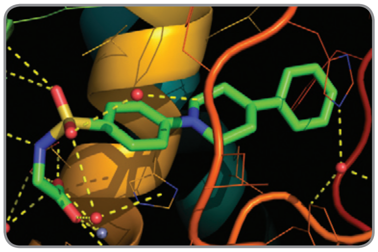
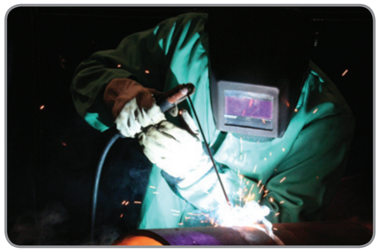
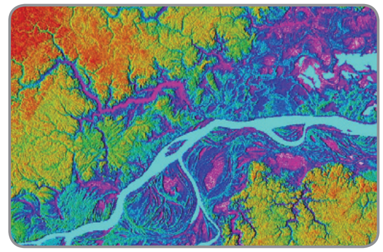
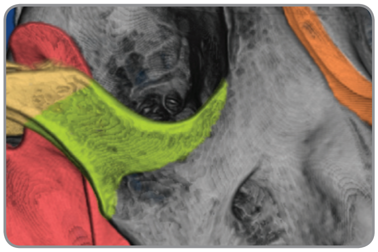
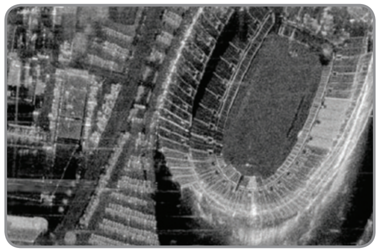
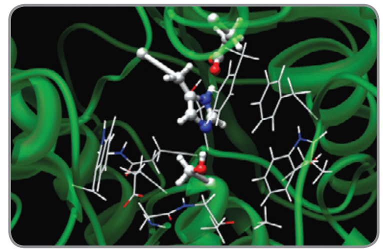
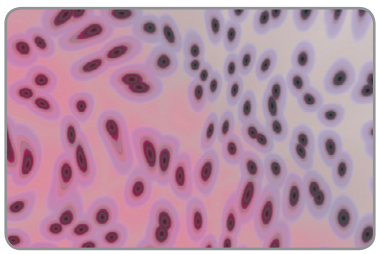







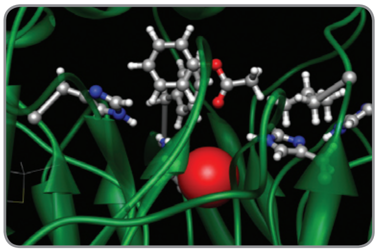



2007 Annual Research Report

Building upon a 20-year legacy of computational innovation and discovery

Empower. Partner. Lead.

Ohio Supercomputer Center



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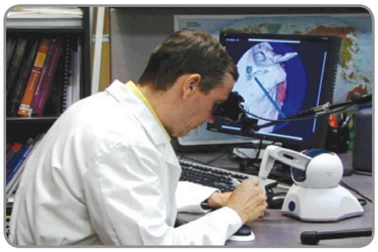
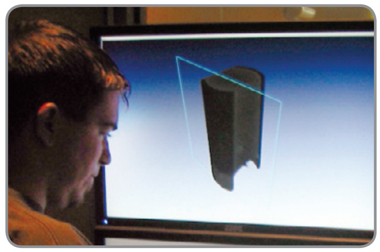
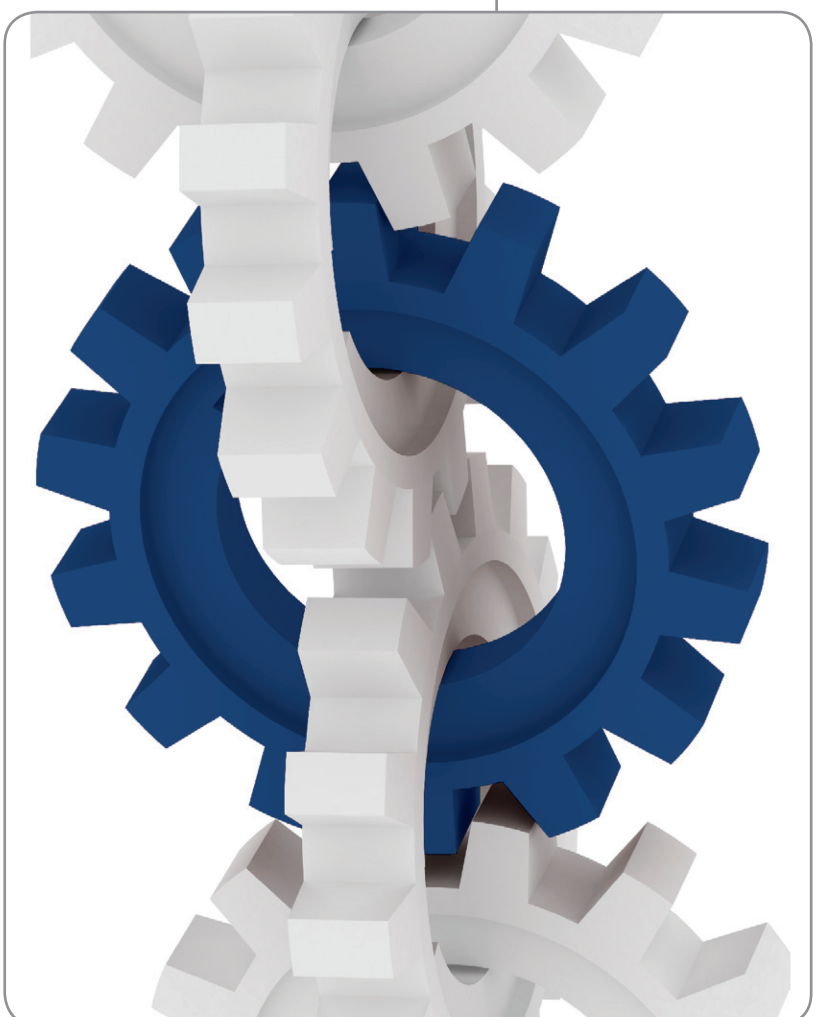




"Clearly, collaboration is

Letter from the Director



key to our success.”

The future competitiveness of organizations, cities, states, and nations in the global marketplace is increasingly reliant on the application of computation to further expand knowledge and increase the speed of communication.

Within this second annual Research Report, you will see how the professional staff of the Ohio Supercomputer Center is responding to this challenge by helping researchers solve complex design, engineering, and scientific challenges. OSC advances these efforts by empowering regional, national, and international clients as they conduct vital research; by strategically partnering with colleagues to develop exciting, new academic, research, and business opportunities; and by demonstrating indispensable leadership in advanced technology and scientific inquiry.

The Center serves a broad spectrum of research clients, offering expertise and specialized support to clients from large, sophisticated computational research programs. At the same time, the staff is developing tools that can meet the needs of a growing number of supercomputer clients - including businesses, students, and faculty - whose primary focus is not computational science. One of our most pioneering projects, Blue Collar Computing™, is high performance computing for small- and mid-sized companies that do not have the time, money, or expertise to invest in supercomputing resources.

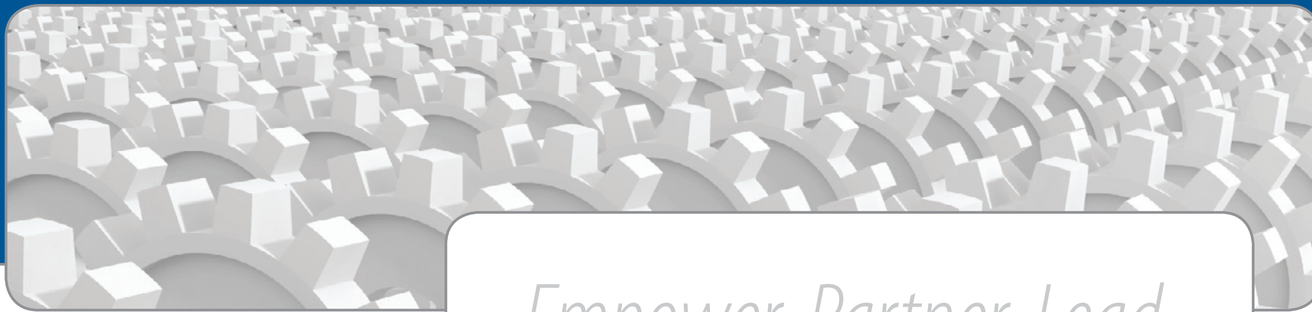
Clearly, collaboration is key to our success. The staff is focused on expanding already strong ties to research centers at all levels of higher education, industry, and state and federal government. As we nurture these relationships, we draw on all of the technical capabilities of our expert staff and a sound infrastructure, including OSCnet - the nation’s leading fiber-optic based statewide network dedicated to research, education, and economic competitiveness.

Also key are effective training and education programs to provide new skills and knowledge for an effective workforce in a new era. The Ohio Supercomputer Center has earned a national reputation for its broad slate of effective educational programs, including those of the recently launched Ralph Regula School of Computational Science. The “virtual” Ralph Regula School coordinates computational science education activities for all levels of learning, from high school students to graduate school students to working adults.

As we mark 20 years of innovation and service at the Ohio Supercomputer Center, we celebrate its creation in 1987 and our many accomplishments. Looking to the future, we clearly see our path - providing essential supercomputing, networking, research, and educational resources to advance innovation and discovery.

Stanley C. Ahalt

Stanley C. Ahalt, Ph.D.
Executive Director
Ohio Supercomputer Center



Empower. Partner. Lead.

Overview

Ohio Supercomputer Center

Within the 2007 Research Report, readers will discover numerous examples that highlight how the Ohio Supercomputer Center *empowers* researchers via high performance computing, advanced networking, and training resources; *partners* with leading scientific investigators in developing joint proposals to regional, national, and international organizations; and *leads* research activities of strategic interest to OSC, the state, and the country.

The Center empowers researchers by assisting them in developing successful proposals, especially following the 2002 establishment of a focused research support program. Based on survey results, Ohio researchers assisted by OSC successfully compete for an estimated $100 million in research funding each year, and for every $1 in research funding OSC receives, our partners throughout Ohio and the United States receive an average of $3.

The Center partners with large numbers of prominent researchers through innovative collaborations. OSC offers these scholars and scientists a wide range of computing resources and has established strong relationships with a variety of state and federal organizations, including the Department of Defense High Performance Computing Modernization Program (DoD-HPCMP), the National Computational Science Alliance (Alliance), the Education, Outreach, and Training - Partnerships for Advanced Computational Infrastructure (EOT-PACI), Sandia National Labs, and Los Alamos National Labs.

More than 30 world-class research staffers lead groundbreaking science and engineering research efforts by leveraging the latest high performance computing and networking solutions. Substantial increases in federal awards to OSC programs during the past few years have pushed annual research program expenditures to more than $5 million for the first time in the group's short history, indicating that OSC's research efforts are translating into continued successes.

A recent report by Battelle Memorial Institute[1] focused on the alignment of Ohio's research and technology portfolios. The report matched core research competencies to technology platforms that could be used to grow the state and regional economies. Similarly, current corporate competencies were matched against industry technology platforms in many of the same fields. Ohio continues to invest new resources towards these areas, and OSC, with several key partners and relationships already in place in these fields, will further focus existing and new resources toward three areas of research:

Biosciences

Using genetic, clinical, imaging, and environmental information to personalize the diagnosis and treatment of patients is profoundly impacting the economics and delivery of medical care. For example, one sector of personalized medicine is molecular-based pharmacogenetic testing that provides right-drug/right-dose information for a specific patient. The development of the relevant approaches, treatments, drugs, and devices requires significant contributions from biological sciences, chemistry, engineering, physics, and medicine.

Advanced Materials

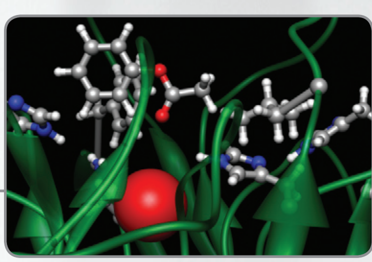
Ohio researchers and scientists are working to advance the field of materials characterization and multi-scale computational modeling and design. A case in point is that in the development of new products and new businesses, a common problem is determining a material that best meets the needs of the product application. The historical process of "build, test, and repeat" is no longer adequate, and the ability to process the materials is almost as important as the materials' performance. Advances in fundamental materials science can be leveraged in several applications, including life prediction and prognosis; corrosion models; energy absorption models; and visualization and virtual prototyping.

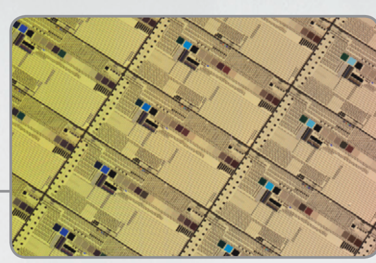
Data Exploitation

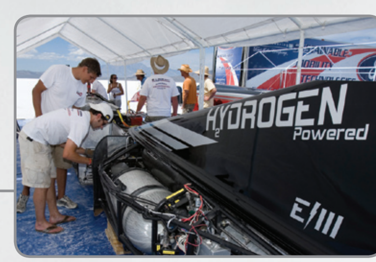
With the increasing ability to measure variables, the amount of data generated as a part of both research and the practice of engineering and medicine has grown astronomically. For example, many new medical devices are designed to pre-screen the data from instruments and discard the majority of it because of the difficulty in handling the data volume – and the volume of the data produced is still overwhelming. Resolving this problem will require a combination of innovative data storage, annotation systems, file systems, advanced I/O, and management systems, as well as analytical software and the computational power to process the data.

The Ohio Supercomputer Center possesses the facilities, personnel, and vision to accelerate the pace of innovation. The burgeoning numbers of researchers accessing OSC computational facilities, collaborating with the Center to advance scientific investigations, and conducting vital scientific studies as members of the OSC research group illustrate how the Ohio Supercomputer Center's philosophy of "Empower. Partner. Lead." is delivering a significant impact felt throughout the state and beyond.

[1] Positioning the State Of Ohio For Economic Growth: Strategically Aligning Ohio's Research and Technology Portfolio, June 2006






HYDROGEN
Powered

The Ohio Supercomputer Center provides a wide array of advanced supercomputing, networking, research, and education resources to empower researchers solving some of the world's most challenging scientific and engineering problems. OSC has garnered an international reputation for supporting top academic and industrial research clients with easy access to dynamic computational power, high-speed networking, and massive data storage. Expert OSC staff support and powerful Web portals accelerate the investigative processes and allow clients to focus more clearly on the science.

Researchers know that OSC will assist researchers in developing successful proposals that will attract funding for innovative scientific, academic, and business endeavors. As a result, Ohio researchers using OSC resources annually receive nearly $100 million in research funding.

OSC serves as a key enabler for the State of Ohio to achieve aspirations in cutting-edge science and engineering, information systems, and advanced industries. From biomedicine and nuclear physics to automotive engineering and computational science, the Ohio Supercomputer Center provides the resources to make evolutionary advances and revolutionary discoveries.

Empower. Partner. Lead.

em·pow·er [em-**pou**-er] verb
(em·pow·ered, em·pow·er·ing, em·pow·ers)
1. To give power, especially legal or official authority.
2. To enable; to equip with an ability.
3. To promote self-actualization.

*The Ohio Supercomputer Center **empowers** research via the use of supercomputing, advanced networking, and training resources.*

This project is one of six interrelated projects to develop antidotes for chemical warfare poisons, funded by the National Institutes of Health-supported program, Countermeasures Against Chemical Threats (CounterACT).

Ultimately, Dr. Hadad's research will provide a computational design of novel enzyme mutants for catalytic destruction of the organophosphinates (OPs), while his colleagues are involved in the experimental verification of the proposed *in silico* mutants. Together, the team will identify competent enzymes able to detoxify lethal nerve gas agents; another project team from Ohio State's plant biology area will produce these bioscavengers in large quantities by combining genes from specific human proteins with genes from algae.

Developing a bioscavenger for chemical nerve agents

Project Lead:
Christopher Hadad, Ph.D.,
The Ohio State University

Research Title:
Mechanistic, Kinetic, Spectroscopic and Computational Evaluations of OP Hydrolysis Activity of Enzymes

Project Team:
- David Lenz, U.S. Army
- Christopher Hadad, Ph.D., The Ohio State University
- Thomas Magliery, Ph.D., The Ohio State University
- Terry Gustafson, Ph.D., The Ohio State University
- Matthew Platz, Ph.D., The Ohio State University

Funding Source:
National Institutes of Health, through the U.S. Army Medical Research Institute of Chemical Defense

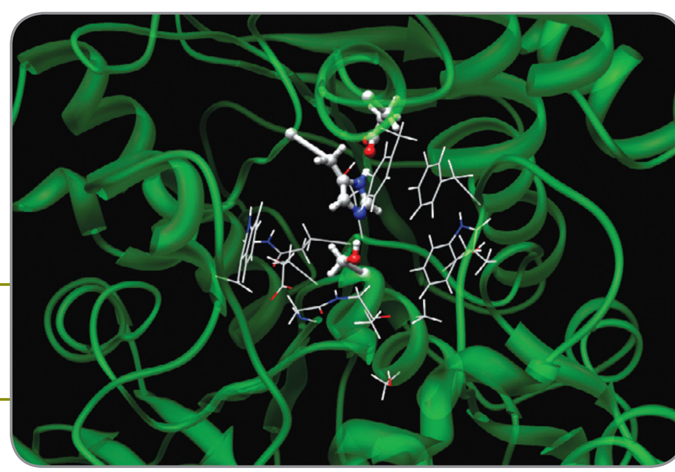
For more information:
www.ninds.nih.gov/funding/research/counterterrorism

Ohio State University chemistry professor Christopher Hadad, Ph.D., is developing measures that will stop, or even prevent, the effects of lethal chemical warfare agents such as the nerve agent sarin. At the center of his research are organophosphinates (OPs), extremely toxic chemicals that attack the central nervous system and can cause deadly convulsions.

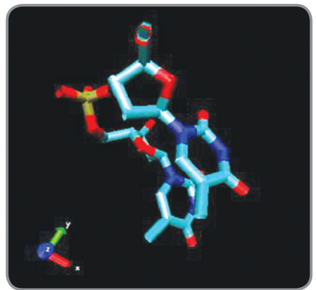
"Because the body continuously processes enzymes, the challenge will be to create a broad spectrum bioscavenger enzyme that is stable in the blood, stays in the body for a period of time, and can process the OPs before they affect a person's nervous system," Dr. Hadad said. "Our goal is to develop one or two biological agents that will improve protection against nerve gas poisoning for soldiers and first responders, and, eventually, serve as a vaccine."

In the first year of this five-year grant, the team extensively turned to the supercomputing resources at the Ohio Supercomputer Center. To illustrate: they used molecular dynamics simulations to study how particular chemicals bind to the catalytic serine, a common amino acid, and Dock 6.0, a program that predicts how OPs bind with the human enzyme paraoxonase.

They've also used Quantum Mechanical/Molecular Mechanical methods to split calculations of the OP reaction process into layers, which greatly improves accuracy. These computationally intensive calculations model the complete reactive system by using an expensive, yet accurate, level of theory for the active site domain of the enzyme, while using a cheaper, and less accurate, molecular mechanics methodology to consider the entire enzyme's structure. The hybrid method provides a study of the complete system without relying on smaller model systems – an aspect especially important for the development of a true bioscavenger.



Sample QM/MM layering of acetylcholinesterase



Demystifying UV light damage

By employing molecular dynamics simulations, an Ohio State University researcher is investigating how DNA is damaged by ultraviolet (UV) light.

The most typical type of damage created by UV light radiation is the cyclobutane pyrimidine dimer (CPD). CPDs interfere with normal cell processing of DNA, which can lead to mutations that cause diseases such as cancer. Recent studies have shown that it takes less than a picosecond, or one-trillionth of a second, for UV light to damage two specific adjacent bases of DNA, thymine-thymine, and create a CPD.

"Because we know the cell's DNA is dynamic, and motions such as helix bending or stacking and unstacking of bases occur relatively slowly, we suspected CPDs form only when the adjacent pyrimidine bases of DNA are favorably aligned for dimerization when excited by photons," said Yu Kay Law, a graduate research associate in biophysics at Ohio State. "Simulating the movements of DNA bases using supercomputers will clarify how CPDs are formed."

Law and his advisor, professor Bern Kohler, Ph.D., verified this hypothesis by using molecular dynamic simulations to model conformational changes of thymidylyl-thymidine in water and with various organic co-solvents, computing at each time step the distance between the two C5=C6 double bonds and their improper torsion angle.

The two parameters were used to find the reactive conformations, which then were used to determine the structure of the dimer precursor. This structure, determined from molecular dynamics simulations, has many similarities with the structure of actual CPDs determined from experiments using nuclear magnetic resonance and X-ray crystallography. The simulations have revealed the motions that make DNA vulnerable to damage, and help to explain why CPDs are formed more readily at certain sequences.

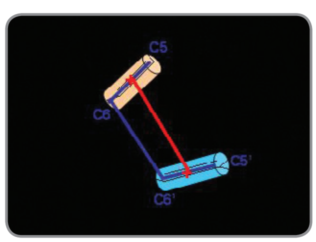
"Conventional experimental means can't be used when investigating a reaction that occurs so quickly," Law said. "With access to OSC's P4 and Itanium clusters, we could simulate these computation-intensive reactions and conduct statistical sampling on a variety of structures."

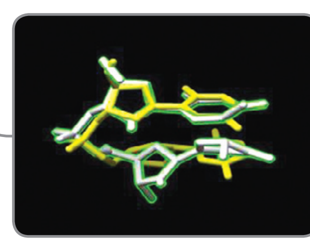
Project Lead:
Yu Kay Law,
The Ohio State University

Research Title:
Ultrafast Photodynamics of Nucleic Acids

Funding Source:
National Institutes of Health, through the National Institute of General Medical Sciences

For more information:
www.chemistry.ohio-state.edu/~kohler/dna.html





Improving semiconductors; Advancing modern electronics

The research of Ohio State University physicist John Wilkins, Ph.D., examines how complex structures form in nature.

His computational research methods range from classical molecular dynamics and more accurate density functional theory descriptions to highly accurate, extremely computationally intensive Quantum Monte Carlo methods. This computational flexibility enables simulations to be performed at the length and time scales required to study different aspects of structural properties and phase transitions.

For example, he and his team are using the resources at the Ohio Supercomputer Center to understand specific types of semiconductor defects at the nanometer level that can influence advances of electronic devices.

"By using our best classical potential for silicon, we're pushing a flexible molecular dynamics simulation to increasingly larger and more realistic semiconductor defect structures, over a broad range of temperatures," Dr. Wilkins said. "The program provides real-time, multi-resolution analysis, combined with still evolving feature detection analysis and visualization software."

The results, Dr. Wilkins hypothesizes, will yield new insights into accurate atomic structures, growth and evolution mechanism, and energetics of atypical semiconductors.

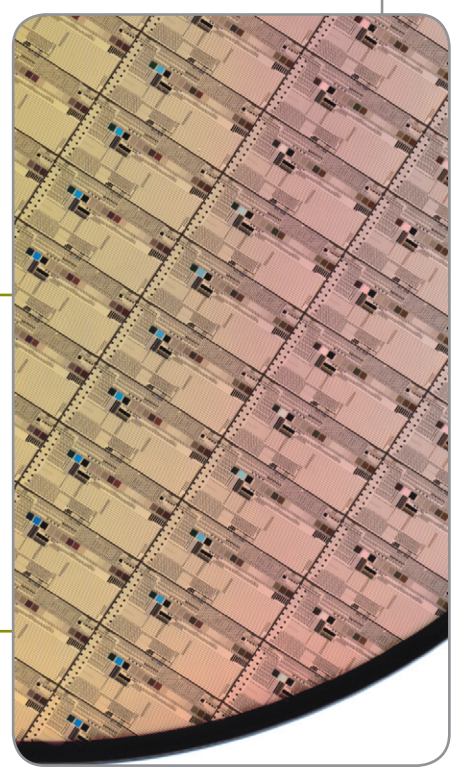
Project Lead:
John Wilkins, Ph.D.,
The Ohio State University

Research Title:
Modeling Dynamically and Spatially Complex Materials

Funding Source:
U.S. Department of Energy

For more information:
www.physics.ohio-state.edu/~wilkins/vita/research/

The Ohio Supercomputer Center is creating a "Center of Excellence" for materials science to support Ohio researchers and scientists, such as Drs. Amar and Wilkins, who are working to advance materials characterization and multi-scale computational modeling and design. Computational materials researchers in Ohio are creating multi-scale models that bridge micro and macro length scales and multiple time scales, and they use Density Functional Theory for molecular level simulation of biological systems coupled with spatial methods typically used for polymers and strongly correlated systems.



Investigating thin-film growth atom by atom

Project Lead:
Jacques Amar, Ph.D.,
University of Toledo

Research Title:
Epitaxial Thin-Film Growth

Funding Source:
National Science Foundation Information Technology Research (ITR) initiative

For more information:
www.physics.utoledo.edu/~jamar

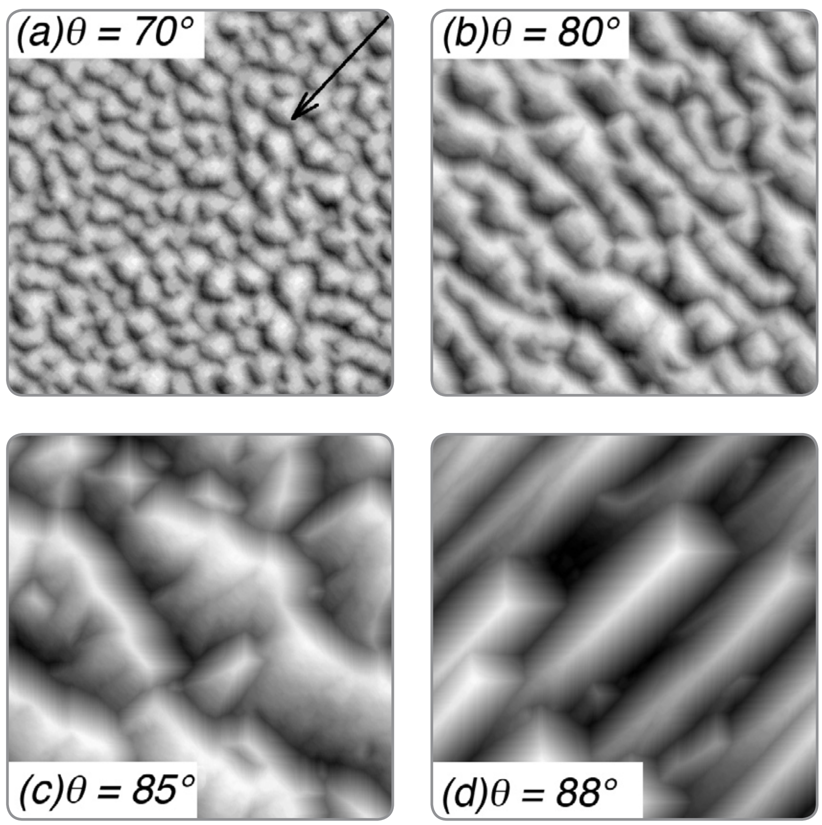
Among several interests studied by University of Toledo physicist Jacques Amar, Ph.D., are the processes behind epitaxial thin-film growth, in which the crystals of the film are aligned with the underlying material.

Thin-film structures can range from fractions of a nanometer to several micrometers in thickness and are used to make semiconductors and solid-state lasers, as well as a variety of other nanostructures such as quantum wells, quantum wires, and quantum dots. These structures are vital in the hybrid microelectronics, microwave, semiconductor, optical, medical, sensor, and related industries.

One of the simplest methods for arranging the atom layers, called Molecular Beam Epitaxy (MBE), enables scientists to create nanostructures by controlling how the thin-films are deposited on a surface. However, neither MBE nor a variety of more complex methods used to grow thin-films is well understood.

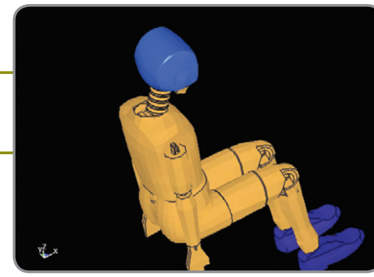
Using supercomputing resources provided by the Ohio Supercomputer Center, Dr. Amar is developing methods to simulate thin-film growth and other non-equilibrium processes over extended time and length scales.

"By carrying out simulations starting from the atomic scale, but ranging up to the micron or sub-micron length-scale, I hope to obtain a fundamental understanding of the key factors and processes which determine thin-film properties," Dr. Amar explained.



Gray-scale pictures of surface morphology obtained from simulations of metal epitaxial growth with different deposition angles θ with respect to the surface normal. The arrow indicates direction of deposition beam. The research was published in *Physical Review Letters*, Volume 98, 2007.

Hybrid III dummy with helmet



Saving soldiers' lives

Some U.S. Army vehicles have various forms of protective seating that absorb some acceleration pulses, or shock waves; this study is part of an effort to update vehicles that do not have such protection, as well as refine those that already do.

Project Lead:
Ala Tabiei, Ph.D.,
University of Cincinnati

Research Title:
Improvised Explosive Devices' Effects on Soldiers in Iraq and Afghanistan

Funding Source:
Army Research Laboratory through the Soldier's Objective Force Electronics Reliability and Survivability Technology Program (SOldier FERST), and directed by the University of Nevada at Las Vegas

For more information:
www.ase.uc.edu/~atabiei

A soldier's ability to survive a mine blast greatly improves if armored vehicles are equipped with energy-absorbing seats, according to recent studies by Ala Tabiei, Ph.D., an aerospace engineer at the University of Cincinnati.

The blast from anti-tank mines or improvised explosive devices, commonly called IEDs, can transfer shock waves from the floor of personnel carriers or other non-tank vehicles to the seats to the occupants, often with such force that it can crush the occupants and severely injure or kill them.

As part of his study, Dr. Tabiei developed and evaluated a new seat design for personnel carriers and other non-tank vehicles that mitigates an explosion's force inside the vehicle. Instead of bolting the seat directly to the floor, he designed a seat attached to steel rails encased in aluminum tubes.

He first created mathematical formulas that represent different aspects of the vehicle. Next, he used special software, LS-DYNA 3D, to create a computer model of the vehicle, including seats, tires and human prototypes, and translate the formulas into a simulation.

By running this data-intensive model more than 500 times on the Ohio Supercomputer Center's Intel Itanium2 computer cluster, Dr. Tabiei was able to perfect the simulation. Once he ensured the model accurately simulated the force and injuries caused by an explosive force, he could reliably test and modify the designs for energy-absorbing seats much faster and with far less expense than conducting full-scale, destructive tests.

Most importantly, computer simulations of the new design showed that the force of a mine blast now moves from the floor to the tubes, crushing them in the process — not the passengers.

"Many fatalities happen because of the acceleration pulses, not because of a direct hit from an exploding device. With an energy absorber between the floor and the seat of the occupant, we can start to mitigate the shock wave," Dr. Tabiei said. "These findings are particularly exciting, because they could contribute to a whole new way of protecting soldiers' lives."

Building fast green cars

Project Advisor:
Giorgio Rizzoni, Ph.D.,
Director, Center for
Automotive Research,
The Ohio State University

Project Title:
Buckeye Bullet 2

Primary Sponsors:
- Ballard Power Systems
- Ford Motor Company
- Rausch

For more information:
www.buckeyebullet.com

Buckeye Bullet 2, the world's first land-speed race research vehicle powered by hydrogen fuel cells, is designed and built by students at The Ohio State University's Center for Automotive Research.

Their goal? To beat the U.S. land speed record for its category set by the first Buckeye Bullet in 2004.

The Bullet 2 team is cautiously optimistic that the streamliner will break that 315 mph record. The long, low, cylindrical racer proved it was well on its way during the 2007 Racing World Finals at the Bonneville Salt Flats in Utah, when it posted a single-run speed of 224 mph — the fastest speed ever recorded for a fuel-cell powered vehicle.

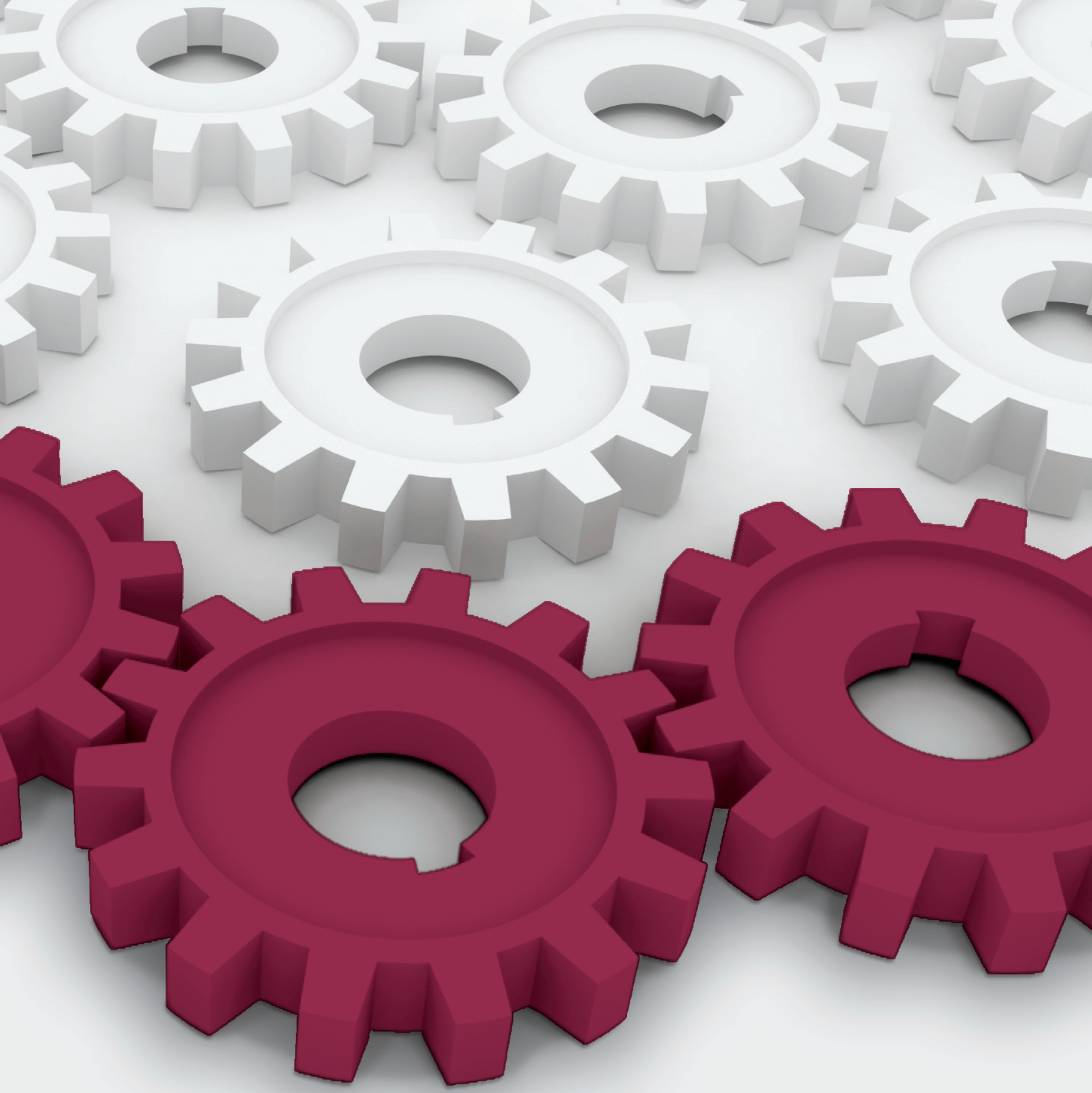
Designers opted to replace the battery concept of the original Bullet with more powerful hydrogen fuel cells last year. However, fuel cells, unlike batteries, don't store energy, and one of the biggest challenges is turbocharging the two 500-pound fuel cells to churn power without overheating.

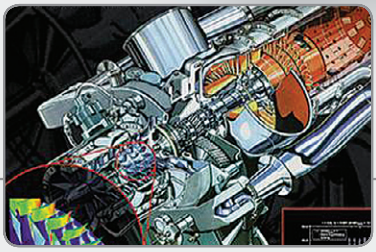
Solving these design challenges is just one way students involved with the Buckeye Bullet project gain hands-on engineering, business, teamwork, and leadership training. Students partner with more than 50 companies from various industries, including the Ohio Supercomputer Center.

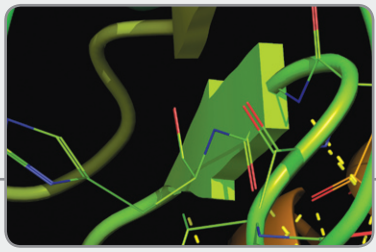
Kimberly Stevens, an OSU senior majoring in aeronautical engineering, tapped the resources at OSC to simulate the shape of the Bullet 2 and, using computational fluid dynamics, model its aerodynamics prior to wind tunnel tests. OSC staff members worked with Stevens to leverage all she could from her programs, especially meshing, batch processing, and fluid-solid modeling.

The entire experience provides team members with a competitive advantage when seeking positions in the global engineering market. Stevens, who plans to begin a master's degree program at Ohio State in 2008, has landed two challenging jobs because of her experience: a co-op position with Honda Research and Development and a research job at Ohio State's Department of Aerospace Engineering.

"Having access to the Ohio Supercomputer Center's resources allows me to apply what I'm learning in class. I have grown to thoroughly enjoy computational fluid dynamics and intend to make a career out of it," Stevens said.







Through strong, catalytic partnerships with Ohio's colleges and universities, businesses, and state and federal labs, the Ohio Supercomputer Center advances leading research throughout the state, the nation, and the world. OSC works alongside researchers, providing superior supercomputing and networking services to energize groundbreaking collaborative activities.

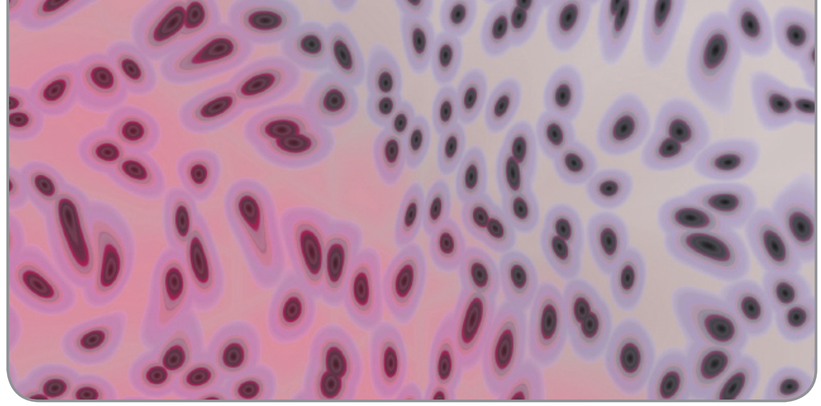
The ability of OSC staff scientists and engineers to create powerful synergies with researchers at other leading organizations places the Center among the national leaders in collaborative technology development and deployment. More specifically, OSC is a partner in many regional and national projects, including those with the Council on Competitiveness, the U.S. Department of Defense, the National Computational Science Alliance, and the U.S. Department of Energy.

The Center will continue to seek out new partnerships and build upon existing collaborations that present unique opportunities for discovery and innovation. OSC scientists, engineers, and other staff experts go far beyond simply supporting research – they are focused on creating deep and specialized partnerships, jointly competing for state, federal, and international funding and developing and executing vigorous research programs.

Empower. Partner. Lead.

part•ner [**pahrt**-ner] verb
(part·nered, part·ner·ing, part·ners)
1. To make a partner of.
2. To join together or associate as partners.
3. To augment with a partner.

*The Ohio Supercomputer Center **partners** strategically with Ohio researchers in developing joint proposals to regional, national, and international organizations.*



VM2M: Improving the fight against cancer

OSC Partners:
- The Research Institute at Nationwide Children's Hospital
- Childrens Hospital Los Angeles
- Children's Oncology Group

Research Title:
Integrated Virtual Microscopy and Molecular Analysis Software for Enhanced Cancer Diagnosis

Funding Source:
U.S. Department of Health and Human Services, through the Ohio Board of Regents

Principal Investigator:
Ashok Krishnamurthy, Ph.D., Ohio Supercomputer Center

Project Team:
- Childrens Hospital Los Angeles: Dennis Mock, Timothy Triche, M.D.
- The Research Institute at Nationwide Children's Hospital: Heather Bao, Tom Barr, William Beyer, Dave Billiter, PMP, Mark Plaskow
- Ohio Supercomputer Center: David Bertram, Jim Gregory, David Hudak, Ph.D., Terry Lewis, Neil Ludban, Siddharth Samsi, Kevin Wohlever

For more information email:
vm2m@osc.edu

The acronym VM2M might stand for Virtual Microscopy to Microarray, but for cancer researchers it means revolutionizing a part of the investigative process.

Expert pathologists depend on microscopy, or the latest use of microscopes, to examine and review diseased tissue. Their conclusions help oncologists form the foundation for treatments.

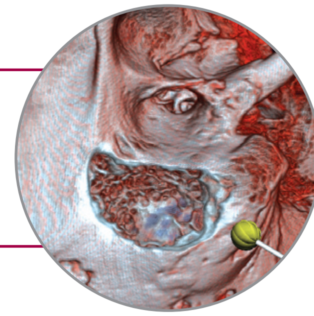
"The different research teams involved are working to create a tool that provides multi-modal views of cancer biopsies that show pathologies of cancerous cells alongside their genetic information," said Dave Billiter, PMP, The Research Institute at Nationwide Children's Hospital. "Our portion involves taking microscopy data virtual, by digitizing the slides of the cancerous biopsies and providing a tool to view them via the Web."

After The Research Institute at Nationwide Children's Hospital creates the microscopy image from the specimen, the tissue sample is sent to the Childrens Hospital Los Angeles, where that research team creates the microarray portion of the project by identifying the genetic information for each tumor.

The Ohio Supercomputer Center researchers, meanwhile, are expanding the capabilities of VIPER (Virtual microscopy Image Pilot EndeavoR), which is the pathology review component of VM2M. The Web-based portal they created enables pathologists to review, annotate, and share tissue specimen images.

Ultimately, VIPER and VM2M will provide cancer researchers with searchable, clinical-genomics software and data-acquisition tools. Multi-modal views of cancer biopsies will show pathologies of cancerous cells alongside their genetic information, an unparalleled - and currently unavailable - resource. Once FDA approval is obtained, the project's collaborators fully expect physicians to use the genetic information available through VM2M to create custom treatments for each person, based on his or her unique situation.

This innovative virtual simulation tool offers a safer, more cost-effective way to teach surgery skills for treating hearing loss, vertigo, infection, or tumors.



Simulator helps train future surgeons

Gregory J. Wiet, M.D., a pediatric otolaryngologist, head and neck surgeon at Columbus Children's Hospital, and experts at the Ohio Supercomputer Center developed a virtual simulation tool that teaches medical residents temporal bone surgery.

Located in the lower part of the skull, the temporal bone encompasses the bones and structures of the ear. Doctors might perform surgery here to implant cochlear implants or hearing aids, treat chronic ear infections, or conduct exploratory surgery.

OSC programmers created an interface system that emulates the multi-sensory environment of the dissection lab. A binocular viewer replicates the view a surgeon would see through a microscope during surgery, and a drill-shaped device creates the pressure and resistance a doctor feels during the surgery. The program generates the sounds of a temporal bone drill.

The system can provide an open-ended dissection of the virtual temporal bone, assist with identifying critical structures through an intelligent tutor, and capture the resident's performance.

"Without a virtual simulation environment, medical residents would learn this surgery by working on cadaveric specimens and training, apprentice-like, in an operating room," said Wiet, who also serves as associate professor of otolaryngology at The Ohio State University College of Medicine. "We've created a safer, cost-effective way to learn fundamental techniques that could not only obviate the initial need for physical bone, but present a greater diversity of bone specimens to enhance training."

The multi-institutional validation study involves more than 30 national and six international otolaryngology programs; this is the fourth year of a five-year study funded by the National Institutes of Health.

OSC Partners:
- Nationwide Children's Hospital
- The Ohio State University College of Medicine

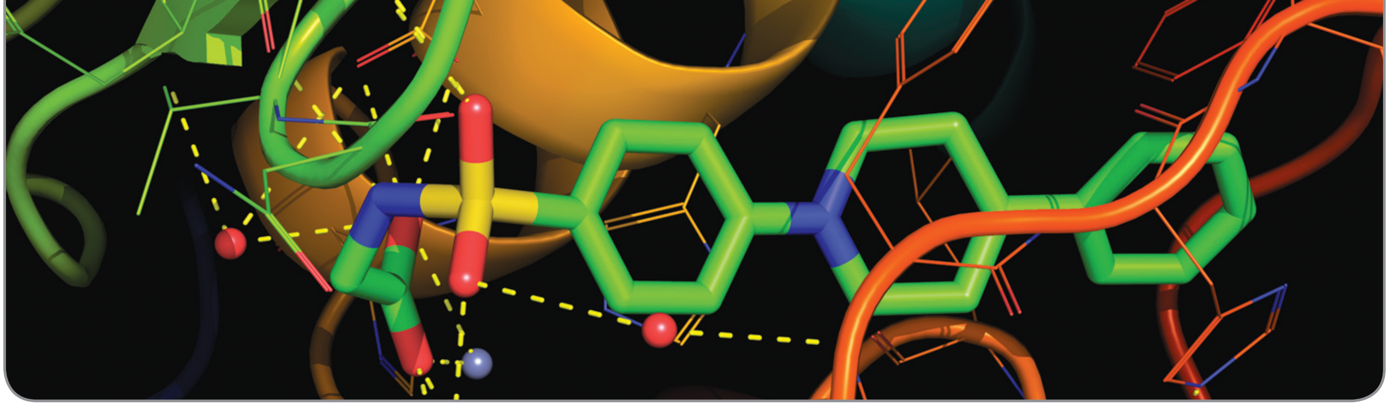
Research Title:
Validation/Dissemination of Virtual Temporal Bone Dissection

Funding Source:
National Institute on Deafness and Other Communication Disorders, through the National Institutes of Health

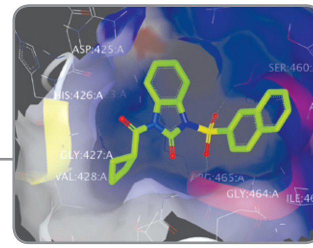
Principal Investigator:
Gregory Wiet, M.D., Nationwide Children's Hospital and Division of Pediatric Otolaryngology, The Ohio State University

Co-Principal Investigator:
Don Stredney, Ohio Supercomputer Center

For more information:
www.osc.edu/research/Biomed/projects/vtbone



Improving drug discovery processes



The Genome Research Institute Discovery Platform, or GRIDP, provides Ohio academic researchers and educators with a user-friendly way to tap into the emerging field of computational drug discovery, encompassing bioinformatics, computational biology, and computational chemistry.

GRIDP gathers currently available computational biology and drug discovery software as well as other computational resources into one intuitive, Web-based interface. While pharmaceutical companies use similar tools that cost hundreds of thousands of dollars, this platform is the first of its kind for academia and harnesses the computational horsepower of the Ohio Supercomputer Center and expertise of the University of Cincinnati Genome Research Institute.

Effectively accessing and using the wealth of structural and chemical data currently available requires significant computing resources, talented programmers, and experienced high performance computing users familiar with the command line environment. GRIDP removes these technical hurdles by providing an intuitive graphical environment that delivers powerful resources, including software through the web. Students can focus on learning and researchers on discovery without being bogged down with technical details.

GRIDP, which was jointly developed by OSC and GRI scientists and programming experts, mirrors the discovery workflow and leads users through tasks such as protein model preparation and evaluation, binding site prediction, ligand preparation and docking/scoring, protein:ligand energy calculations, and chemical property analysis such as Lipinski's rules and distribution/absorption.

By modeling the interaction between target proteins and putative drug candidates, researchers can dramatically focus the set of compounds that need to be tested to a number that becomes reasonable — hundreds rather than tens of thousands. This allows academic researchers to play in an arena formerly reserved for big pharma.

"The most striking comment from biologists since we've launched GRIDP this summer is, 'I didn't know this was possible.' GRIDP opens a new realm of possibility, especially in drug discovery," said Matt Wortman, Ph.D., a researcher at the University of Cincinnati's Genome Research Institute and one of the lead investigators in GRIDP's development. "It gives researchers an entirely new research tool for discovering novel, biologically active chemicals."

OSC & UC PRESENT GRIDP OHIO'S DISCOVERY PLATFORM

OSC Partner:
University of Cincinnati's
Genome Research Institute

Research Title:
Genome Research Institute
Discovery Platform

Funding Source:
U.S. Department of Health
and Human Services' Health
Resources and Services
Administration, through
the Ohio Board of Regents

Principal Investigators:
Matthew D. Wortman, Ph.D.,
University of Cincinnati's
Genome Research Institute

Co-Principal Investigators:
Steven Gordon, Ph.D.,
Ohio Supercomputer Center

For more information:
www.gridp.org

Streamlining chemistry with cyberinfrastructure

With the Computational Chemistry Grid, chemists can focus on their science, not the nuts and bolts of their computing.

Led by the University of Kentucky's Center for Computational Sciences in partnership with four supercomputing sites around the nation, the Computational Chemistry Grid is a virtual organization that provides access to high performance computing resources via a Web services production infrastructure that includes an intuitive desktop client, user support, and associated services.

"Prior to this, if chemists needed to access the computational chemistry software applications on our systems, they needed to learn how to use UNIX, move input files from their hard drives to our servers, and understand how to run the applications on our high performance computing systems," said Jim Giuliani, Science and Technology Support Group lead, Ohio Supercomputer Center. "But, GridChem, with its desktop client, automates these steps and reduces the effort needed to leverage our resources."

GridChem, a Java-based interface, seamlessly incorporates the hardware, software, and middleware resources computational chemists need to conduct their work, all through a secure Internet portal.

For example, once the scientists click "Run" on the portal interface, GridChem packages up their data, ships it to the target system, configures the job based on established scheduling policies at the remote site and submits the job for execution. The clients have several point-and-click utilities that allow them to monitor the status of their jobs and view a history of all jobs submitted, without having to log into each system. And, once a job has completed, they can browse the remote storage and download results to their desktop.

Giuliani and his colleagues at the Ohio Supercomputer Center lead the education, outreach, and training effort, ensuring that computational chemists have all the tools and training they need to easily submit, monitor, and manage their jobs on supercomputing systems and software around the country – from the convenience of their own computer.

Cyberinfrastructure refers to software that enables scientists to exploit cutting edge technology resources, including computer and data servers, visualization devices, instruments and networks, for advancing research in science and engineering.

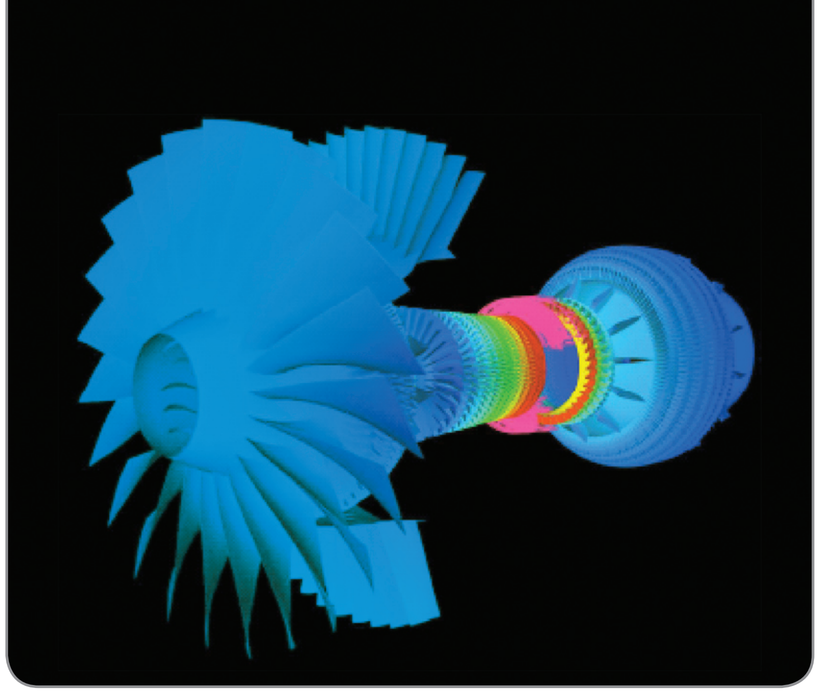
OSC Partners:
- University of Kentucky, Center for Computational Sciences
- Louisiana State University, Center for Computation and Technology
- National Center for Supercomputing Applications
- Texas Advanced Computing Center

Research Title:
Computational Chemistry Grid (CCG): Production Cyberinfrastructure for Computational Chemistry

Funding Source:
National Science Foundation, National Middleware Initiative

Principal Investigator:
John Connolly, Ph.D., Center for Computational Sciences, University of Kentucky

For more information:
www.gridchem.org



Building better, faster jet engines

OSC Partner:
The Ohio State University

Research Title:
Turbomachinery Modeling and Simulation

Funding Source:
Advanced Virtual Engine Test Cell, Inc.

Principal Investigator:
Jen-Ping Chen, Ph.D.,
The Ohio State University

For more information:
aerospace.eng.ohio-state.edu/people/faculty/chen/Dr.Chen.html

Aerospace engineers such as Ohio State University professor Jen-Ping Chen, Ph.D., depend on modeling and simulations of turbomachinery, the alternating sections of spinning and fixed blades in a jet engine's compressor and turbine, because the multiple stages and extreme temperatures make it difficult to conduct experimental measurements.

Inside a jet engine, a series of spinning and fixed blade rows called a compressor compress the air, which then moves into the combustor. The air then mixes with the fuel and is ignited, pushing hot gas out the back of the engine. A second series of spinning and fixed blade rows called a turbine extracts energy from hot gas as it flows past to keep the compressor turning and gives the airplane power. By increasing the loading, or compressing more air and pushing it through the engine, engineers get more thrust with a smaller physical size - which improves the efficiency and cost of jet engines.

Using TURBO, a computational fluid dynamics application for multistage turbomachinery, Dr. Chen simulates the airflow through multiple compressor and turbine stages. By also modeling the movement of the blade rows relative to each other, this code is capable of accurately computing the unsteady interactions between blade rows.

The Ohio Supercomputer Center is working with Dr. Chen and his research team to provide access to high performance computing resources and consulting assistance for these data-intensive simulations. He recently ran several 584-processor TURBO jobs on OSC's IBM e1350 system during the installation testing of the new system; this gave his team unfettered access to the system for nearly two weeks.

"These multiple-blade-row simulations can be useful in investigating problems of stage matching, or aligning the air movement between the spinning and fixed blades," said Dr. Chen. "Constraints on the flow field in a multistage machine are quite different from those in an isolated rotor. Although the flow in a single stage shows similarities with that in a multistage configuration, the finer details of airflow are sufficiently different to prevent extrapolating single-stage data to multi-stage configurations."

The Amazon River, the second longest river in the world, measures 4,000 miles from its source to its mouth, drains a territory of more than 2.5 million square miles, is fed by more than 100 tributaries, discharges between 30 million and 70 million gallons of water a second, and deposits a daily average of 3 million tons of sediment near its mouth.

Tracking Amazon flood patterns

Using the high performance computing and support resources of the Ohio Supercomputer Center, Ohio State University Earth scientist Doug Alsdorf, Ph.D., and his colleagues successfully predicted flooding patterns for 5,000 square miles of the central Amazon floodplain.

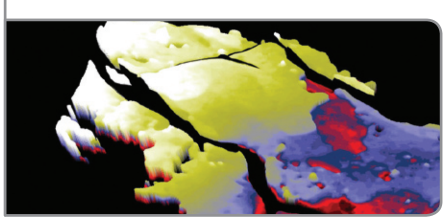
This was the first time a hydrodynamic model of this scale was successfully used to resolve complex floodplain flow patterns. Until this work, hydrologists didn't know much about the Amazon's seasonal floods.

"Almost no data existed on the Amazon's flooding behavior over large areas, such as where the waters rise first, the elevations, or how fast the waters ebb," Dr. Alsdorf said. "To understand the hydrological and biogeochemical processes in the ecosystem, it was critical to find a way to understand the flood patterns."

Water level gauges typically register a change in water elevation over time. However, these are sparsely placed on the Amazon and only in the main channels. So the researchers turned to the Shuttle Radar Topography Mission and other satellites for records of floodplain topography, water levels, and highly accurate water level fluctuations.

The researchers took the enormous amount of satellite data and simulated water movement through the Amazon floodplains, using the computer program LISFLOOD-FP. At Dr. Alsdorf's request, OSC researcher Judy Gardiner, Ph.D., adapted the program to run quickly and efficiently on multiple processors of the Center's Cray supercomputer.

"With Judy's help, we went from four weeks of compute time on a desktop to less than four days," Dr. Alsdorf said. "Because of this, we were able to tweak the formulas and do multiple runs, ultimately resulting in a much better simulation." The results suggest that water flows through the floodplain in a much more complex way than previously thought. The flood levels also do not always correlate directly to the main channel levels, but were influenced by topography as well as local and far-reaching hydraulic factors created by the flood itself.



OSC Partner:
The Ohio State University

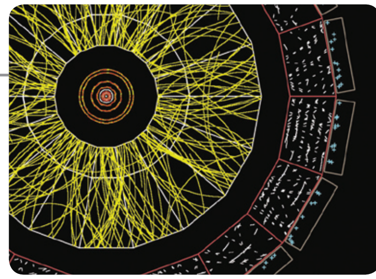
Research Title:
Modeling Large-Scale Inundation of Amazonian Seasonally Flooded Wetlands

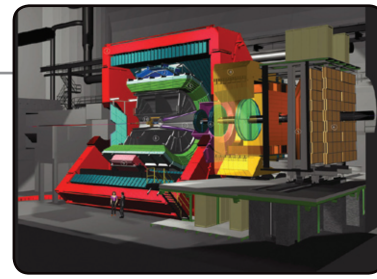
Funding Sources:
- Petrobras S.A.
- Piatam Project
- NASA
- UK Royal Society

Principal Investigator:
Doug Alsdorf, Ph.D.,
The Ohio State University

Co-Principal Investigators:
- Matthew Wilson, Ph.D., University of Exeter, Cornwall, UK
- Paul Bates, Ph.D., University of Bristol, Bristol, UK
- Bruce Forsberg, Ph.D., Instituto Nacional de Pesquisas de Amazonas, Manaus, Brazil
- Matthew Horrit, Ph.D., Halcrow Group, Ltd., Wiltshire, UK
- John Melack, Ph.D., University of California, Santa Barbara
- Frédéric Frappet, Ph.D., University of California, Irvine
- James Famiglietti, Ph.D., University of California, Irvine

For more information:
earthsciences.osu.edu/water





Understanding the 'big bang' in a billionth of a trillionth of a second

OSC Partners:
- The Ohio State University
- University of Houston
- Lawrence Berkeley National Laboratory
- Lawrence Livermore National Laboratory

Research Title:
Developing Extensions to Grid Computing for ALICE at the LHC

Funding Source:
National Science Foundation

Principal Investigator:
Thomas J. Humanic, Ph.D., The Ohio State University

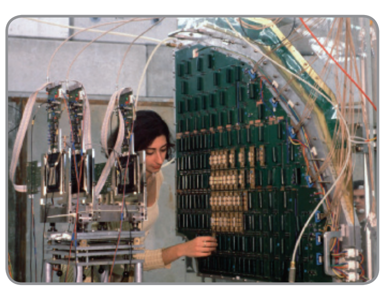
For more information:
www.physics.ohio-state.edu/HIRG/experiments.html

The ALICE experiment, short for A Large Ion Collider Experiment, is a massive effort to study the birth of matter involving a collaboration of more than 1,000 physicists, engineers, and technicians from 30 countries. The Ohio Supercomputer Center serves as a key resource for hosting data and analysis codes in North America.

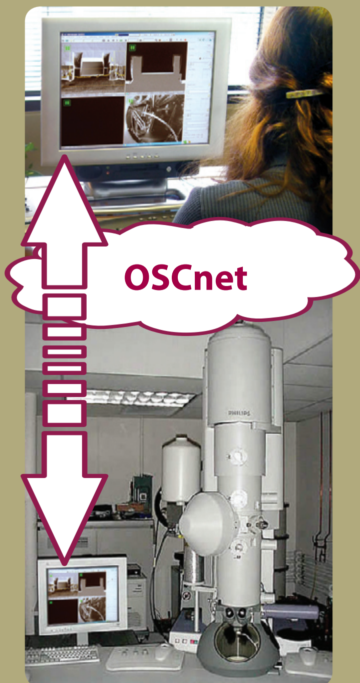
ALICE researchers are working to recreate the "Big Bang" on a small scale by generating heavy ion collisions within the Large Hadron Collider at CERN, the European Laboratory for Nuclear Research in Switzerland. They will examine a rare matter called quark-gluon plasma (QGP), which hasn't existed in nature since 20 - 30 microseconds after the universe formed. Because QGP exists for only about one billionth of a trillionth of a second, it cannot be studied directly.

ALICE physicists will accelerate two lead nuclei to nearly the speed of light and collide them at unprecedented temperatures and densities. The collaboration's challenge is to visualize particles expelled from the collisions, distinguishing the formation of QGP from the other more common phenomena. Intricate detection instruments will measure the position of a particle to a fraction of a millimeter, plot its path among millions of other particles, and record approximately 1.25 gigabytes of data per second - or as much as three DVDs per minute - on the momentum, charge, and velocity of particles.

This data will be distributed through high-speed connections for processing by the "Grid," a global network of computer clusters at scientific institutions. OSC will provide 300,000 CPU hours through the end of 2007 and one million hours in 2008. Researchers currently are responding to final data challenges prior to the first experiments, expected in mid-2008. ALICE already has yielded many valuable second-order benefits in areas such as distributed computing, mass data storage and access, software development, and instrument design.



Remote Site
Client using RICE software to access the electron microscope.



OSU CAMM
Electron microscope

OSC Partners:
- The Ohio State University
- Miami University
- Ohio University

Research Title:
Visualization, Imaging, and Modeling: Shared Instrumentation in Materials Research and Education

Funding Source:
Ohio Board of Regents

Principal Investigator:
Hamish Fraser, Ph.D.,
Center for the Accelerated Maturation of Materials,
The Ohio State University

Co-Principal Investigator:
Ashok Krishnamurthy, Ph.D.,
Ohio Supercomputer Center

For more information:
www.osc.edu/research/networking/projects/telemicroscopy

RICE: Removing roadblocks to sharing scientific instruments

The Ohio Supercomputer Center and its partners are enabling researchers around the state and beyond to remotely access some of Ohio's most valuable and expensive scientific instruments over the Internet.

Remote access to instrumentation such as electron microscopes, NMRs, Raman spectrometers, and ion accelerators demands high-resolution video image transfers with simultaneous, real-time mouse and keyboard controls.

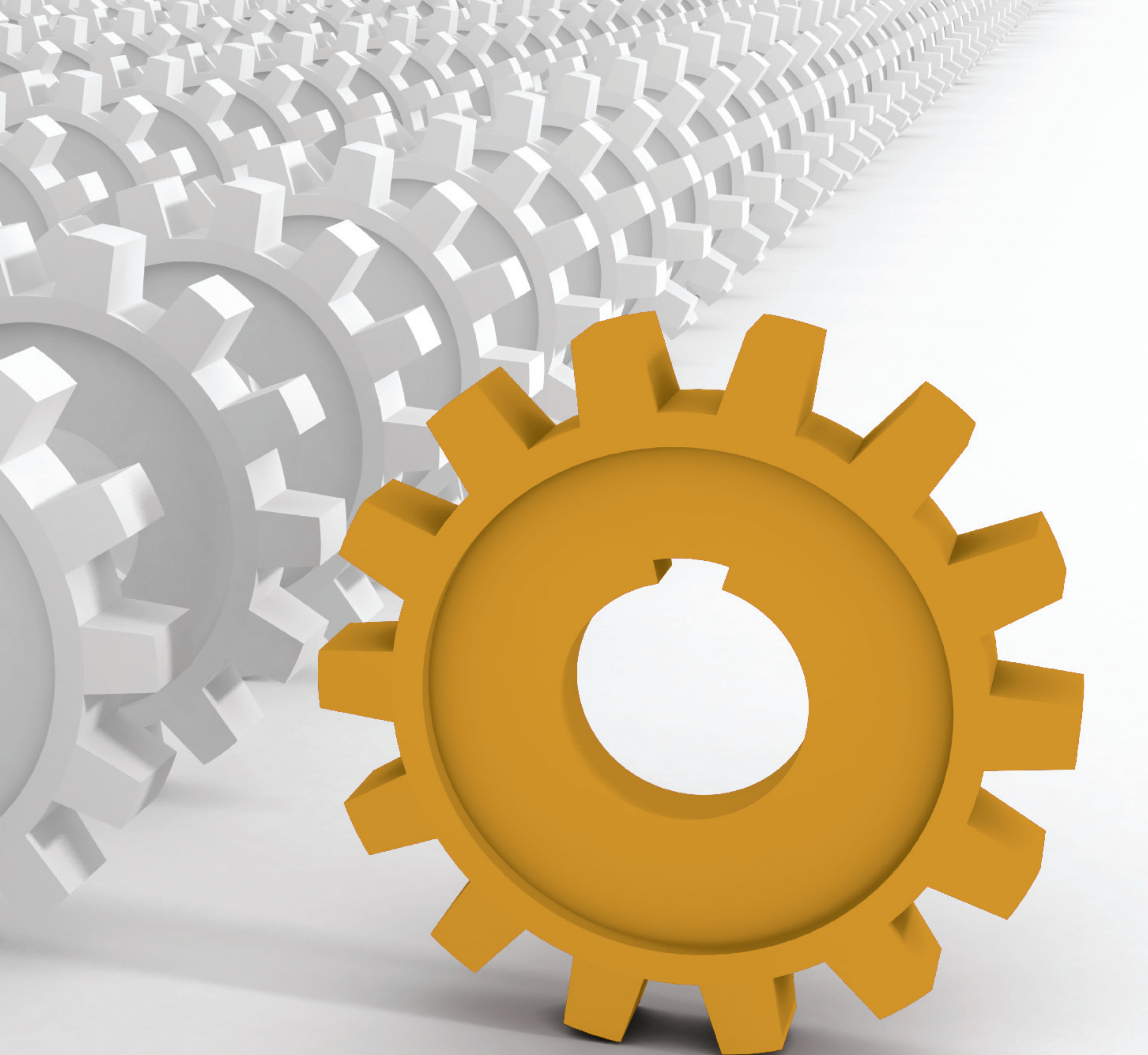
"With such high-bandwidth demands, end-user quality-of-experience during 'tele-observation' or 'tele-operation' is affected by last-mile network bandwidth limitations," said Prasad Calyam, a systems developer and engineer at OSC. "Quality-of-experience is also highly sensitive to network traffic congestion. Improper mouse and keyboard movements due to delays caused by network bottlenecks could result in physical damage to instruments that are prohibitively expensive to repair."

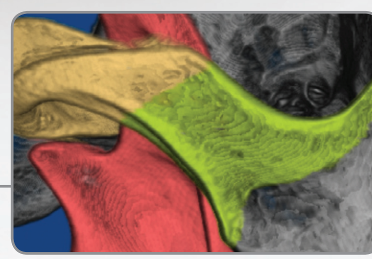
OSC, with assistance from the Center for Advanced Maturation of Materials at The Ohio State University, has modeled several objective and subjective measurements in remote access sessions. These tests have been conducted under different network conditions - in LAN environments and across OSCnet, Ohio's statewide, fiber-optic research and education network. Based on user needs and the modeling experience, OSC engineers developed the Remote Instrumentation Collaboration Environment (RICE) software. RICE is a remote access application that features multi-user session support, user-control management, live video feeds between labs, and collaboration tools such as Voice-over IP and chat. This technology also can support image archival/retrieval for managing image data sets collected during remote instrumentation sessions.

"The ultimate goal is to integrate RICE into existing cyberinfrastructure for a remote instrumentation service that is easy to use and maintain," said Mr. Calyam. "Such a service can foster research and training activities that drastically shorten the development process involved in innovations related to materials modeling, cancer research, and the like."

This type of service also will improve user convenience, significantly reduce costs and, ultimately, decrease duplication of instrumentation investments across the state, he said.

RICE
Remote Instrumentation Collaboration Environment
an initiative of the Ohio Supercomputer Center





Over the course of two decades, the Ohio Supercomputer Center has become a recognized leader in supercomputing, networking, research, and education. That recognition comes, in part, through the concentrated efforts of a world-class, in-house research staff that excels in a variety of scientific disciplines.

The OSC research group's exceptional skills and knowledge have garnered the Center prominence and respect among colleagues throughout the state, across the nation, and around the world. These scientists have built a sterling reputation as a staff of invaluable experts in the fields of supercomputing, statewide networking, data management, biomedical applications, and a host of emerging disciplines.

The Center plays a key role in fueling innovative projects, such as the national Blue Collar Computing™ initiative to deliver essential high performance computing to small- and mid-sized companies, the creation of powerful Web-portals to access and manipulate complex computational resources, and "side-by-side" remote and shared instrumentation. The Ohio Supercomputer Center continues to lead vital science and engineering research endeavors that leverage limited public and private monies and benefit science, business, and the general populace.

Empower. Partner. Lead.

lead [lēd] verb
(led, lead·ing, leads)
1. To show the way, especially by going in advance.
2. To guide or direct in a course.
3. To go or be at the head of.

*The Ohio Supercomputer Center **leads** research activities of strategic interest to OSC, Ohio higher education, and the State of Ohio.*

Online computational tool revolutionizes traditional welding processes

Lead Researchers:
- David Hudak, Ph.D., Ohio Supercomputer Center
- Sudarsanam Suresh Babu, Ph.D., Edison Welding Institute

Funding Sources :
Ohio Board of Regents

For more information:
calculations.ewi.org

Engineers at heavy-manufacturing and energy industries today have access to a new online welding simulation tool, E-Weld Predictor, thanks to the Ohio Supercomputer Center's Blue Collar Computing™ initiative and a partnership between OSC and Edison Welding Institute (EWI).

This on-demand product will allow welding engineers to evaluate the changes in temperature profiles, material microstructures, residual stresses, and welding distortion to reduce the number of experimental trials during the design of welded joints – and ultimately improve productivity and profitability.

Currently, experimental welding procedure trials can be cost prohibitive due to the myriad of geometrical, process, and material combinations. By using E-Weld Predictor, engineers can explore a wide range of "what if" combinations and simulations. This results in a decrease in prototype costs and quicker production because E-Weld Predictor manages the "heavy-lifting" associated with evaluating multiple alternatives. The number of trials also will be reduced since only the most promising welding procedures are sent to the mock-up stage.

OSC programmers worked with EWI on the engineering application and collaborated on the user interface design, developing the final Web layout and the middleware. The Center also is hosting the application on its supercomputers.

"For the last two decades, simulation tools of this kind were only accessible to large-scale industries who could afford the expertise, technology, and infrastructure required to take advantage of these simulation tools. However, the launch of this service levels the playing field," said Henry Cialone, CEO of EWI.

The first launch of E-Weld Predictor is focused on arc welding processes and is primarily for steel pipe and plate weld simulation. Additional processes and applications, including automotive applications, will be evaluated for rollout in future versions. Meanwhile, a similar partnership with PolymerOhio will bring the same supercomputing access to small- and medium-sized plastics and polymer companies throughout Ohio.

"Blue Collar Computing democratizes supercomputing."

Blue Collar Computing:
High performance computing for the rest of us

Blue Collar Computing™, an initiative of the Ohio Supercomputer Center, helps take the same supercomputing systems and applications used almost exclusively by Fortune 500 companies and makes them scalable, accessible, and affordable to small- and medium-sized companies.

"When small businesses can harness cutting-edge supercomputing technology, they have greater opportunities to retain, or regain, competitive footing in the global market," said Stan Ahalt, Ph.D., executive director of OSC. "The benefits reaped from Blue Collar Computing will result in a full-spectrum surge of innovation and scientific advancement."

For example, advanced computational technologies provide companies with innovative tools that allow for the virtual development of new and improved products, such as cars, pharmaceuticals, and financial products.

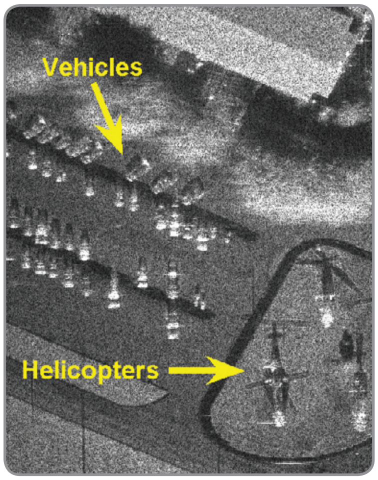
Virtual modeling and simulation also provide companies with a competitive edge through improved manufacturing processes designed to bring products to market quicker, reducing development time, cost, and labor. Simulation makes choosing between alternative processing methods far easier, better analysis and documentation of capabilities help with efficiency, and improved factory and workflow layouts increase productivity. All of these factors can dramatically improve a company's bottom line.

"Similar to the time when desktop computing was considered the primary workhorse for industrial productivity, today's workhorse is supercomputing," Dr. Ahalt said. "Blue Collar Computing democratizes supercomputing."

Collaborating Institutions:
- Edison Welding Institute
- PolymerOhio
- Procter & Gamble
- Council on Competitiveness
- University of Southern California

For more information:
www.bluecollarcomputing.org

Blue Collar Computing™
an initiative of the Ohio Supercomputer Center



Improving homeland security through surveillance

Lead Researcher:
Juan Carlos Chaves, Ph.D.
Ohio Supercomputer Center

OSC Project Team:
- Stan Ahalt, Ph.D.
- Ashok Krishnamurthy, Ph. D.
- Alan Chalker, Ph.D.
- John Nehrbass, Ph.D.

Research Title:
Detection of Moving Targets in Heterogeneous Radar Clutter Scenarios

Funding Source:
U.S. Department of Defense, High Performance Computing Modernization Program User Productivity Enhancement and Technology Transfer (HPCMP PET)

For more information:
www.osc.edu/research/pet

Surveillance of the ground by air- and space-borne sensors has proven to be essential to military and intelligence organizations. Specifically, the U.S. Department of Defense's 2006 Quadrennial Defense Review highlights the need for "a highly persistent capability to identify and track moving ground targets in denied areas."

Of all the sensing technologies available, ground moving-target indication (GMTI) radar has important advantages because of features such as day/night/all-weather operation and foliage, obscurants, smoke, and dust penetration. But GMTI radar data from targets also includes echoes from ground clutter, and the radar motion strongly degrades the performance of target detection for a conventional moving target.

Space-time adaptive processing (STAP) is a signal- and image-processing technique that compensates for the radar's platform motion. Engineers must carefully develop and efficiently implement the robust STAP algorithms, as the technique's high-dimensional vectors and matrices render it computationally intensive.

To improve efficiency, Ohio Supercomputer Center experts developed technology for DoD researchers that simplifies developing complicated algorithms such as STAP and significantly reduces the simulation times by connecting to and interacting with a supercomputer – while still using MATLAB software or related applications designed for basic desktop computers. (See a related story on SSHToolbox on page 29.)

"On my PC, it took almost 246 hours to complete a STAP simulation with 128 thresholds. On the ARL MSRC (Army Research Laboratory MSRC) system, it took 7 hours, which is 35 times faster. This is a tremendous improvement!" said Freeman Lin, Ph.D., Air Force Research Laboratory Sensors Directorate's Electromagnetic Scattering Branch, based at Hanscomb AFB, Massachusetts.

Advancing technology for the U.S. Armed Forces

The User Productivity Enhancement and Technology Transfer (PET) program within the U.S. Department of Defense's High Performance Computing Modernization Program (HPCMP) ensures DoD researchers make the best use of the military's computing capacity. PET gathers and deploys the best ideas, algorithms, and software tools emerging from the national supercomputing infrastructure by contracting with academic leaders, including the Ohio Supercomputer Center.

OSC leads projects in Signal & Image Processing (SIP) and Integrated Modeling and Test Environments (IMT). SIP provides the extraction and analysis of key information of sensors, signal intelligence, and navigation assets, while IMT deals with the collection, storage, processing, and analysis of test data, and models for verifying, synthesizing, directing, and understanding test results.

OSC researchers are addressing needs that include improved algorithms for signal/phenomena exploitation, enhanced means of data transmission and storage, use of life-cycle software development tools, increased use of commercial off-the-shelf tools, and comprehensive and persistent training.

OSC also manages the overall PET program for the MOS consortium, one of two prime contractors for the PET program, which includes Mississippi State University, the Ohio Supercomputer Center, Science Applications International Corporation, Computer Sciences Corporation, University of Tennessee at Knoxville, University of Alabama at Birmingham, University of Texas at Austin, and the University of Hawaii. OSC staff members provide strategic oversight as well as daily management for this $13 million per year contract.

Improving HPC accessibility

A key element in enabling customers to use high performance computing technology is the ability to access supercomputing systems in a simple, straight-forward manner.

Many U.S. Department of Defense (DoD) high performance computing researchers, particularly those in the Signal Image Processing (SIP) area, develop and run programming codes with MATLAB or related development tools such as MatlabMPI, StarP, and pMatlab. These development tools are convenient because they are completely self-contained on a desktop computer.

When MATLAB researchers need access to supercomputers, they desire to connect to and interact with the high performance computers but are reluctant to leave their comfortable desktop MATLAB environment. Often they choose not to use HPC resources because the loss of productivity is too expensive.

With the SSHToolbox, OSC experts have empowered users to be able to have the best of both worlds. SSH stands for Secure Shell and is the most widely used protocol/tool for connecting to remote high performance computing resources. The toolbox supports the DoD-mandated Kerberized authentication protocol and is used for interacting with DoD, government, industry, and systems. Customers include Boeing, NASA, the Pentagon, Air Force, Army, Navy, and universities.

"The toolbox provides simple commands for users to connect to a remote system, run code, send and retrieve results, and disconnect," said John Nehrbass, technical fellow/director of SIP, Ohio Supercomputer Center. "In essence, the SSHToolbox allows a complicated HPC application to be implemented so that it is as easy to use as clicking a mouse."

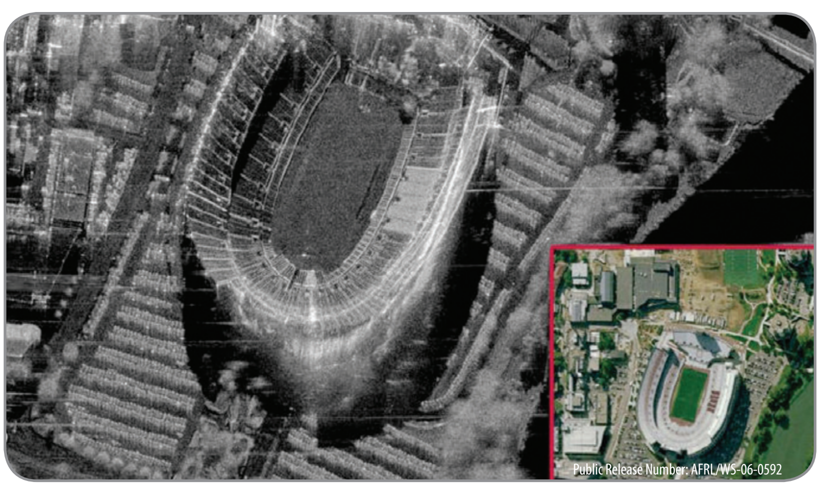
Since the main component of the toolbox is written in C and packaged as a dynamic link library (DLL), the toolbox also can be extended to work with other programming languages such as Java, Python, and Octave. The complexity of the DLL interface and most of the security needs are hidden from the user, making this a very easy to use and powerful toolbox. MATLAB-style documentation for the toolbox also makes it easy to obtain help on various aspects of the toolbox, and a GUI-based installer enables distribution.

Lead Researcher:
John Nehrbass, Ph.D.,
Ohio Supercomputer Center

OSC Project Team:
- Siddharth Samsi
- Tanner Suttles
- Ben Smith
- Stan Ahalt, Ph.D.
- Ashok Krishnamurthy, Ph.D.
- Alan Chalker, Ph.D.
- Juan Carlos Chaves, Ph.D.
- Judy Gardiner, Ph.D.
- Brian Guilfoos
- Jose Unpingco, Ph.D.

Research Title:
Interfacing PC-based MATLAB Directly to HPC Resources

Funding Source:
U.S. Department of Defense, High Performance Computing Modernization Program User Productivity Enhancement and Technology Transfer (HPCMP PET)



General Dynamics created this high-resolution synthetic aperture radar image of Ohio Stadium. The SSHToolbox provides the capability for AFRL/SN researchers to routinely generate similar quality images using both high performance computing and a custom MATLAB GUI designed by OSC researchers.

Employing intelligent peripherals to improve computational performance

While continued developments in processing speeds and disk densities improve computing over time, the most fundamental advances come from changing the ways in which components interact. A research group at the Ohio Supercomputer Center is investigating ways to dramatically increase computational performance using object-based storage devices (OSDs) to augment the processing ability of a parallel file system.

Delegating responsibility for some operations from the host processor to intelligent peripherals such as OSDs can improve application performance. Traditional storage technology is based on simple fixed-size accesses with little assistance from disk drives; however, OSDs offer improvements in performance, scalability, and management by permitting clients to securely and directly access storage.

Yet, OSDs do not provide all the functionality needed by a parallel file system.

"We are examining multiple aspects of the mismatch between the needs of a parallel file system, in particular PVFS2, and the capabilities of OSD," said Pete Wyckoff, Ph.D., a research scientist with OSC. "Our work will examine techniques to accommodate this high performance usage model."

The Parallel Virtual File System (PVFS) provides an open-source, scalable input/output subsystem for machines ranging from small cluster computers to the largest peta-scale supercomputers and allows communication over various devices at high speeds.

Object-based storage devices are expected as commodity items in the near future, but no physical devices are yet available. At present, researchers use a software emulator to enable a storage server to behave as an object-based disk.

If the research is successful, OSDs will result in computers that can process data and produce results faster. Consequently, problems that hinge on the use of massive amounts of data, such as energy exploration, environmental modeling, and patient safety, will be easier to solve.

Lead Researcher:
Pete Wyckoff, Ph. D.,
Ohio Supercomputer Center

Project Team:
- Dennis Dalessandro, Ohio Supercomputer Center
- Ananth Devulapalli, Ohio Supercomputer Center
- Nawab Ali, The Ohio State University

Research Title:
Applicability of Object-Based Storage Devices in Parallel File Systems

Funding Source:
National Science Foundation

For more information:
www.osc.edu/research/network_file/projects/object

Improving Web server performance

Due to the cost of network processing, high-end Web servers in the near future will be unable to handle the continually increasing demand of more clients ever hungrier for more content. In fact, it is already commonplace today to use multiple servers to host a single Web site. Solutions such as multi-core systems or TCP Offload Engines have provided some relief, but are limited approaches because of the way they deal with memory.

However, a technique known as Remote Direct Memory Access (RDMA) has the capability to fully saturate high-speed networks while leaving the CPU free to do other tasks. RDMA not only moves the protocol processing to the network adapter, but also moves data directly from user space. This eliminates the need for costly memory copies.

While RDMA has proved successful in the high performance computing realm, it is not used widely because of compatibility issues with existing network infrastructures. But a new adaptation of RDMA called iWARP enables RDMA over ordinary TCP/IP-based networks. (See the iWARP below for more details.)

Leveraging iWARP, the research team at the Ohio Supercomputer Center has created a module (mod_rdma) that enables the popular Apache Web server to use RDMA to send and receive client data.

"In our study, we have outfitted a Web server with 10 gigabit iWARP hardware and used client-machines running iWARP-software modified wget and Apache bench programs," said Dennis Dalessandro, networking researcher for OSC. "The result improves Web server performance, both in throughput and client request rate."

Lead Researchers:
- Dennis Dalessandro
  Ohio Supercomputer Center
- Pete Wyckoff, Ph.D.
  Ohio Supercomputer Center

Research Title:
RDMA Enabled Apache (mod_rdma)

Funding Source:
- U.S. Department of Energy, ASC Program
- NetEffect, Inc.

For more information:
www.osc.edu/research/network_file/projects/rdma

Downloading at warp speed

As network speeds have increased to 10 gigabits per second and beyond, today's CPUs have been unable to sustain the increased network processing requirements while at the same time meeting computational needs. However, specialty network solutions, such as InfiniBand, have long been available to solve this problem. The downside is the incompatibility with the existing TCP/IP based networking infrastructure that is common today.

iWARP, though, bridges the gap between high performance networking and TCP/IP compatibility. The term iWARP refers to a set of published protocol specifications that provide remote read- and write-access to user applications, without operating system intervention or intermediate data copies. The result is higher throughput and lower latency transfers. While hardware implementations of iWARP have begun to emerge, a software implementation is useful to serve as a transition mechanism and for protocol testing and research.

Another benefit provided by iWARP is single-side acceleration. In other words, only one end of a connection needs to have iWARP hardware to see local advantages, if the other side is equipped with iWARP. This is particularly attractive for the very common single-server, many-client scenarios.

Experiments conducted by Ohio Supercomputer Center researchers show that, with single-side acceleration, the sender system load drops from 35 percent to 5 percent, and receiver load drops from 90 percent to less than 5 percent, for 1 gigabit-per-second communication.

Lead Researcher:
Pete Wyckoff, Ph.D.,
Ohio Supercomputer Center

OSC Project Team
- Dennis Dalessandro
- Ananth Devulapalli

Research Title:
Software Implementation and Testing of the iWARP Protocols

Funding Source:
Sandia National Labs

For more information:
www.osc.edu/research/network_file/projects/iwarp

Expanding supercomputing by improving programmer productivity

Project Lead:
David Hudak, Ph.D.,
Ohio Supercomputer Center

OSC Project Team:
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- Neil Ludban
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- Juan Carlos Chaves, Ph.D.
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- Brian Guilfoos
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- Siddharth Samsi
- Jose Unpingco, Ph.D.

Funding Source:
- U.S. Department of Energy
- U.S. Department of Defense, High Performance Computing Modernization Program User Productivity Enhancement and Technology Transfer (HPCMP PET)

For more information:
www.bluecollarcomputing.org

Blue Collar Computing™
an initiative of the Ohio Supercomputer Center

Supercomputers are only as useful as the software they can effectively run. In order to expand that base of software, it must be easier to write and debug code on massively parallel systems. The Ohio Supercomputer Center's high-level language initiative addresses this pressing need through a combination of software development, a robust production services environment, and in-house research and consulting.

"By taking this holistic approach to generating efficient supercomputing applications for our researchers, we're able to capitalize on all the components within the cycle of innovation - development, experimentation, and analysis - and continuously improve our services," said David Hudak, Ph.D., senior research scientist, Ohio Supercomputer Center.

For example, OSC researchers developed ParaM, a collection of internally and externally developed software, including bcMPI, pMatlab, and GNU Octave, that also incorporates a launcher and installer to facilitate downloading the program. ParaM is installed and supported on OSC clusters as part of its production services environment, along with MatlabMPI, MATLAB DCE, and Star-P. iPython is slated for installation soon.

"Providing our user community these various software options serves dual purposes," Dr. Hudak said. "The variety enables researchers to select parallel computing languages they most prefer, and just as important, it creates a test bed for exploring these systems."

ParaM and bcMPI

MATLAB, a commercial mathematical modeling package, and GNU Octave, its open source counterpart, are leading choices for computational science and numeric application prototyping. Researchers at the Ohio Supercomputer Center developed ParaM to improve the potential for applying these high-level languages to larger problems in these domains.

ParaM enables developers to directly write parallel code in MATLAB with either a "message passing" or "global array" parallel programming model. By leveraging the GNU Octave interpreter, ParaM works on a wide variety of machines that don't support MATLAB, such as Itanium and POWER processors, and it uses modern interconnects like Infiniband and Myrinet.

bcMPI was developed as part of the ParaM project; it is a software package that implements message passing interface (MPI) extensions for MATLAB and GNU Octave. It consists of a core library that interfaces to the MPI library, a toolbox for MATLAB, and a toolbox for Octave.

bcMPI implements a subset of the MPI application program interface. The MATLAB language bindings are simpler than the standard bindings for C or Fortran: data types are detected at run time, received data is returned by value, and data communication functions accept variable number of parameters. Where possible, compatibility with MatlabMPI has been maintained.

Both ParaM and bcMPI are open source programs. They are available for download at www.bluecollarcomputing.org/applications/bcMPI/download.shtml.

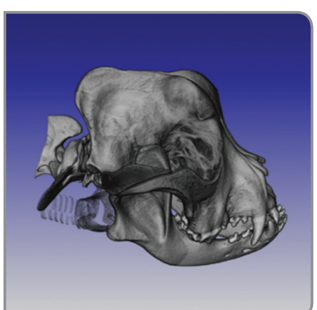
Using innovation to teach veterinary students

Project Leads:
- Mary Ann McLoughlin, D.V.M., The Ohio State University
- Don Stredney, Ohio Supercomputer Center

Research Title:
Employing Simulation Technologies for Veterinary Surgical Training to Support the Effort to Reduce Animal Use: Accelerating Adoption

Funding Source:
The Alternatives Research & Development Foundation

For more information:
www.osc.edu/research/Biomed/projects/animals



Veterinary schools nationwide are continually seeking new methods to reduce the use of live animals in surgical training. Yet, the question remains whether this reduction negatively affects the surgical proficiency veterinary students and residents require prior to graduation.

The Ohio State University College of Veterinary Medicine is collaborating with the Ohio Supercomputer Center to address both issues.

OSC researchers are applying technologies employed for human medical training to veterinary medicine. Working in coordination, OSC and the College of Veterinary Medicine have created computer models of a dog's head, pelvis and spine, using non-invasive imaging techniques such as computed tomography and magnetic resonance imaging.

The computer models will be used in simulations for teaching regional anatomy and procedural surgical techniques – without harming any animals. For example, in the study's first year they integrated the spine data with software that provides interactive drilling, developed from human temporal bone simulation (see story on page 17), to emulate laminectomies, a surgical procedure for dogs with intervertebral disc disease.

After the simulations are incorporated into the veterinary surgical curriculum, the team will conduct studies to validate their usefulness and effectiveness in the veterinarian curriculum.

"The implications for teaching anatomy through computational modeling extends far beyond medical or veterinarian colleges," said Don Stredney, director of OSC's Interface Lab and research scientist for biomedical applications. "In the near future, I think all levels of education will use computational modeling, especially in middle and high school. Instead of dissecting frogs in biology class, there could be a standardized curriculum incorporating computational models and simulations that all schools use, thereby reducing the need for purchased, expensive, and dwindling physical specimens."

Facilitating large-scale visualization and computation

The gaming industry, with its consumer demand for realistic, smooth, 3-D images, is without a doubt advancing the graphics hardware market exponentially. In recent years, commodity-based graphics chips or graphical processing units (GPUs) have become more programmable and easier to use for general purpose applications (GPGPU).

Researchers are starting to use these single process, multiple data parallel processors to accelerate image processing algorithms and line of sight calculations, in addition to real-time deformation calculations.

Understanding that demand for this technology will only continue to grow, the Ohio Supercomputer Center installed a GPGPU/Visualization cluster in 2007. The system's configuration contains:

- 36 AMD Opteron 2.6GHz dual-core CPUs
- 36 NVIDA Quadro FX 5600 GPUs
- Infiniband Dual Port HCA card
- 144 gigabytes of RAM
- 13,500 gigabytes SATA hard disk

Each Quadro FX 5600 card has 1.5 gigabytes of onboard, high-speed memory and is capable of 330 peak gigaflops. Combined, the 36 GPUs of the cluster are capable of 11,800 peak gigaflops, and, most importantly, are fully programmable. This level of memory, speed, and programmability is a necessity for realistic graphics and a boon for researchers wanting to use GPGPU for their data sets.

"Our goal is to create an environment for Ohio's researchers to tap the latest graphics technology, whether it's for GPGPU computation or visualization," said Dennis Sessanna, director of hardware - Interface Lab, Ohio Supercomputer Center. "In addition to the hardware, the cluster is running GPU-accelerated application program interfaces such as CUDA, Cg, and GLSL. These interfaces make it easier for non-programmers to use the GPUs for their studies.

"Initial performance studies show that some common scientific algorithms completed 50 to 100 times faster on the GPGPU/Visualization cluster than they would have on a comparable CPU-based supercomputer," Sessanna said. "However, not all algorithms will perform this well on a GPU. We're helping our clients determine what applications can be optimized for the graphics processor."

The cluster also enables researchers to access the cluster's graphics cards and perform data-intensive visualizations in real-time, from viewing 3-D medical data to creating simulation models. The resulting images are then interactively streamed back to their desktop.

Project Lead:
Dennis Sessanna,
Ohio Supercomputer Center

OSC Project Team:
- Don Stredney
- Ashok Krishnamurthy, Ph.D.

Research Title:
HHS-OBOR: Cluster Computing Capacity

Funding Source:
Ohio Board of Regents

For more information:
www.osc.edu/research/Biomed/interface.shtml

Two of the GPGPU/Visualization cluster nodes are located in OSC's Interface Lab. One system is connected to a four-panel video wall (above) and the other to a passive stereo projection system.

"Seeing is believing" and other benefits of high-definition videoconferencing

High-definition videoconferencing (HDVC) is rapidly becoming an alternative to the traditional standard-definition videoconferencing systems for applications in fields as diverse as education, health care, justice, and entertainment.

"The Ohio Supercomputer Center is playing a major role in the deployment of HDVC systems across Ohio universities, hospitals, and research labs," said Prasad Calyam, an OSC system developer and engineer. "Additionally, various collaboration technologies, including tele-presence, have been tested at OSC for integration with HDVC systems."

To illustrate: OSC and Nationwide Children's Hospital in Columbus – the largest neonatal center in the country – are working with Adena Regional Medical Center, an hour's drive to the south, to use HDVC to improve medical care for babies and provide comfort to their families.

The goal of the project is to improve remote medical consultation by allowing specialists in Columbus to view distressed newborns with exceptional clarity, examine detailed X-rays, take online electronic stethoscope readings, and consult with attending physicians in Chillicothe. This arrangement also will provide high-definition tele-visits to help reassure working families whose newborns have been transferred to Columbus for extended periods.

"Since HDVC is a recently developed technology, the network requirements and security issues for large-scale deployments are not well understood," Calyam explained. "To address these issues, OSC engineers have conducted several studies to characterize HDVC network traffic in terms of bandwidth consumption and end-user quality-of-experience under different video encoding rates and network health conditions."

In addition to the neonatal example above, OSC engineers have conducted studies of HDVC's usability and reliability by deploying systems at the Organ-Transplant Preparation and Consultation Services office of Lifeline of Ohio, the Game Research and Immersive Design Lab at Ohio University and its partner site at Shawnee State University, and the Tele-Music Operations site at the Cleveland Institute of Music.

Lead Researcher:
Prasad Calyam,
Ohio Supercomputer Center

OSC Project Team:
- Pankaj Shah
- Terry Lewis
- Arif Khan

Funding Sources:
- American Distance Education Consortium
- Ohio Board of Regents

For more information:
www.osc.edu/networking/videocon

Computational Science Minor:
Enhancing the academic portfolio

Students at nine Ohio college and university campuses began adding valuable computational science skills to their academic portfolio with the August launch of a new, virtual minor program being coordinated by the Ralph Regula School of Computational Science.

Computational scientists use computers – especially supercomputers – to create mathematical models that help them simulate and understand complicated mechanical and natural processes. Computational science has produced enormous advances in areas such as product prototyping, DNA sequencing, behavioral modeling, global climatic predictions, drug design, financial systems, and medical visualization.

One well-known example of computational science is modern weather forecasting, where vast amounts of data are combined with sets of mathematical formulas in a computer program called a weather model to develop forecasts. These forecasts are far more accurate and timely than were possible before computer modeling was available.

Another important example is the use of computer models to simulate and test new products prior to manufacturing. The use of "virtual prototypes" sharply reduces or even eliminates the slow and expensive process of building and testing physical prototypes.

"Computational science and the use of modeling and simulation have been cited by prominent federal committees and panels as keys to continued United States competitiveness in science and engineering," said Steve Gordon, Ph.D., director of the Ralph Regula School.

The Ralph Regula School of Computational Science is a statewide, virtual school, administered by the Ohio Supercomputer Center, that serves as a coordinating entity for a variety of computational science education activities. The Ralph Regula School does not offer degrees or program certificates on its own, but instead draws upon the resources and expertise of Ohio's colleges and universities to develop and offer coursework for academic programs and certificates.

Project Lead:
Steve Gordon, Ph.D.,
Ohio Supercomputer Center

Funding Sources:
- National Science Foundation
- Ohio Board of Regents

Partner:
Ohio Learning Network

Collaborating Institutions:
- Capital University
- Central State University
- Columbus State Community College
- Kent State University
- Sinclair Community College
- The Ohio State University
- University of Cincinnati
- Wittenberg University
- Wright State University

For more information:
www.rrscs.org

Ralph Regula School of Computational Science
an initiative of the Ohio Supercomputer Center

The Ralph Regula School: Providing the workforce with computer simulation and modeling skills

The Ralph Regula School of Computational Science (RRSCS) is a statewide virtual school focused on computational science - the use of computer modeling and simulation to solve complex business, technical, and academic research problems.

Businesses recognize computational science as an essential tool for innovation and use it to develop new products. Researchers do the same to expand the frontiers of knowledge. In collaboration with the Ohio Supercomputer Center, the Ohio Board of Regents, the Ohio Learning Network, and Ohio's colleges and universities, the Ralph Regula School ensures that Ohio has the skilled people needed to support the use of this new approach to innovation.

The Ralph Regula School relies on participating colleges and universities to confer degrees and certificates and offer their expertise to the multi-institutional, interdisciplinary undergraduate minor launched in 2007, cultivate and maintain curricula standards for computational science degree programs and certificates, and to use technology resources to teach courses and programs in the most convenient and effective way for students.

The competencies created by participating faculty for Ralph Regula School programs have been reviewed and approved by a business advisory committee, meaning that when these students enter the workforce, they will have the specific skills sought by employers.

Other RRSCS projects under way include:
- Industry-focused certificate and college co-op programs
- A high school elective within the Ohio Project Lead The Way curriculum
- Online tools for teachers in the classroom and researchers
- Model associate degree program in computational science

OSC Research Grants

July 1, 2006 to June 30, 2007

Funding Source	Topic	OSC Contact	Partners
Agricultural Telecommunications Program	Tri-State Aquaculture Outreach Using Technology	Robert Dixon, Ph.D.	The Ohio State University
The Alternative Research & Development Foundation	Employing Simulation Technologies for Veterinary Surgical Training to Reduce Animal Use: Accelerating Adoption	Don Stredney	The Ohio State University
Argonne National Laboratory	Forwarding I/O with Portals in PVFS	Pete Wyckoff, Ph.D.	
AVETeC	Sharing Data by Linking Parallel File Systems in the Wide Area	Pete Wyckoff, Ph.D.	
National Science Foundation	CPATH T: NEWPATH: Nurturing, through Entrepreneurship, IT World Leaders	Elaine Landwehr	The Ohio State University
National Science Foundation	Computational Science Program for Ohio Community and Technical Colleges	Steve Gordon, Ph.D.	Battelle Memorial Institute Cal Poly Capital University Owens Community College Stark State Community College Sinclair Community College
National Science Foundation	Applicability of Object-Based Storage Devices in Parallel File Systems	Pete Wyckoff, Ph.D.	
New Mexico Institute of Mining & Technology	Finite-State Modeling Analysis of Electrical Power Grid	Judith Gardiner, Ph.D.	
Ohio Board of Regents/The Center for the Accelerated Maturation of Materials	Remote Telemicroscopy	Steve Gordon, Ph.D.	The Ohio State University
Ohio Board of Regents	GRIDP Project	Steve Gordon, Ph.D.	University of Cincinnati Genome Research Institute
Ohio Department of Education	Summer Institute for Gifted Students	Elaine Landwehr	The Ohio State University
Rivers Unlimited	OSU GIS Project	Steve Gordon, Ph.D.	
The MathWorks	Summer Institute for Gifted Students	Elaine Landwehr	
University of Illinois Gelato Federation	Storage Layout Optimizations to Improve Parallel Distributed File System Performance	Pete Wyckoff, Ph.D.	

Funding Source	Topic	OSC Contact	Partners
U.S. Air Force Aeronautical Systems Command	HPC Technology Support	Richard Pritchard, Ph.D.	
U.S. Air Force Materiel Command, U.S. Air Force Research Laboratory	High Performance Computing Innovation Service Portal Study	Dave Hudak, Ph.D.	University of Southern California
U.S. Air Force Research Laboratory	Automatic Target Recognition Center's Summer Internship Program	John Nehrbass, Ph.D.	Jacobs Technology
U.S. Air Force Research Laboratory	HPC Technology Support	John Nehrbass, Ph.D.	
U.S. Army Research Laboratory	Object Detection, Localization, and Tracking Using Multiple Sensors	Ashok Krishnamurthy, Ph.D.	
U.S. Department of Defense High Performance Computing Modernization Program	PET – Integrated Modeling and Test Environments	Ashok Krishnamurthy, Ph.D.	Mississippi State University
U.S. Department of Defense High Performance Computing Modernization Program	PET – Overall Program Management	Richard Pritchard, Ph.D.	Mississippi State University
U.S. Department of Defense High Performance Computing Modernization Program	PET – Signal/Image Processing	Stan Ahalt, Ph.D.	Mississippi State University
U.S. Department of Defense High Performance Computing Modernization Program	PET - Productivity and Performance Evaluation	Juan Carlos Chaves, Ph.D.	Mississippi State University
U.S. Department of Defense High Performance Computing Modernization Program	PET - Run SIP Codes from Desktop on HPC	John Nehrbass, Ph.D.	Mississippi State University
U.S. Department of Defense High Performance Computing Modernization Program	PET - Simplify Uniprocessor IMT Code Transitions to HPC	Alan Chalker, Ph.D.	Mississippi State University
U.S. Department of Education	Ralph Regula School of Computational Science	Steve Gordon, Ph.D.	
U.S. Department of Health and Human Services/Ohio Board of Regents	VM2M: Integrated Virtual Microscopy & Molecular Analysis Software for Enhanced Cancer Diagnosis	Ashok Krishnamurthy, Ph.D.	The Research Institute at Nationwide Children's Hospital Childrens Hospital Los Angeles Children's Oncology Group
U.S. Environmental Protection Agency/Centers for Disease Control	Human Health Assessment of Air Pollutants in India	Moti Mittal, Ph.D.	

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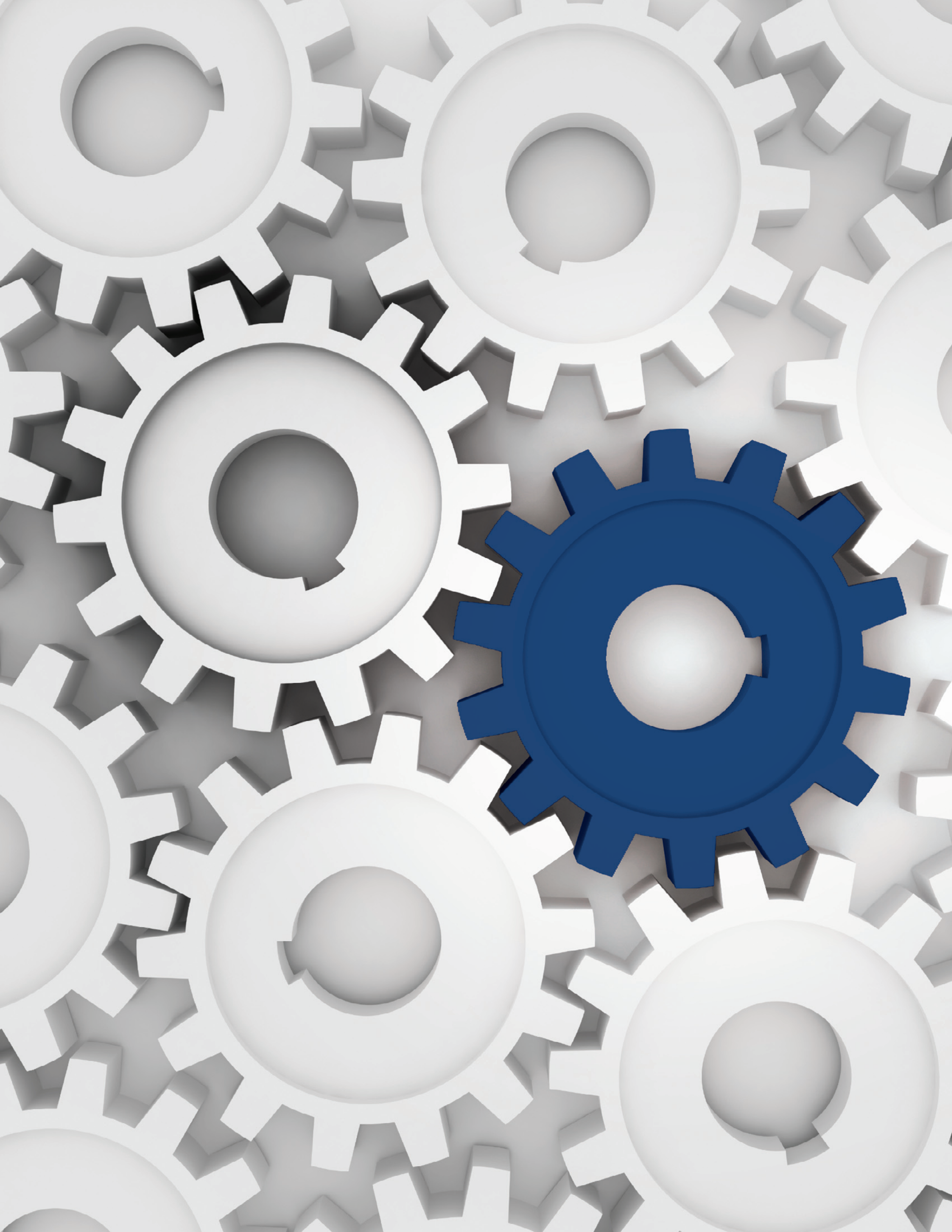

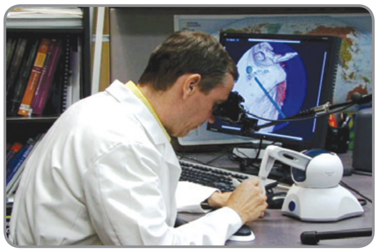

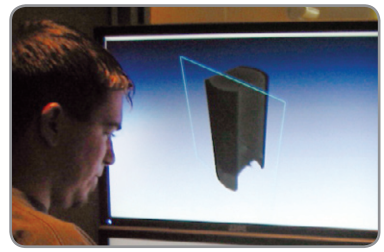
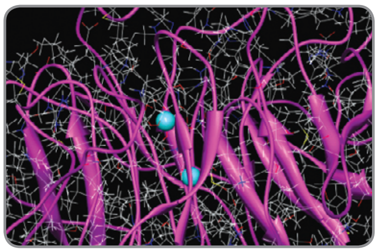

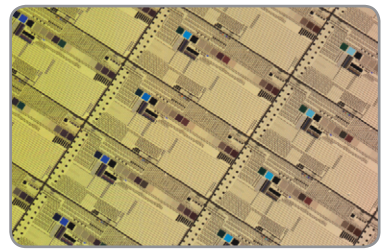

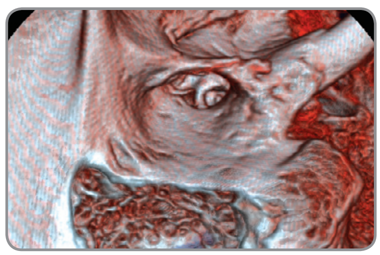
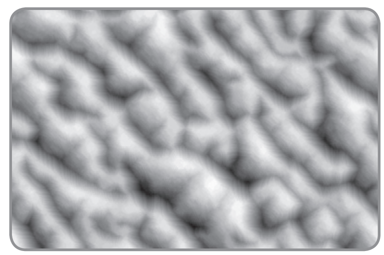

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