analytical modeling have advantages such as simplicity, less time consumed and limited data needs. The disadvantages include oversimplification of physical phenomenon and the need for approximations related to atmospheric turbulence. Moreover, the empirical models are usually site-specific."

Studying the airflow patterns inside a farmhouse, graduate student Srikar Velagapudi is focusing on predicting minute particulates and various gases. Numerical simulations will be used to calculate the velocity, pressure and temperature values for individual indoor spaces, providing a detailed airflow distribution inside the original geometry.

Biodiesel exhaust is the center of graduate student Akhil Kadiyala's studies; he collected indoor air quality data at two points inside a test bus operating on biodiesel. He obtained the ambient concentrations of PM2.5 and gases (inputs) from the Environmental Protection Agency. To model bus geometries, he obtained test bus plans from the Toledo Area Regional Transit Authority and simulated a preliminary 3-D turbulence model to help predict in-vehicle pollutant concentrations.



Predicted concentration of particulates from the edge of a farm field in Ohio during pre-application (a), application (b) and post-application (c) of biosolids.

Project lead: Ashok Kumar, University of Toledo
Research title: CFD modeling of outdoor and indoor air pollution problems
Funding source: Department of Agriculture, Department of Transportation
Web site: http://bit.ly/OSC-RR-Kumar

TRANSPORTATION SYSTEMS

Marano, Wollaeger evaluate PHEV energy management

Intelligent Transportation Systems (ITS) research focuses on new technologies that can improve vehicle systems, such as safety, energy management and traffic management. ITS innovations enable users to be better informed and make safer, 'smarter' use of vehicles and transportation networks.

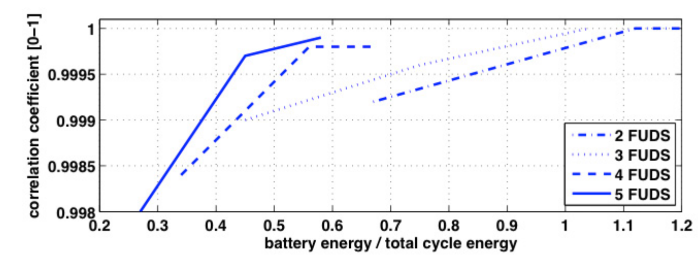
James Wollaeger, a former Ohio State University graduate student in electrical and computer engineering, investigated the use of ITS theories and applications to improve energy management systems of plug-in hybrid electric vehicles (PHEVs). These vehicles are a particular challenge to control engineers, because they operate with two power sources – an internal combustion engine (ICE) and a battery-powered electric motor (EM).

Wollaeger centered his studies on a power-flow based model of Ohio State's Challenge X vehicle and the dynamic equations that form the vehicle model. The vehicle was designed for a 2004 competition, where student teams converted small SUVs into hybrid electric vehicles. The simulator was modified from its original form to reflect a prototypical PHEV.

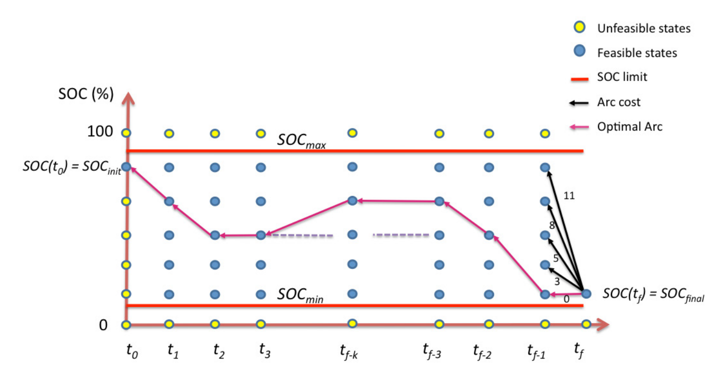
"We set the simulation resolution at 500 watts, which resulted in about 40,000 possible states-of-charge for each time step," explained Vincenzo Marano, Ph.D., a senior research associate at OSU's Center for Automotive research who assisted Wollaeger. "Because of the huge number of possible solutions – which required a large amount of memory and resulted in long runtimes – we leveraged Ohio Supercomputer Center resources to solve this optimization problem."

Wollaeger implemented a control strategy, called the Adaptive Equivalent Consumption Minimization Strategy (A-ECMS), and compared its solution to the global optimal solution. Applying a dynamic programming algorithm to determine the optimal power split between the two power sources established the global optimal solution and produced a state-of-charge profile that would consume the least fuel over the driving cycle. The usable energy in the battery is defined as between 95 percent and 25 percent, because of battery life concerns. Wollaeger's studies yielded the first implementation studies of the Finite Horizon A-ECMS control strategy on a PHEV operating across varying road load conditions.

"We have shown that this control strategy is successful in minimizing the fuel consumption in PHEVs that have no velocity prediction error," Wollaeger said. "In a world where more data is available every day, tomorrow's vehicles should be designed to take advantage of that data to optimize fuel consumption by advanced energy management control systems."



Linear correlation with respect to battery capacity: As the battery size of a PHEV increases, the optimal state-of-charge profile shows a higher correlation coefficient to a linear fit.



Calculation of the optimal state-of-charge profile for a model based upon the Ohio State Challenge X vehicle shown above.

Project lead: Vincenzo Marano, The Ohio State University
Research title: ITS in energy management systems of PHEVs
Funding source: The Ohio State University
Web site: http://bit.ly/OSC-RR-Marano

RESEARCH **LANDSCAPE**

Ohio's strengths in basic and applied research are broad and deep, spanning a multitude of academic, business and industrial interests. The spectrum of clients served by the Ohio Supercomputer Center encompasses many fields of study, from establishing secure, firewall-free network architecture to improving injection molds for manufacturing, as highlighted on the following pages.

PARALLEL COMPARISONS

Bokhari conducts comparisons of system architectures

Surveying the wide range of parallel system architectures offered in the supercomputer market, a former Ohio State University graduate research student sought to establish some side-by-side performance comparisons.

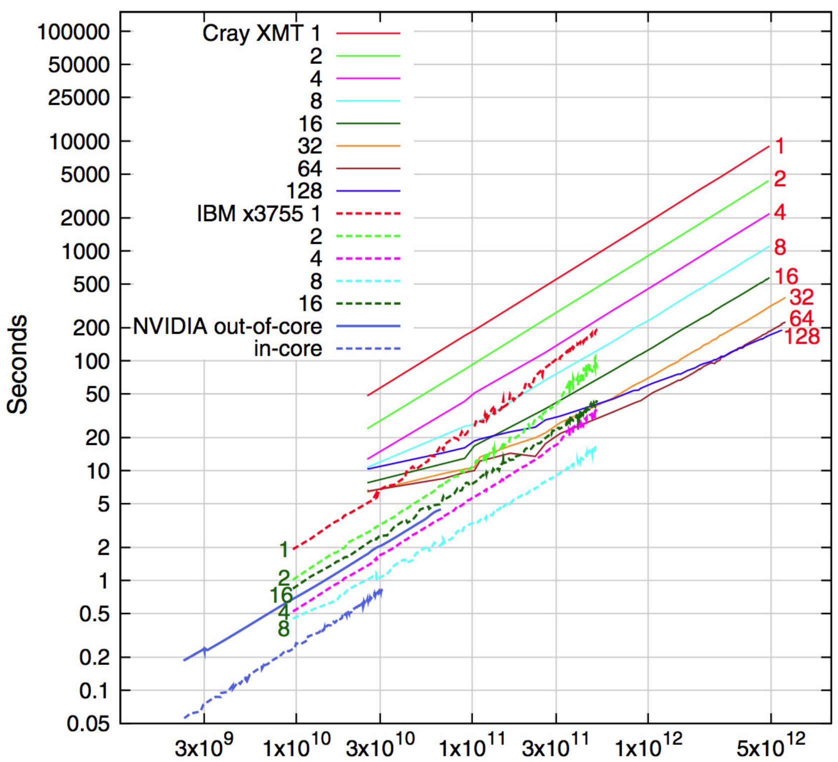
"We explored the parallelization of the subset-sum problem on three contemporary but very different architectures: a 128-processor Cray massively multithreaded machine, a 16-processor IBM shared memory machine and a 240-core NVIDIA graphics processing unit," said former computer science and engineering graduate student Saniyah Bokhari. "These experiments highlighted the strengths and weaknesses of these architectures in the context of a well-defined combinatorial problem."

Bokhari evaluated the conventional central processing unit architecture of the IBM 1350 Glenn Cluster at the Ohio Supercomputer Center and the less-traditional general-purpose graphic processing unit architecture available on the same cluster. She also evaluated the multithreaded architecture of a Cray Extreme Multithreading (XMT) supercomputer at the Pacific Northwest National Laboratory's Center for Adaptive Supercomputing Software.

Each of the architectures Bokhari tested fall in the area of computing where multiple processors are used to tackle pieces of complex problems "in parallel." To solve the subset-sum problem she used an algorithm that takes a period of time that is proportional to the number of objects entered, multiplied by the sum of their sizes. Also, she carefully timed the code runs for solving a comprehensive range of problem sizes.

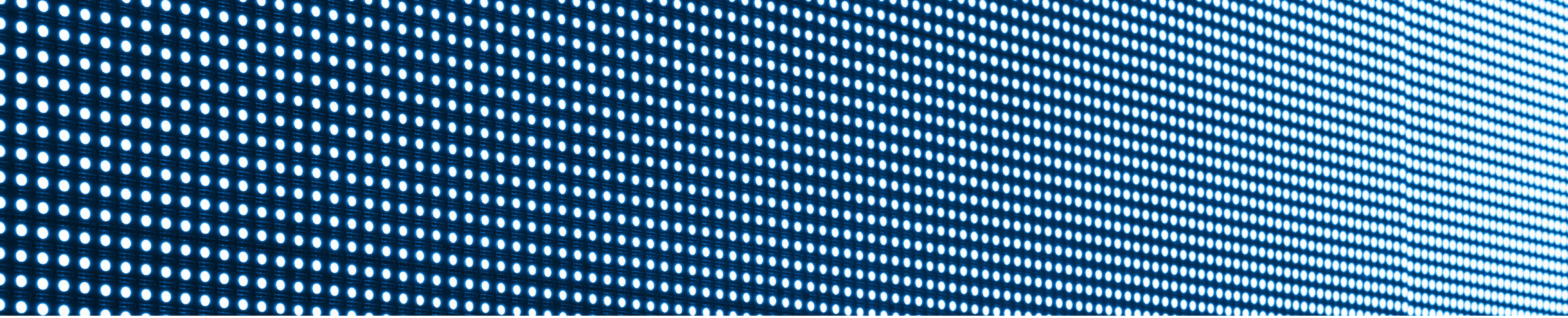
Bokhari's results illustrate that the subset-sum problem can be parallelized well on all three architectures, although for different ranges of problem sizes. Bokhari concluded that the graphical processing unit (GPU) architecture performs well for problems whose tables fit within the limitations of the device memory. Because GPUs typically have memory sizes in the range of 10 gigabytes (GB), such architectures are best for small problems that have table sizes of approximately 30 billion bits.

She found that the IBM x3755 performed very well on medium-sized problems that fit within its 64-GB memory, but had poor scalability as the number of processors increased and was unable to sustain its performance as the problem size increased beyond 300 billion bits. The Cray XMT showed very good scaling for large problems and demonstrated sustained performance as the problem size increased, she said. However, the Cray had poor scaling for small problem sizes, performing best with table sizes of a trillion bits or more.



Comparison of performance measures of parallel supercomputers that employ various architectures: (1) Cray XMT, 128 proc, 500 MHz, 1-TB; (2) IBM x3755, 2.4-GHz Opterons, 16-core, 64-GB; (3) NVIDIA FX 5800 GPU, 1.296 GHz, 240 cores, 4-GB device memory.

Project lead: Saniyah Bokhari, The Ohio State University
Research title: Parallel solution of the subset-sum problem: an empirical study
Funding source: The Ohio State University
Web site: http://bit.ly/OSC-RR-Bokhari

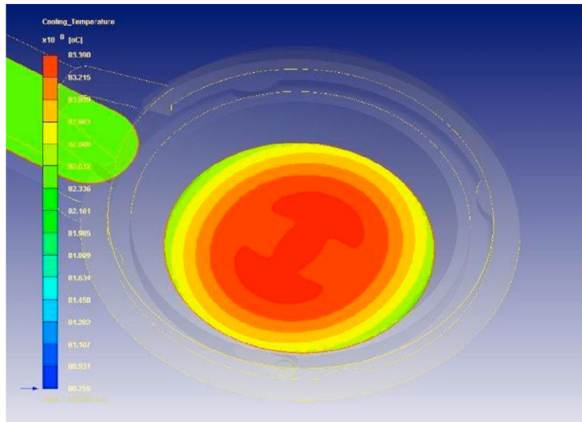


INJECTION-MOLDED LENSES

Greenlight Optics

Greenlight Optics simulation reduces manufacturing time

Optical functions are being incorporated into a rapidly increasing number of applications in a wide range of commercial, research and consumer markets. To enable the exploration and deployment of new applications, Greenlight Optics provides its clients with the design, development, prototyping and manufacturing of integrated optical systems, specializing in LED illumination, projection displays, imaging systems and instrumentation.



Three-dimensional simulation of an injection-molded lens, showing cooling temperature gradients.

Based in Loveland, Ohio, company officials agreed in 2011 to collaborate with the Ohio Supercomputer Center on a demonstration project with the National Digital Engineering and Manufacturing Consortium, or NDEMC, an initiative of the U.S. Economic Development Administration and led by the Council on Competitiveness. OSC provides resources to 13 of the 20 board-approved NDEMC projects.

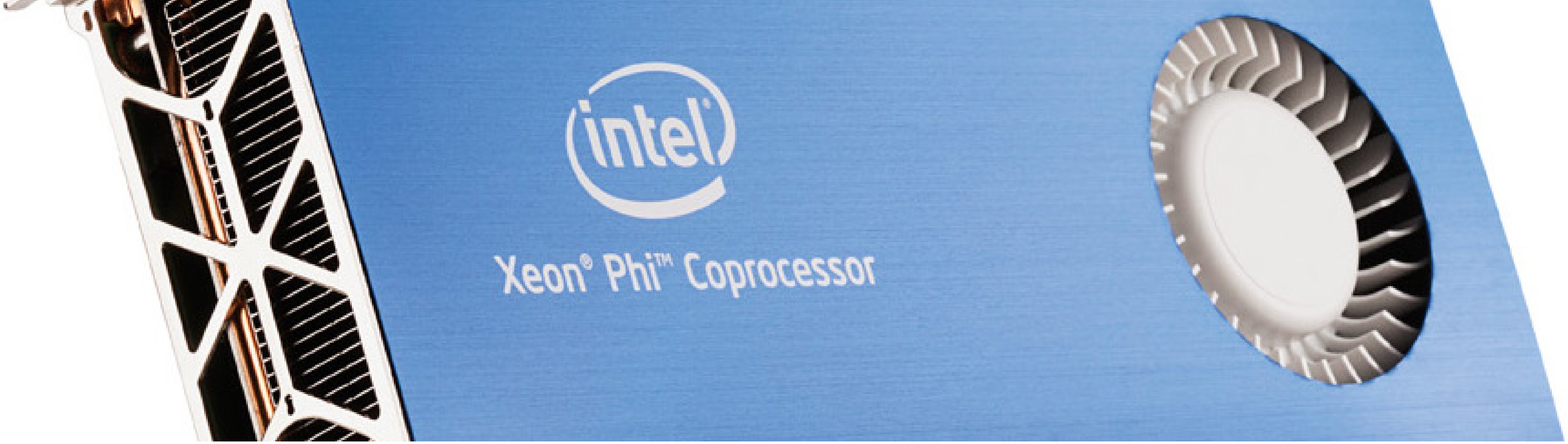
NDEMC's pilot project, The Midwest Project for SME-OEM Use of Modeling and Simulation is the first large-scale public-private partnership of the U.S. government, original equipment manufacturers, state and university computing centers, the State of Ohio, and other non-governmental organizations. The project provides education, training and access to computing resources to small- and medium-size businesses to develop modeling and simulation skills within their manufacturing workforce.

Initially, Greenlight Optics investigated the use of modeling, simulation and analysis to conduct thermal modeling of systems incorporating high-brightness LED light sources. While that particular application didn't result in any production-related achievements, the company's engineers quickly identified an even better candidate.

"Through the Ohio Supercomputer Center, we were able to model thermal properties involved in producing an injection-molded lens used for collimating LED light," said Michael O'Keefe, the managing partner of business for Greenlight Optics. "With the modeling software, we were able to accurately predict a problem with the lens and, subsequently, to reduce the manufacturing cycle time by 64 percent." This type of cycle time reduction while maintaining precision optical quality is a key part of Greenlight's strategy of developing and manufacturing new optical products in Ohio.

For their computational modeling needs, Greenlight Optics accessed Moldex3D software through the Polymer Portal, an online "one-stop resource" developed by PolymerOhio, Inc. and OSC as part of a project funded by the National Institute of Standards and Technology's Hollings Manufacturing Extension Partnership (NIST MEP). The portal bundles access to commercial software modeling and simulation services with training in computation and 3-D modeling.

Project lead: Michael O'Keefe, Greenlight Optics
Research title: NDEMC demonstration project: Thermal modeling software technologies
Funding source: Economic Development Administration
Web site: http://bit.ly/OSC-RR-Greenlight



Intel's Many Integrated Core (MIC) accelerator. Ohio Supercomputer Center engineers began a collaboration with Intel on application development and testing more than a year ago.

APPLICATION DEVELOPMENT

Hudak leads group evaluating new processor technologies

The Xeon Phi co-processor is based upon a new technology developed by Intel Corporation to provide greater compute performance through massive parallelism and designed to fit many high-performance computing applications. The first Xeon Phi-based HPC system, Stampede, will be deployed in early 2013 at the Texas Advanced Computing Center as part of the National Science Foundation's Extreme Science and Engineering Discovery Environment (XSEDE) program.

In conjunction with a larger project, David Hudak, Ph.D., program director for cyberinfrastructure and software development at the Ohio Supercomputer Center (OSC), recently led a research team that examined the performance of different HPC algorithms on pre-release Xeon Phi hardware. The group included OSC staff members John Eisenlohr, Ph.D., a systems developer and engineer, and Karen Tomko, Ph.D., a senior researcher in computer science. Kurt O'Hearn, an undergraduate student at Grand Valley State University, worked with the team as part of an XSEDE student engagement project.

"The unique design of the Xeon Phi architecture required the specification of application parallelism for maximum performance," Hudak explained. "It is important for application developers to experiment and gain experience on the best way to structure applications to exploit the Xeon Phi."

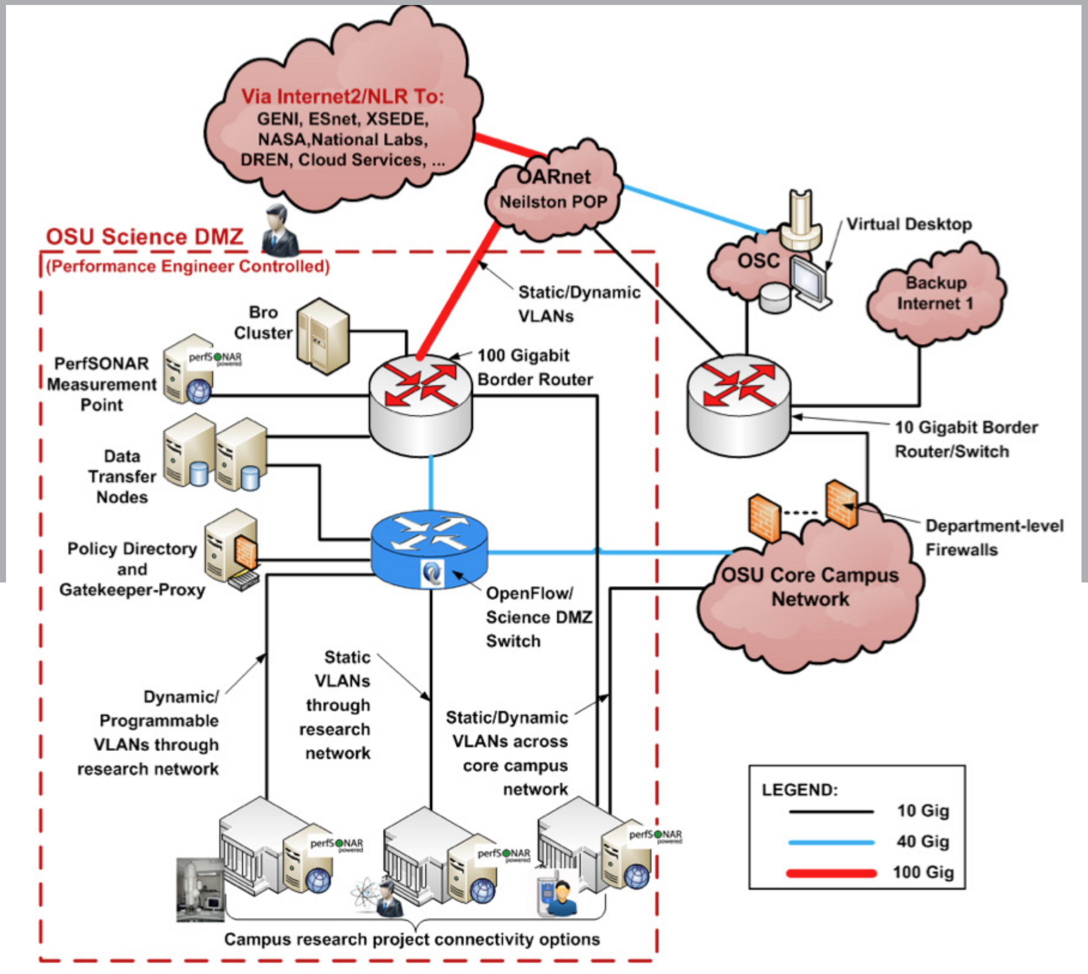
To achieve this end, Hudak's group performed a detailed performance analysis of a well-known communication-avoiding QR factorization algorithm (CAQR), compared CAQR performance between the first- and second-generation Xeon Phi chips and restructured the algorithm for improved performance.

"QR factorization is a linear algebra routine fundamental to solving commonplace problems in the sciences and engineering," said Hudak. "As such, it has been extensively studied on all major HPC architectures: vector, MPP, SMP, cluster, multi-core cluster and GPU cluster."

The parallelization of the CAQR algorithm proved non-trivial due to load imbalance caused by the decreasing amount of matrix to be factored as the algorithm progresses. To better understand the behavior of the algorithm on the Xeon Phi, timing methods were used to measure the total execution time and the four main kernels.

The team concluded that CAQR execution time on the Xeon Phi is sensitive to both matrix shape and tile shape and that the optimal tile shape appears to correlate with cache size (larger tiles perform better with larger caches). They also found that the execution time for two kernels dominates for larger thread counts, indicating a need for improved collective operations.

Project lead: David Hudak, Ohio Supercomputer Center
Research title: Parallel application development for the Intel Xeon Phi platform
Funding source: Intel, Ohio Supercomputer Center
Web site: http://bit.ly/OSC-RR-Hudak



A logical network diagram of the Science DMZ network that will help scientists collaborate over the Internet with minimal interference from security measures.

HIGH-SPEED RESEARCH NETWORK

OSU, Missouri and OH-TECH collaborate to design Science DMZ

Since its inception, the Internet has sped the pace of scientific discovery, but the necessary firewalls that protect institutions from malicious online activity often hinder data sharing among research partners.

To help solve this problem, a research team from The Ohio State University, the University of Missouri and the Ohio Technology Consortium are working to create a safe and resilient network architecture dubbed the "Science DMZ" – a play on the term "demilitarized zone." In this case, instead of being a neutral area between warring nations, the DMZ will be a sub-network on the Internet where institutions normally protected by firewalls will be able to freely and safely share information with each other.

"We, as researchers, need the Internet to effectively collaborate with colleagues around the world, but using it poses a challenge," said Caroline Whitacre, Ph.D., vice president for research at Ohio State and principal investigator of the project. "Researchers haven't been able to widely adopt networking advances, mainly due to limitations in the traditional cyberinfrastructure equipment, policies and engineering practices that are already in place on university campuses for our protection."

For example, the Internet2 consortium provides a high-speed connection between campuses across the country, but it can't quickly pass information through a university's local firewalls. At this point, dataflow slows, and a bottleneck forms.

With a million-dollar federal grant, the researchers will create an experimental research network – a prototype for scientific collaborations around the world to follow. Ultimately, the researchers aim to identify the software, hardware, methods and protocols that will allow scientists to securely move data past local firewalls. The project will provide the flexibility required by researchers, such as HPC users at the Ohio Supercomputer Center, while keeping the infrastructure integrity necessary for the safe, smooth functioning of campus networks.

"The research team also will allow for 100 Gigabit-per-second connectivity into the project, to leverage the soon-to-be-lit 100 Gbps statewide network being deployed by the Ohio Academic Resources Network (OARnet)," said Prasad Calyam, Ph.D., research director for networking and virtualization for OH-TECH's Research and Innovation Center and a co-PI on the project. This is in addition to integrating relevant advanced networking technologies, such as communications protocols, measurement tools and transport services.

"We hope that reducing or removing the bottlenecks will encourage much more research and more collaboration across regional, national and international networks," Whitacre said.

Project lead: Caroline Whitacre, The Ohio State University
Research title: CC-NIE Integration: Innovations to transition a campus core cyberinfrastructure to serve diverse and emerging researcher needs
Funding source: National Science Foundation
Web site: http://bit.ly/OSC-RR-Whitacre

COMPRESSED SENSING

Ziniel exploits structure to improve imaging techniques

Most digital cameras today feature large, multi-megapixel CCD arrays that record incoming light intensity at each pixel location. Typically, as this data is collected, the camera immediately compresses the resultant image into a JPEG file, which reduces time and storage requirements, but in essence "throws away" most of the information that it had collected without a noticeable reduction in quality.

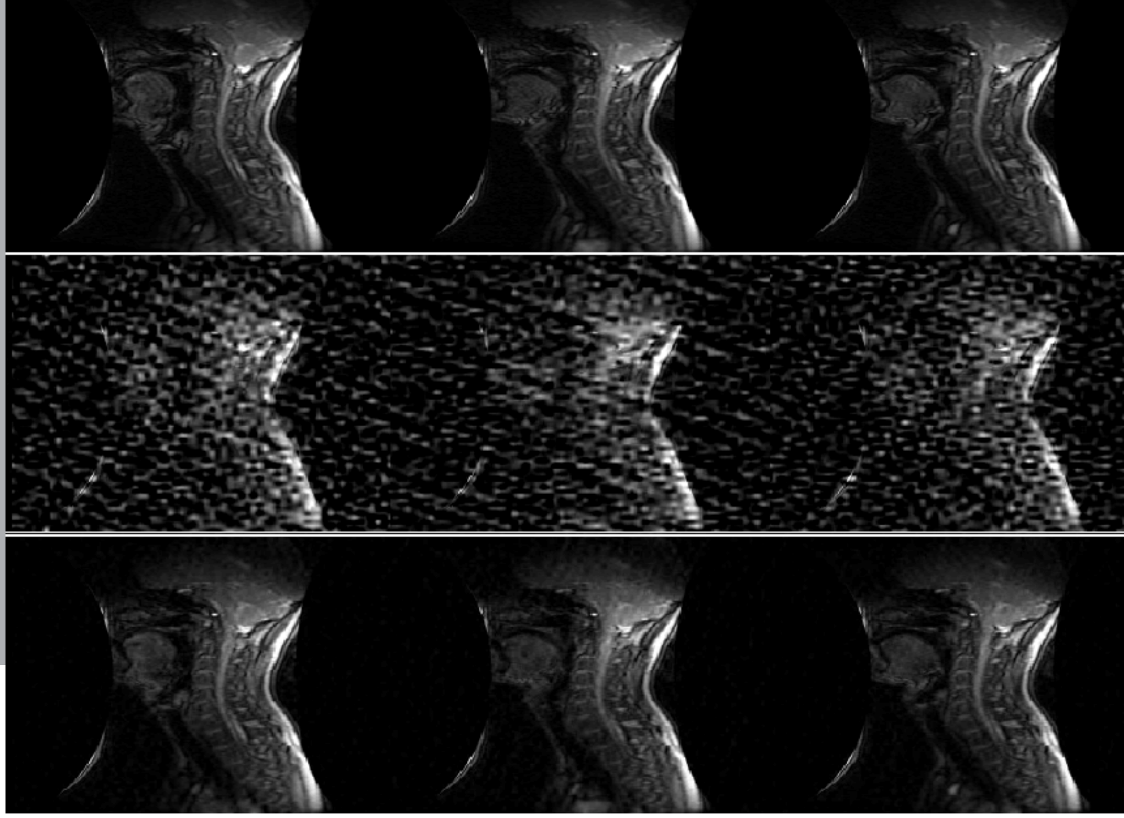
For more than a decade, research on this compressed sensing (CS) has focused on developing more intelligent, more efficient sampling methods. Since compressed sensing does not require hardware with higher and higher sampling rates, the implications are enormous across a wide range of applications, such as radar, medical imaging, remote sensing and hyperspectral imaging.

Justin Ziniel, a doctoral student in electrical and computer engineering (ECE) at The Ohio State University, seeks to extend traditional CS to the scenario in which the underlying signal being recovered has non-trivial structure that can be exploited by observing that, not only does each image have a succinct representation, but each image also is highly similar to its neighbors (in time). Exploiting this structure with compressed sensing allows for more undersampling without a reduction in quality, relative to standard techniques.

"Exploiting structure often comes at the cost of substantially increased computational complexity," explained Ziniel. "We've developed a wide range of message passing algorithms for dramatically speeding up the computation time."

The Ohio Supercomputer Center has been extremely important to Ziniel and his colleagues, Sundeep Rangan, Ph.D., an associate professor of ECE at the Polytechnic Institute of New York, and Philip Schniter, Ph.D., an associate professor of ECE at Ohio State. They must be able to characterize the performance of their algorithms against competing techniques across a wide range of different problems that might be encountered. This typically means averaging the performance on hundreds or thousands of different problems over thousands of realizations.

"This process would take way too long if we had to rely on a single desktop, but by farming out the work to many OSC nodes, we can condense many CPU months' worth of work into just a few hours or days," Ziniel said. "This has allowed us to achieve a much more comprehensive characterization of how our algorithms perform under many different settings than would otherwise be possible."



Three frames of an MRI image sequence of the larynx. The top row consists of fully sampled data that would ordinarily be produced from an MRI machine. The second row is an example of a "traditional" compressed sensing recovery with access to only 16 percent of the complete data. The third row is a recovery on the same 16 percent of data using proposed algorithms that take advantage of the image structure.

Project lead: Justin Ziniel, The Ohio State University
Research title: A general framework for structured sparse signal recovery
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The Ohio Technology Consortium (OH-TECH) functions as an umbrella organization for the Ohio Board of Regents' statewide technology infrastructure, offering innovative technology resources and services for Ohio colleges and universities, health care facilities, K-12 schools and state and local government. The consortium members include the Ohio Supercomputer Center, OARnet, eStudent Services, OhioLINK and the Research and Innovation Center. OH-TECH leverages the strengths of each of these organizations, enabling each to concentrate on its core mission. Ultimately, OH-TECH maximizes efficiencies to benefit Ohio education and research, positively impacting the economic outlook for our state.

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