Research Report 2015–16

Ohio Supercomputer Center

An OH·TECH Consortium Member

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Chancellor John Carey directs the Ohio Department of Higher Education and oversees the strategic initiatives of the Ohio Technology Consortium and its member organizations in support of the state's technology infrastructure needs.

"Research and innovation are fundamental requirements for a vibrant economy in the 21st century, and the Ohio Supercomputer Center provides Ohio researchers with the essential tools and services to advance that critical work."

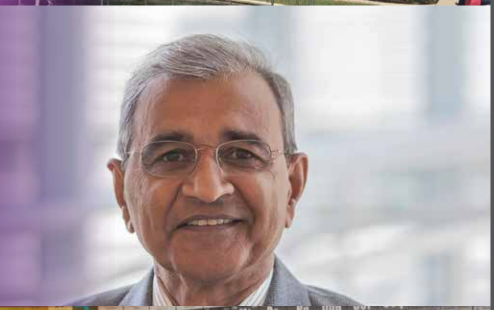
— *John Carey, Chancellor, Ohio Department of Higher Education*

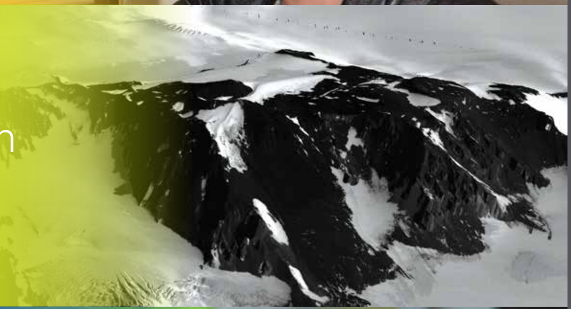
OH·TECH | Ohio Technology Consortium
A Division of the **Ohio Department of Higher Education**

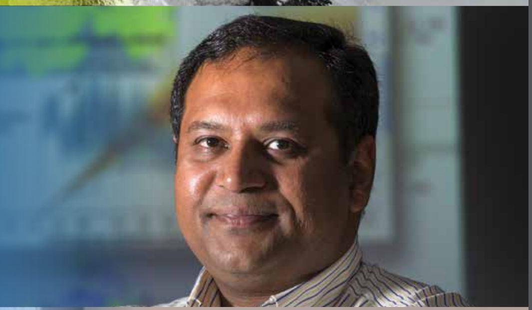
The Ohio Technology Consortium (OH-TECH) serves as the technology division of the Ohio Department of Higher Education and comprises a suite of technology and information member organizations unsurpassed in any other state: OSC, OARnet, OhioLINK and eStudent Services. Their consolidation under the OH-TECH banner allows each organization to pursue assorted synergies and efficiencies.

Ohio Supercomputer Center

The Ohio Supercomputer Center (OSC) addresses the rising computational demands of academic and industrial research communities by providing a robust shared infrastructure and proven expertise in advanced modeling, simulation and analysis. OSC empowers scientists with the services essential to making extraordinary discoveries and innovations, partners with businesses and industry to leverage computational science as a competitive force in the global knowledge economy and leads efforts to equip the workforce with the key technology skills required for 21st century jobs.







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OSC mission focuses on people

In 2016, the Ohio Supercomputer Center arrived at another crossroads. We began installation of the most powerful supercomputer in the history of the center. We swapped out almost all of our storage and other infrastructure, essentially rebuilding OSC's production infrastructure from the ground up. We also are undergoing a leadership transition with the departure of the former executive director. With all this change, what, if anything, remains the same? In short, our mission.

"At the Ohio Supercomputer Center, our duty is to empower our clients, partner strategically to develop new research and business opportunities and lead Ohio's knowledge economy."

Examined closely, you will notice that the mission statement doesn't mention our "cutting-edge supercomputer clusters" or "immense and fast storage systems." There are several reasons for that. First, the people who conduct their research by leveraging our supercomputing services are the central focus of what we do. Their work advances scientific discovery and spurs technological innovation. Furthermore, very few people find it interesting to read a story of a computer chip that is incrementally faster than the one we used the year before, but there is no doubt people are captivated with research stories about the spread of the Zika virus, strategies to mimic shark skin to improve airflow around jet plane surfaces and design of future materials or new types of batteries that could more safely and efficiently power electric cars.

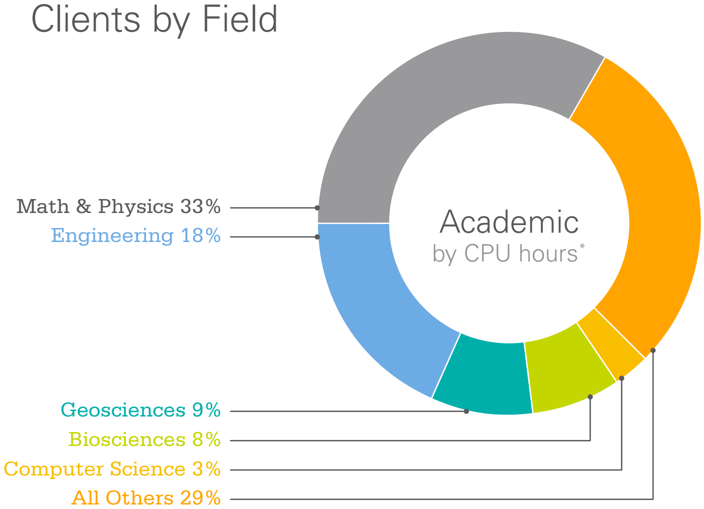
Secondly, the highest value aspect of OSC is found in the many services we provide, not in the rows of hardware and labyrinth of cables. Our clients often lack the time or the skills to scale up their work and really use a supercomputer to its full capabilities. As a result, our hardware is too frequently "driven like a Ferrari in first gear," observes David Hudak, our interim executive director. To address this, we offer services that are increasingly focused on client engagement, training, facilitation and software development.

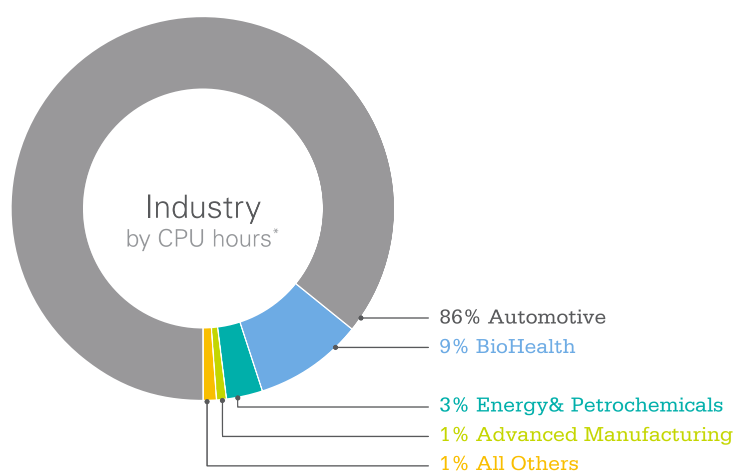
Lastly, the aspect that truly makes OSC run are the people behind our services: help desk experts eager to find a solution to any issue that arises, operations engineers who design and maintain the machinery at the data center, programmers who continue to develop new and easier access channels, coders who examine lines and lines of data to find a single command that could slow a job. As a prime example, our Virtual Environments and Simulation Group possesses great expertise with an extraordinarily powerful set of tools, which could be used in many cases to help bring even higher levels of insight to new and existing research.

Advancing academics

One of our primary goals at OSC is to advance the academic research ecosystem encompassing the students, staff and faculty of the colleges and universities of Ohio. One of our largest client communities is that of the graduate student who does a lion's share of the computational work for the principal investigators in academia. Grad students turn their research into theses and dissertations to complete their education. Faculty members leverage our resources across generations of graduate students, with those close to graduation sharing expertise with those new to the lab. Additionally, faculty members can cite access to our services in grant proposals demonstrating that they have the resources needed for their proposed projects. When appropriate, we also provide them with letters of commitment for specialized services or expertise. In some cases, members of our staff collaborate fully in the project as co-investigators.

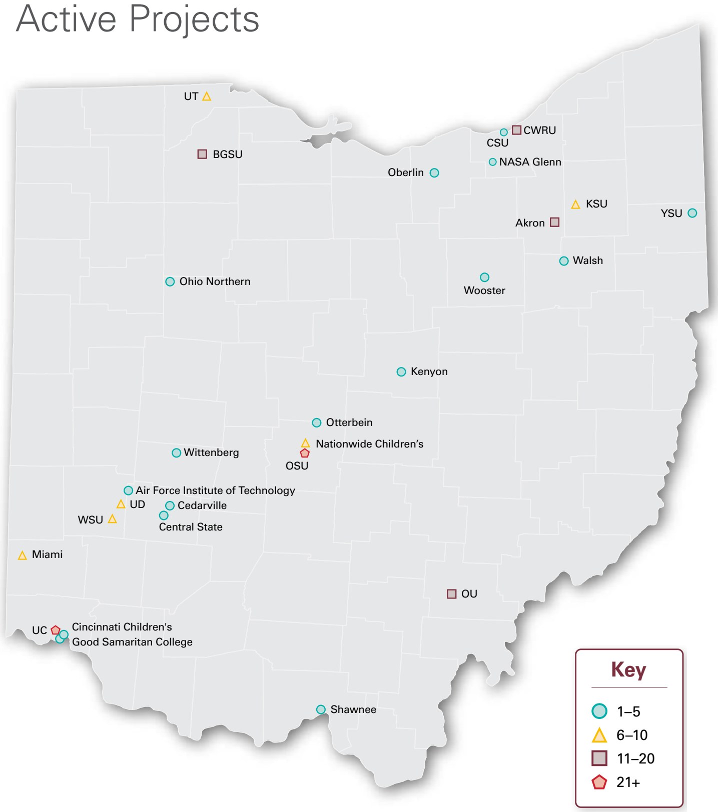
Clients by Field



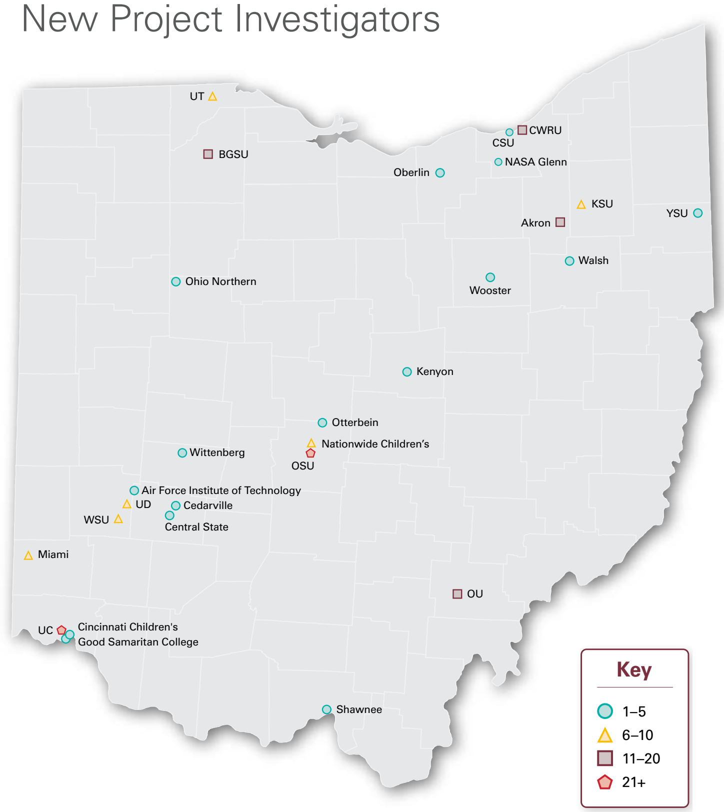


*All data CY2015

Active Projects



New Project Investigators



We provide university deans and department heads with faculty recruitment materials that help draw even higher numbers of leading computational scientists to their campuses. Having direct access to our cutting-edge supercomputing services helps make quality academic programs even more competitive, enhancing national proposals and collaborations and improving the quality of academic programs.

We also provide classroom services to professors who leverage access to OSC services to teach a wide range of engineering and science courses, everything from pharmacy to aerospace engineering. In the summer, OSC hosts a residential institute for high school boys and girls and another for middle school girls, augmenting the STEM education they receive at their local schools and preparing them for the technology economy of today and tomorrow.

Assisting industry

Since OSC was created in 1987, it has been one of our charges from the General Assembly and the Department of Higher Education to boost the research capacity of manufacturing and other industries around the state. From the concept of Blue Collar Computing, coined more than a decade ago, to that of AweSim, a program that today promotes online modeling and simulation apps and tools, OSC always has been at the forefront of simulation-driven design.

Many people, especially in industry, find supercomputers too daunting and expensive to integrate into the R&D process. Our engineers have been working hard to provide new services and innovative tools, such as OSC OnDemand—our "one stop shop" for access to our high performance computing resources—to make access to supercomputing simpler and more intuitive.

Providing new solutions

Finally, to address the constantly rising demand for computing capacity, we installed a new system in our data center—the most powerful system in the center's history. However, the new Dell/Intel-Xeon Owens Cluster was just the beginning. We literally rebuilt our entire computing infrastructure, producing dramatic increases in all aspects of storage and interconnecting network speeds. In addition, we've been working with our data center partners at the State of Ohio Computer Center to enhance the physical computing environment, including a viewing vestibule to make our suite more secure and visitor-friendly.

Plans for the future include adding GPUs to the Owens Cluster, replacing the Oakley Cluster, further expanding our project storage and replacing/upgrading sections of our tape backup systems. All of this work is being done with an eye toward supporting our mission to support those clients who are driving discovery and innovation across Ohio and beyond.

Biological Sciences

On a daily basis, each one of us asks ourselves: Where do we come from? Where are we going? And how can we thrive? The study of modern biology seeks to answer those questions on a broader scale to improve each one of our lives in some significant way. The biosciences represent a vast, eclectic and fascinating field. Research being done at the Ohio Supercomputer Center illustrates the breadth of critical work being done to understand life, including everything from evolutionary questions to focused issues of fighting cancer, improving human hearing and developing plants to boost economies.

Bioinformatics Tools

Carstens gauging how statistical models fit various genetic data

In less than 10 years, the way genetic data has been collected has sped up in a major way. Previously, collecting data from a species was done one gene at a time, on an individual-by-individual basis, but new sequencing technologies allow researchers to process hundreds of thousands of genes at a time.

That massive uptick has created a huge need for bioinformatics tools. Bryan Carstens, Ph.D., and researchers in his lab within the Department of Evolution, Ecology and Organismal Biology at The Ohio State University are working to create these bioinformatics tools through the Ohio Supercomputer Center (OSC).

The Carstens lab relies heavily on statistical models to determine parameters for evolutionary processes, such as mutation, selection, genetic drift, migration and phylogenetic diversification. While there are plenty of software packages available for these processes, there hasn't been a lot of attention dedicated to assessing how well one model fits a given empirical data set.

"The work we do is looking at fitting statistical models to genetic data, and we do this to learn about the evolutionary history of different species," Carstens said. "Sequencing now is massively parallel so it's ideal for a parallel computing environment."

Carstens has several projects with OSC, some of which are packaged into a larger one: Developing bioinformatics tools for evolutionary genetics. Those projects include: Developing P2C2M (Posterior Predictive Checks of Coalescent Models), a package that evaluates the fit of coalescent models; developing Phrapl, which evaluates coalescent model selection; genome assembly for the carnivorous plant Sarracenia alata; and using bGMYC, a species delimitation software, to evaluate sequence data from more than 20,000 Malagasy ants. In addition, other lab researchers are working on predicting the future geographic distributions of threatened and endangered species under differing models of climate change.

Carstens' lab is seeking to understand demography of specific species because it allows for more precise inferences about changes in natural selection, how strongly the selection has been and other related questions.

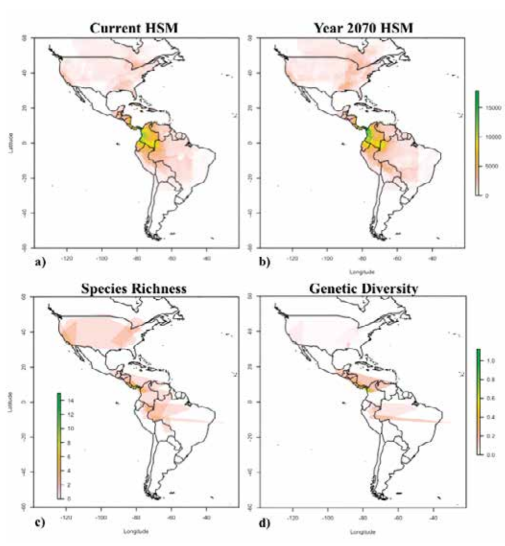
That insight helps gain understanding into many areas such as fighting disease. For example, some stricken by cancer might have a genetic variance that can be pinpointed to develop a treatment that has worked for someone with a similar genotype.

Another example relates to conservation. For instance, why are certain species of birds, like blue jays or cardinals, plentiful while others are rare?

"It's a mistake to assume an abundant species has always been abundant," Carstens said. "If you're a conservation manager and you're trying to make decisions about how to allocate resources, it becomes useful to know some species have undergone a dramatic expansion because it looks like they're able to thrive in human-moderated environments versus another species that has declined since the time of European colonization. This history, you can't really get it any other way."

That makes high performance computing critical to bioinformatics, which may require thousands of computing hours for the statistical analyses necessary to understand a genetic data set.

"What happens at one part of the genome is very likely to impact some other part of the genome," Carstens said. "As geneticists, we need to understand the statistical properties and distributions of our analyses by replicating them over and over. If we do one analysis and don't have replication we often can't interpret it. So what we need to do is thousands of different analyses with slightly different parameters and positions to understand how much confidence we should place in the answers we've gotten. And that's only possible in a parallel computing environment, so it's a huge competitive advantage to house my research program at The Ohio State University because of OSC's resources." •



► Left: Bryan Carstens, Ph.D., and researchers in his lab within the Department of Evolution, Ecology and Organismal Biology at The Ohio State University are working to create these bioinformatics tools through the Ohio Supercomputer Center.

► Geographic distributions of American amphibians, under current and projected climatic regimes. Carstens' analysis of intraspecific genetic diversity can contribute to the identification of regions that should be targeted for conservation.

Project Lead: Bryan Carstens, Ph.D., The Ohio State University
Research Title: Developing bioinformatics tools for evolutionary genetics
Funding Source: National Science Foundation
Website: carstenslab.osu.edu

Hearing Loss

Sotomayor group examines molecular-level mechanics of hearing

The difference between hearing and a lifetime of silence sometimes lies in the integrity of tiny inner ear proteins.

Before Marcos Sotomayor, Ph.D., began studying these proteins, very little was known about hearing at the molecular level. The Sotomayor Research Group, part of the department of chemistry and biochemistry at The Ohio State University, models the intricate structures of these proteins using Nanoscale Molecular Dynamics (NAMD) software run through the Ohio Supercomputer Center (OSC)'s Oakley Cluster. The group aims to more deeply understand the mechanics of hearing and what can impair it.

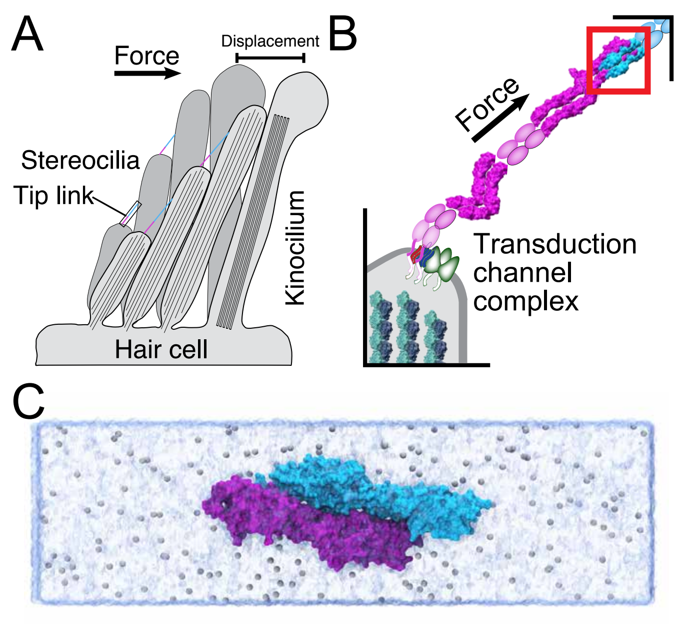
We experience sound when pressure from sound waves is transformed into an electrical signal sent to the brain. Vibrations push on tiny, hair-like structures in the cochlea called stereocilia, which are arranged in bundles. Each stereocilia is connected to its neighbors by protein filaments called tip links. When the stereocilia bend, the tip links stretch, opening an ion channel that allows potassium to flow into the cell, generating an electrical signal the brain interprets as sound. Hearing loss occurs when tip link proteins are mutated in hereditary deafness or when they stretch too far and break.

"If you go to a rock concert and put your ear next to the speaker, some tip links may break and your threshold for hearing goes up for a few hours, maybe a day, and the next day you recover, as tip links regenerate," Sotomayor said. "In some cases, a person's tip link proteins are mutated and tip links never form, leading to deafness."

To study tip link proteins more closely, Sotomayor's group puts the tip link protein DNA into bacteria to produce the protein. They then crystallize the proteins, which allows them to use X-ray crystallography to obtain the protein structure. This structure is then modeled and tested at length in computer simulations through the use of OSC. With the speed of HPC processing, researchers can stretch, break and test the proteins under certain conditions to observe their limitations and function.

"The details matter here," Sotomayor said. "Each atom is important. So that requires very large computations for long time scales, and in that sense, using Oakley has been really, really nice for us."

By gaining a basic understanding of the structure and function of tip link proteins, Sotomayor's work could have great potential in treating hearing disorders, such as hereditary deafness. •



▶ Sound mechanotransduction. (A) Inner-ear hair cells sport a bundle of stereocilia that deflects in response to sound-induced forces. (B) Tip links, made of two proteins named protocadherin-15 (magenta) and cadherin-23 (cyan) pull on mechanosensitive channels to elicit sensory perception. (C) Simulation of the "handshake" interaction between protocadherin-15 and cadherin-23 essential for hearing.

Project Lead: Marcos Sotomayor, Ph.D., The Ohio State University
Research Title: Molecular mechanisms of cadherin dynamics and force transduction
Funding Source: National Institutes of Health
Website: research.cbc.osu.edu/sotomayor.8

Botanical Alternatives

Cornish developing substitute for rubber shortfall

Sometimes numbers can be startling.

For instance, natural rubber is used in 50,000 commercial products, including 400 medical devices, because of its unique properties with regard to resilience, elasticity, abrasion and impact resistance, efficient heat dispersion and malleability at cold temperatures. It's a critical raw material that developed countries simply can't live without.

How about another number: 1.5 million, as in metric tons of natural rubber the U.S. may suffer in supply shortfall by 2020. That is unless Katrina Cornish, Ph.D., has anything to say about it.

The Endowed Chair and Ohio Research Scholar of Bioemergent Materials in the Department of Food, Agricultural and Biological Engineering at Ohio State is working to develop a domestic natural rubber crop—Taraxacum kok-saghyz, also known as TK, Buckeye Gold and the Rubber Dandelion—in Ohio and the U.S.

"Rubber is a critical raw material, and we should care about doing this because it will help prevent a catastrophic depression and an economy collapse in the developed world," Cornish said. "As we're able to produce (TK) on a commercial scale, we'll make hundreds of thousands of new jobs for the U.S."

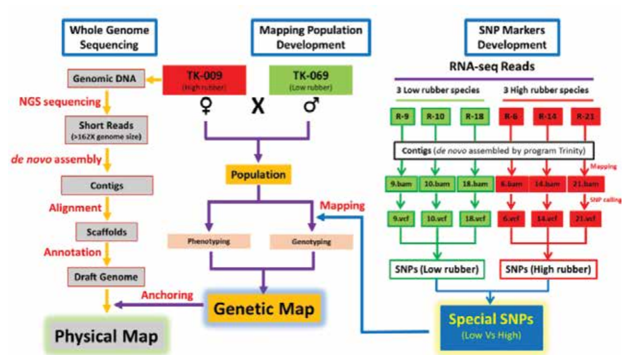
The dandelion rubber crop, a cousin of the common dandelion, is being investigated and developed as a supplement or replacement for certain types of imported natural rubber and produces high quality rubber for the rubber industry—especially tire manufacturers.

One of the key first steps to getting TK domesticated so it can be grown as a real crop is genome sequencing. TK is genome resource poor because of its large genome size and large fraction of highly repetitive DNA. That's where the powerful Ohio Supercomputer Center clusters come in.

"OSC is allowing us to assemble and annotate genomes as well as validate markers, and it's led to discovery," Cornish said. "Without OSC we would be terribly dead in the water."

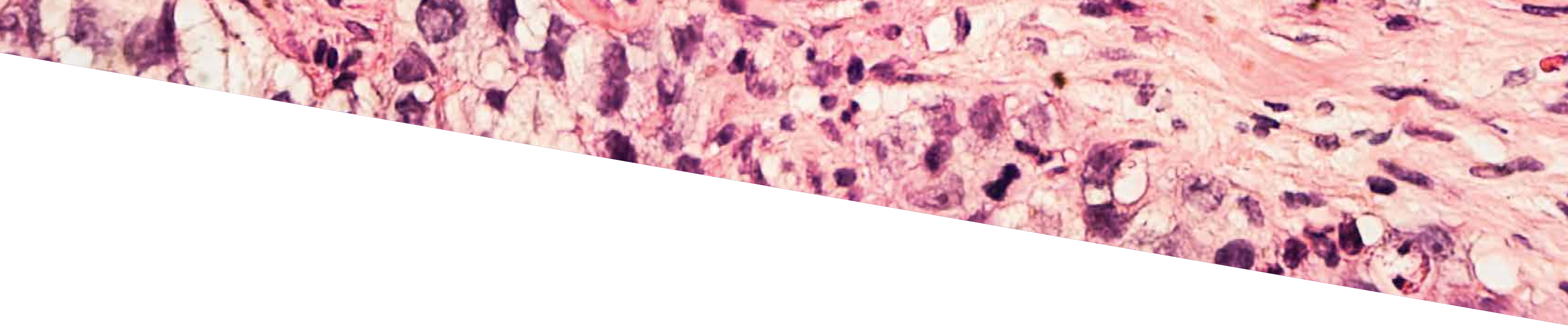
Cornish's project with OSC focused not only on genomic DNA and sequencing, but also an application of these resources to TK domestication and breeding.

"What we're developing are high-tech applications of the annotated genome for crop domestication," Cornish said. "If we look at wild TK plants and ask, 'What would we like it to be?' If it is something that can be edited, we can go to a relative and look for genes to modify and edit to produce the trait we want." •



The workflow diagram illustrates TK whole genome sequencing, mapping population development, and SNP markers development. The majority of bioinformatics analysis were executed through OSC resources.

Project Lead: Katrina Cornish, Ph.D., The Ohio State University
Research Title: TK whole genome sequencing
Funding Source: The Ohio State University
Website: cornishlab.cfaes.ohio-state.edu



Estrogen Receptors

Yang investigates signaling mechanisms' role in cancer

A critical first step oncologists must take after finding a patient has breast cancer is to look for overexpressed hormone receptors in the cancer cells.

This determines the type of therapy that will be used to most effectively combat the disease. While it is well known that point mutations of hormone receptors are associated with several types of cancer, still elusive is a mechanistic understanding of how these receptors function at the molecular level. Sichun Yang, Ph.D., assistant professor at Case Western Reserve University, is working to understand the signaling mechanisms of two critical domains in estrogen receptors, using computer modeling resources at OSC.

"We're going to come out with a structural model regarding how these molecular domains work together," Yang said.

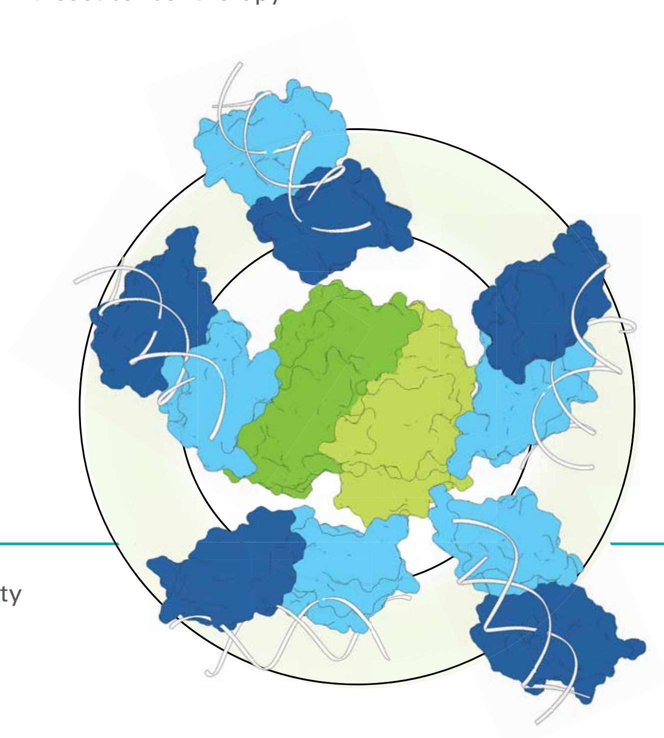
Estrogen receptors are proteins found on the surface of cells that receive signals from the hormone to direct activity within the cell. While they are critically important for healthy cells in regulating female reproductive functions, their presence in breast cancer cells work against the body. Nearly 75 percent of all breast cancers are estrogen-receptor positive, which means the presence of estrogen triggers tumor growth. To treat ER-positive breast cancer, doctors use hormone therapy to block estrogen from binding to receptors in the cancer cells, reducing their chance of survival and proliferation.

Yang's group focuses on two domains in ER that are essential for cell communication: one binds to DNA while the other binds molecules called ligands. The latter of the two is where a cancer drug would bind to the cell. Discovering how these two domains talk to each other could accelerate drug discovery for improved breast cancer therapy.

Yang's lab uses a hybrid approach in which computer simulations of the domains garnered from high-resolution structures (recently published at the Journal of Structural Biology; doi: 10.1016/j.jsb.2016.08.001) on OSC's Oakley and Ruby clusters are used to inform structural models in the lab. Driven by experimental discovery on ER, Yang's next step could mean the most to breast cancer patients.

"We're kind of excited in that we now have some ideas of how these molecules work, we're moving toward the next stage of drug discovery," Yang said.

The next step of a drug discovery project is to identify environmental substances that may have an effect in humans similar to an effect produced by a naturally occurring estrogen. This could predict highly promising substances for the design of improved breast cancer therapy. •



▶ Right: Sichun Yang's lab focuses on basic and translational studies of estrogen receptor (ER), a key molecule in breast cancer biology.

Project Lead: Sichun Yang, Ph.D., Case Western Reserve University
Research Title: Multifaceted modeling of estrogen receptor
Funding Source: National Institutes of Health
Website: theyanglab.org

Industrial Engagement

Businesses that thrive can do so in any number of ways, but it all ties back to leaders who are intelligent and innovative. Since the moment of its creation, the Ohio Supercomputer Center has strived to give manufacturers of all shapes and sizes the best tools needed to stay competitive, lean and at the forefront of their industry. How? By leveraging high performance computing and simulation-driven design, companies are able to access expertise and fine-tune their knowledge banks in support of rapid, cheaper development of consumer goods.

Valve Performance

Clippard, Kinetic Vision team up to eliminate flow inconsistencies

When your business is manufacturing valves, predictable and controlled fluid flow is essential. So when Clippard Instrument Laboratory Inc. encountered a proportional valve that wasn't delivering consistent performance, they knew they needed to take a closer look at the issue.

After reaching out to the Ohio Supercomputer Center's (OSC) AweSim program, they were able to do just that—down to the micron.

Doug Robertson, director of engineering at Clippard—a community-oriented company near Cincinnati—and his team initially approached AweSim to help the company segue into the world of high performance computing (HPC) modeling and simulation. Their original project was to predict the performance of a spring in one of their electromagnetic proportional valves. Ideally, the amount of fluid that flows through the valve is controlled by, and proportional to, the amount of electricity running to a solenoid coil that pulls on the spring. Early on, however, the test data on the prototype valve showed a nonlinear trend for flow versus electric current. This was inconsistent with the flow analysis of the computer-aided design (CAD) files of the valve.

In collaboration with AweSim partner Kinetic Vision, a Cincinnati-based engineering service provider, the team

▶ Using simulation through OSC's AweSim program, the team discovered a defect in the valve manufacturing process that allowed Clippard to ultimately produce a more efficient product.

Project Lead: Doug Robertson, Clippard Instrument Laboratory Inc.
Research Title: Spring response simulation
Funding Source: Clippard Instrument Laboratory Inc.
Website: clippard.com

▶ Clippard Instrument Laboratory Inc. has been manufacturing industrial equipment in Cincinnati since 1941.

took a two-pronged approach to finding what was causing the discrepancies between the performance of the physical valve and the computer model.

"One thing we did for them was nondestructive inspection," said Jeremy Jarrett, vice president at Kinetic Vision. "We also helped with finite element analysis. It was really the blend of those two things together which really helped them solve their problem."

By first performing an industrial computed tomography (CT) scan of the assembled valve, the team compared the prototype with the computer model of the valve. They then built a finite element model from the industrial CT scan. From this model, they found that the problem was not with the computer design of the valve, but in the manufacturing process Clippard was using.

"It became obvious that our machine surface was not the shape that we thought it was and that we had asked our computer-controlled machines to (manufacture) for us," said Rich Humason, engineering manager at Clippard.

Because the CT technology scans the entire assembled valve, Kinetic Vision was able to provide Clippard with complete imaging of the entire valve, every piece down to a micron-level view. Thanks to the results provided through modeling and simulation and a quick turnaround, the Clippard team was able to make changes in their computer translation to correct the issue and manufacture a better product.

"The depth, detail and the granularity of this information—they're able to really inspect their parts after they're put together," Jarrett said. "We're actually measuring these parts as they're assembled so they can really see what's going on with the component in its operating state."

As an AweSim charter partner, Kinetic Vision's engineering experts perform their intricately detailed analyses, scans and inspections through OSC resources.

"Having the supercomputer at your disposal makes this type of methodology possible," Jarrett said. "We are solving high fidelity finite element models directly generated from microCT data—it really helps enable that technique to even happen because the models have to be much more detailed."

Since the valve solution, Clippard has developed new methods to measure their material surface, improving processes from initial computational design to the finished product. According to Robertson, modeling and simulation has saved the team valuable time and resources.

"There's no doubt we're sold on simulation," Robertson said. "I'm not sure if we ever really would have put our finger on that as specifically as we were able to without that simulation in our hands." •

Energy Generation

First Solar optimizes semiconductor properties in crystalline structures

The performance of semiconductor devices such as solar cells, detectors, etc., depends strongly on the properties of materials used in their fabrication.

Deep understanding of these properties and the ability to tune them is critical for the development of new generations of advanced photovoltaics and electronics. First Solar, the world's largest manufacturer of thin-film solar panels, is using resources from the Ohio Supercomputer Center (OSC), to predict and optimize semiconductor properties in crystalline structures such as cadmium telluride (CdTe).

Although the efficiency of commercial CdTe photovoltaic material has grown dramatically in recent years, the advances in performance and stability of CdTe devices are achieved mostly through costly experimentation and process development while lacking theoretical guidance.

"Our research is aimed at theory-driven understanding and optimization of CdTe-based solar cells performance and stability for clean energy generation," said Dmitry Krasikov, development engineer at First Solar.

CdTe semiconductor, used for decades in X-ray detectors, has recently become the material of choice for the multi-gigawatt-per-year, thin-film photovoltaic industry. The semiconducting properties of CdTe is determined by the structures of pure crystals and imperfections, or defects. While the word "defects" often carries negative meaning, it is the defects in CdTe that make them useable in practical applications.

Though CdTe crystals always contain some intrinsic imperfections, engineers can intentionally introduce defects to give semiconductors unique, application-specific properties. The concentrations of defects and their positioning in the device structure define the electrical behavior of the device. These depend strongly on the process conditions, such as annealing temperatures, quenching rates and field operation conditions. Concentrations, spatial distributions and charge states of defects can change as a results of different diffusion, reaction and ionization processes. To understand and describe these processes, engineers first need to know the fundamental parameters of defects and reactions.

First Solar uses theoretical calculations of the parameters of defects and reactions, such as defect formation energy, reaction energy and energy barriers of elementary processes, to feed the models describing the formation and evolution of defect concentrations and recharge of the defects. These accurate, state-of-the-art methods require considerable parallel computational resources to treat systems large enough within a reasonable time frame.

"This is why we are using OSC supercomputer resources in our work," Krasikov said.

Through First Solar's research and development, their large-scale solar farms can deliver energy to utilities at prices that are lower than fossil fuels. •

▶ Above: To date, First Solar has sold 13.5 gigawatts worth of solar panels, enough to power more than 2 million homes in the United States.

Below: First Solar's factories produce solar panels at a rate of approximately one every second.

Project Lead: Dmitry Krasikov, First Solar
Research Title: Optimizing semiconductor properties of cadmium telluride for solar cell application
Funding Source: First Solar
Website: firstsolar.com

Component Analysis

ANSOL adopts cluster computing to enhance analysis, boost business

Advanced Numerical Solutions (ANSOL) is proof the industrial engagement efforts of the Ohio Supercomputer Center (OSC) are quite beneficial to the "little guy."

ANSOL is a small consulting software company located in Hilliard, Ohio, just outside of Columbus. The company writes special software for finite element analysis (FEA) of gear boxes and transmissions for large automotive and aircraft companies, such as Boeing, GM and Ford, to name a few.

Since 1988, ANSOL has worked with OSC, but recently amped up its usage as it gets pushed by its clients to make sure it's using the fastest computers possible.

"There's no way we could compete with bigger companies if it weren't for OSC," said Sandeep Vijayakar, Ph.D. president at ANSOL. "Having a cluster of our own is not in the realm of possibility for us. A large company can afford that.

"All the mathematics are implemented by us but we do need the compilers, debuggers, profiling tools, etc., so there's a bunch of tools at OSC we use to speed up the program."

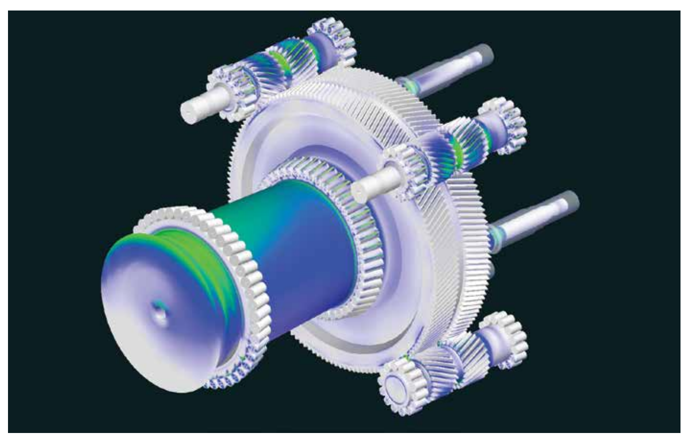
As companies continue to want more and more analyzed, ANSOL's models have become significantly bigger, causing challenges that need to be addressed now rather than later.

"People have been throwing everything into the computer models, and we've reached the point we can't do some of these models in single computers anymore; that's why we've been trying to get our software to work on clusters," Vijayakar said. "A lot of our customers have supercomputers of their own, but it takes a lot of work to convert a standalone computer program to a parallel one."

To help with this, ANSOL recently received a grant from NASA to start a feasibility study to move the company's software into a cluster environment. That started recently with small examples run on OSC's Oakley Cluster.

ANSOL's proposal to NASA was to create a new computational method for generating the data needed to create decision-making strategies for condition-based monitoring algorithms that can differentiate between a healthy system or a defective or damaged system. The only means available for this currently are physical testing, which is expensive and time-consuming.

"It's going to allow us to do things that were simply not possible before," Vijayakar said. "Once this works out, there will be a lot of projects coming from our existing customers." •



► ANSOL writes special software to perform finite element analysis of gear boxes and transmissions for large automotive and aircraft companies. That software provides uniform 3D finite element analysis for all components of a gear box, including the bull gear (above) and power takeoff unit (top).

Project Lead: Sandeep Vijayakar, Ph.D., Advanced Numerical Solutions LLC
Research Title: Transmission and gear box development for automotive and aerospace companies
Funding Source: Advanced Numerical Solutions LLC, NASA
Website: ansol.us

E-commerce Marketplace

Nimbis develops access strategies to promote modeling, simulation

Nimbis Services Inc., a charter partner of the AweSim industrial engagement initiative led by the Ohio Supercomputer Center (OSC), has been delving into access complexities and producing, through innovative e-commerce solutions, an easy approach to modeling and simulation resources for small and medium-sized businesses.

"Nimbis is providing, essentially, the e-commerce infrastructure that allows suppliers and OEMs to connect together in a collaborative form, where they can do joint product development or share tools, applications, libraries, licenses, etc.," said Bob Graybill, Nimbis president and CEO. "AweSim represents a big, giant step forward in that direction."

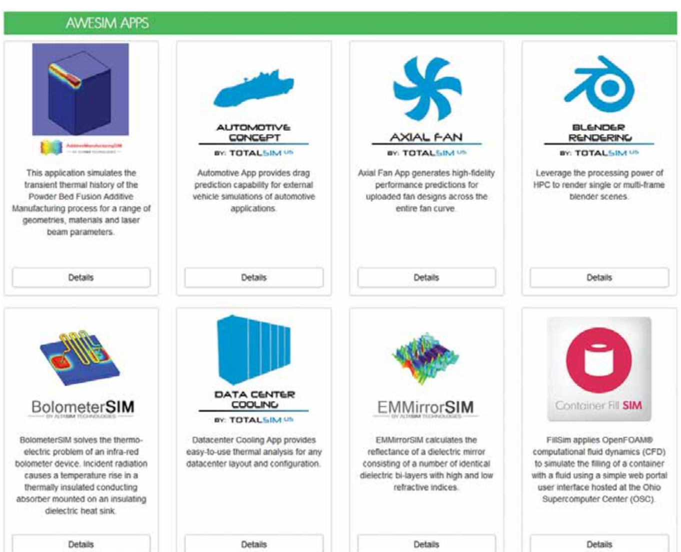
The AweSim program, and its predecessor program Blue Collar Computing, have identified several obstacles that impede widespread adoption of modeling and simulation powered by high performance computing: expensive hardware, complex software and extensive training. In response, the public/private partnership is developing and promoting use of customized applications (apps) linked to OSC's powerful supercomputer systems. These apps mask many of the inherent intricacies behind web portals created with partnering engineering service providers (ESPs).

"We have successfully created an e-commerce marketplace that is both intuitive and user-friendly," Graybill explained. "However, users must be willing to use it. Unfortunately, a lot of small and medium-sized manufacturers are not ready, or they simply don't feel comfortable with engineering e-commerce sites. Sometimes they need the confidence and wisdom that comes from an ESP standing with them to actually get started using modeling and simulation."

From a technical perspective, e-commerce sites have been around for a while. In the mid-1980s, Compuserve offered one of the first examples of e-commerce as we know it today—the Electronic Mall; a service where users could purchase items directly from 100+ online merchants. Amazon and eBay transformed e-commerce in the mid-1990s, and online sales in the United States are expected to reach $335 billion in 2016.

"There's a major difference between what we have done and what's 'generically' available out there," said Graybill. "Ours is not static. It has to interface with OSC's dynamic computing resources on the backend, monitor resources consumed, manage licenses, provide secure connect connections, and we make it all as transparent as possible for the end-user."

Nimbis is already pushing ahead on their next challenge—developing cloud-based collaborative communities of interest with embedded marketplaces targeting manufacturing supply chains, DoD trusted microelectronics and collaborative research institutes initiatives. •



▶ A screenshot shows only a few of the many apps that have been made available through the AweSim e-commerce marketplace that Nimbis developed in collaboration with the Ohio Supercomputer Center and the AweSim industrial engagement program there.

Project Lead: Robert Graybill, Nimbis Services Inc.
Research Title: Developing a collaborative e-commerce marketplace for HPC-powered modeling & simulation
Funding Source: Ohio Third Frontier program
Website: awesim.org

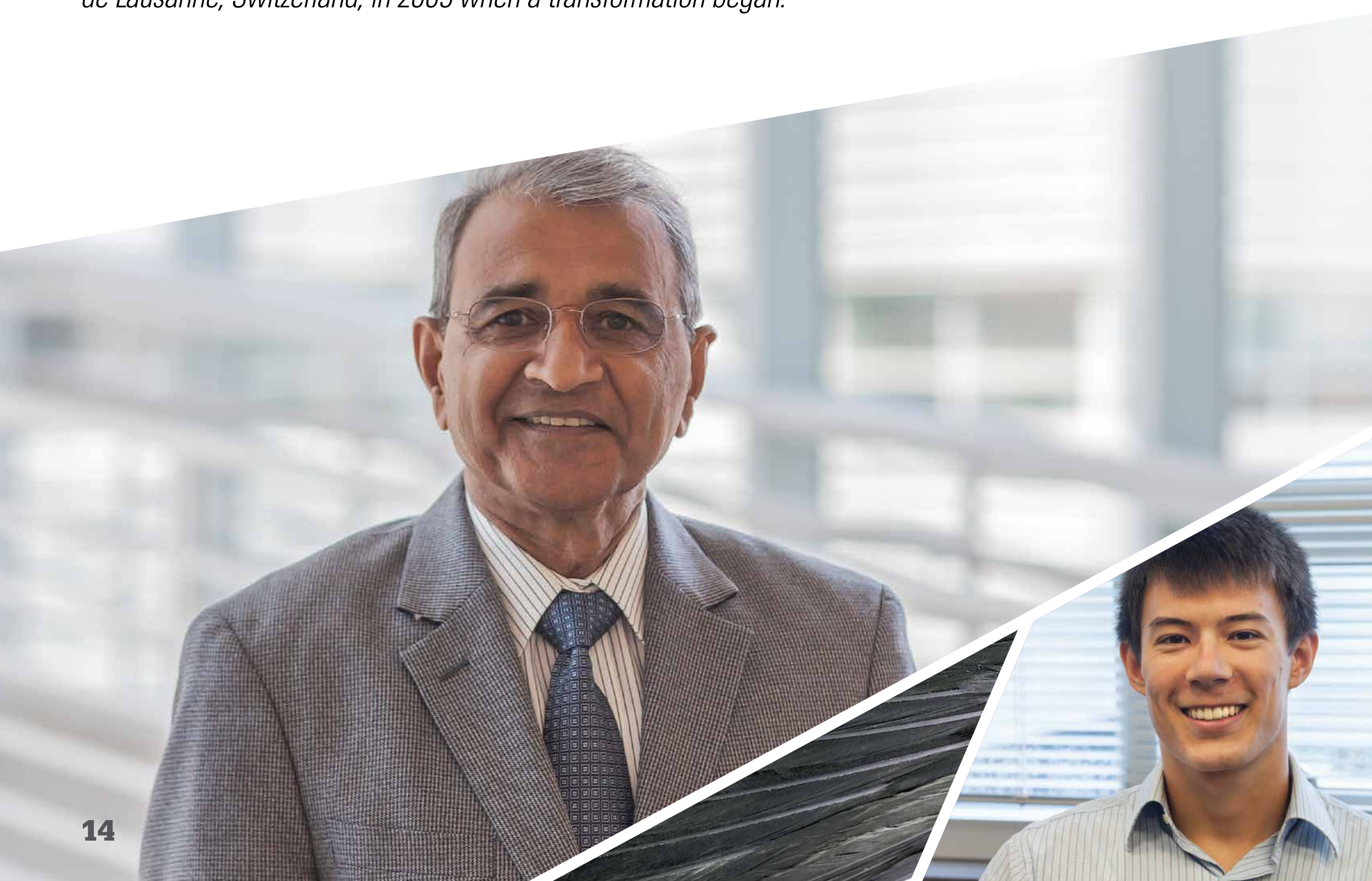
Advanced Materials

How can shark skin make cars cruise more efficiently? How can explosives help us invent more useful, environmentally safe products? Can molecules be introduced to polymers to expand their use in our daily lives? And, speaking of explosives, are we close to unlocking the secret to safer variations? Computational science investigations conducted on powerful Ohio Supercomputer Center systems are helping researchers in business and academic labs crack these difficult questions.

Drag Reduction

Bhushan studies bird beaks, shark skin to glean answers from nature

Bharat Bhushan, Ph.D., was on sabbatical at École polytechnique fédérale de Lausanne, Switzerland, in 2005 when a transformation began.



After reading an article in a trade magazine on the lotus leaf's water repellant properties, Bhushan's industrial research launched down a greener, livelier new path.

"I became fascinated," said Bhushan, Ohio Eminent Scholar and the Howard D. Winbigler Professor in the Department of Mechanical and Aerospace Engineering at The Ohio State University. "That article and my research in this area have transformed me from a science geek to a nature lover."

Prior to 2005, Bhushan never dreamed he'd be studying lotus leafs or geckos or sharks or black skimmer birds, nor that supercomputers would help him do it all.

"I've been a beneficiary of the Ohio Supercomputer Center (OSC) for a long time; many of the things we're doing wouldn't be possible without it," Bhushan said. "I'm an engineer by trade and had worked in various science and technologies prior to 2005 but had not done anything related to nature to that point."

Bhushan was looking for surfaces that repel water and reduce friction, a major problem in the industry in which he had been involved. It turned out, nature had answers.

"Nature provides a wealth of information and uses basic materials," he said. "We're not trying to mimic nature, but we like to be inspired by nature."

Recently, Bhushan's research has focused on black skimmer birds and shark skin to understand drag reduction. For the first time, he discovered that the beak of black skimmers can reduce drag in water as reported in a Philosophical Transactions of the Royal Society paper in August 2016. Black skimmer birds are the only birds known to do fly fishing, in which they soar just above water and dip their beaks in to grab fish. Sharks, meanwhile, have skin perfectly evolved for drag reduction to cut through water at high speeds.

The secret to both black skimmer birds' beaks and shark skins lies in the riblet structures that contain microgrooves aligned in the direction of fluid flow, allowing water to move efficiently over the surfaces. Studies have shown these riblet structures allow for drag reduction by controlling the vortices formed in turbulent flow.

This feature results in a drag reduction up to 10 percent when compared to even a smooth, flat surface. Bhushan's lab uses computer modeling to explore drag reduction, dimensions of vortices and segmented riblet surfaces. Understanding these drag-reduction properties could improve air flow over cars and aircraft or fluid flow through pipelines for a more efficient transfer of oil, gas and coal.

To understand how riblet structures and vortices reduce drag, Samuel Martin, a Ph.D. candidate and co-author on Bhushan's recent study, performed computer simulations on OSC's Glenn and Oakley clusters.

"Each simulation has a slightly different riblet geometry, such as different spacing or height," Martin said. "By running simulations I see how water flows over these riblets and how the drag or the vortex formations are in these models and how riblets reduce drag."

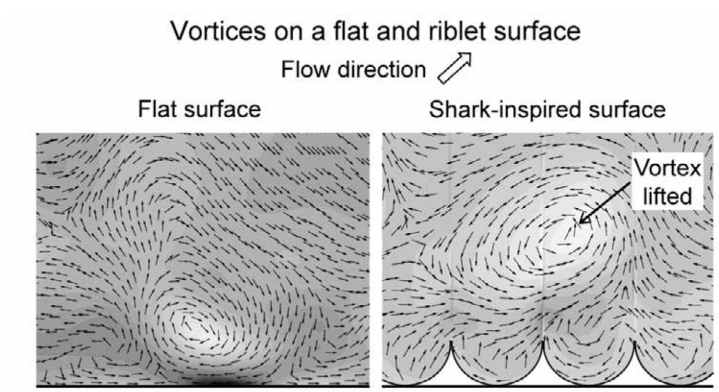
Martin creates numerous models to analyze riblet spacing, and each model needs to run for a long time to see how well the average drag performs.

"On a cluster, I can run multiple jobs parallel and get more data quickly," Martin said.

Bhushan said without supercomputing capabilities the work couldn't be done, but because it can, the clues he's unlocking could be invaluable.

"Nature has 10 million species and each one has a unique structure that provides functionality we can use to our advantage," Bhushan said. "It's exciting to know what nature has to offer." •

▶ Left: Bharat Bhushan, Ph.D., The Ohio State University; Inset: Samuel Martin, a Ph.D. candidate and co-author



▶ Computer simulations on OSC's Glenn and Oakley Clusters showed how riblet structures and vortices found on the beaks of black skimmer birds and sharks reduce drag. Each simulation had a slightly different riblet geometry with regard to spacing and/or height, creating the need for numerous models to analyze the riblet spacing.

Project Lead: Bharat Bhushan, Ph.D., The Ohio State University
Research Title: Computational modeling to explore drag-reducing geometries inspired by biomimetics including black skimmer and shark skin
Funding Source: The Ohio State University
Website: nlbb.engineering.osu.edu

Electrolyte Design

Hall group pursues knowledge that will lead to advanced polymers

To enable the rational design of future materials, such as batteries that could more safely and efficiently power electric cars, a research group at The Ohio State University is developing an innovative modeling approach to reveal the details of the microscopic structure and dynamics in microphase-separated polymer electrolytes.

"Safe batteries of high energy density and low cost are an underlying requirement to meet multiple societal needs, such as reducing carbon and pollutant emissions by switching to electric cars," said Lisa Hall, Ph.D., the HC Slip Slider Professor of Chemical and Biomolecular Engineering at Ohio State.

"This has driven research into solvent-free, non-flammable battery electrolytes in recent years," Hall said. "Such electrolytes are inherently safer in case of battery failure or damage. Certain microphase-separated polymer electrolytes would also save weight, because they are mechanically robust enough to be used in conjunction with a solid lithium electrode—one-tenth the weight of a typical graphitic electrode."

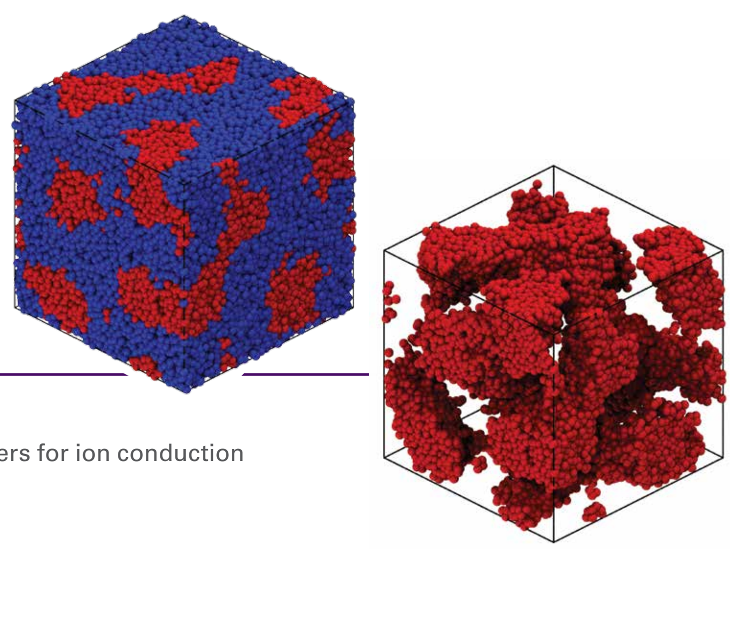
However, Hall points out, ion conductivity of these polymer electrolytes is lower than that of conventional electrolytes, a feature that impedes their adoption in batteries. It remains unclear how to adjust the many material parameters to improve conductivity, in part because the mechanism of ion conduction is not well understood.

Using simple models, we can build a general picture of how salt and tapering affects microphase separation and ion conduction across the whole class of microphase separating polymers. This can yield general guidelines for how to choose future materials, in contrast to atomistic simulations, which would show a detailed picture of one or a few particular chemical systems. Additionally, the time and length scales of interest in these systems would be difficult or impossible to reach using fully atomistic simulations or other very detailed modeling. Therefore, we propose to create, test, and use what we conceive of as the simplest possible microscopic models that accurately describe microscopic morphology and ion transport in salt-doped microphase separated polymers.

In moving to a salt-doped system, we need a model with more detail than SCFT and that includes local packing effects. We have already implemented such a model in both fDFT and MD (as is a major component of the proposed work, except without salt) and compared the resulting density profiles as a function of taper length.

This work will create, optimize, and use simple models of neat and salt-doped microphase separating copolymers. In contrast to prior work, this model will both include long-ranged electrostatics and show the details of ion dynamics and conduction in such materials. Additionally, we will study for the first time how tapering the copolymer composition between the blocks changes the phase diagram and the location of ions within the microphase separated structure and the effects of this on ion conduction. Besides the interest in using tapering as an additional control variable to allow optimization of material properties, the change in the interface as a function of tapering will allow this work to develop a better scientific understanding of the effect of the interface on conduction (versus considering only pure diblock materials).

Thus we expect to elucidate the major mechanism of ion transport and how it depends on the morphology. The models' results along with comparisons with other theory and experiments will significantly broaden our knowledge of the morphology, thermodynamics, and dynamics of microphase separated polymer electrolytes and suggest new polymers to be used in improved electrolytes in the future. •



► Right: The "double gyroid" structure shown in this simulation is a desirable structure because regions of both chemical types of polymers (red and blue in the first image) are continuous in three dimensions. The second image is the same structure with the blue regions made invisible.

Project Lead: Lisa Hall, Ph.D., The Ohio State University
Research Title: Simulation and theory of tapered diblock copolymers for ion conduction
Funding Source: National Science Foundation
Website: hallgroup.engineering.osu.edu

Glass Transition

Simmons seeks understanding of molecule additives on polymers

One of the grand challenges in materials science is discovering exactly how materials form glasses.

David Simmons, Ph.D., an assistant professor in the University of Akron's Department of Polymer Engineering is trying to understand at the fundamental level the relationship between the molecular structure and the way a material forms a glass.

"There's a big-picture fundamental challenge in polymers, and in a lot of other materials, which is the question of how these materials solidify through a process known as the glass transition," Simmons said. "This is a process in which they go from a melt or liquid to a solid without crystallizing. So unlike a metal or a diamond, they don't have this beautiful lattice structure on the molecular side—they look disordered and yet they seem solid."

After 50 or even 100 years of studying this problem, it's still not understood why this happens. Using the Glenn Cluster at the Ohio Supercomputer Center to perform a massive number of simulations, Simmons' project "Tuning glass formation with molecular additives" aimed at gaining understanding into this age-old question.

"What this project focuses on is how can we rationally and efficiently choose a molecule we can introduce to a polymer to widen its use range," Simmons said. "Imagine you're making some massive amount of a polymer and it softens at 80 degrees Celsius and you want to use it for some application, like cooking, at a higher temperature. How do you do that?"

The choices include either the very expensive path of making a new polymer, or modifying what's already there to get it to stay solid at a higher temperature while keeping it processable.

"The purpose of this project is to use computer simulations to understand how we go about designing molecules to add to a polymer to tune its properties so we can use it for more applications without dramatically increasing the cost," Simmons said.

Simmons' project required simulating 50 to 100 different temperatures using a software called Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) with each simulation based on a different time scale.

"We're doing multiple replicas for statistics and then we might be doing 50 or 100 different molecular structures so we can learn trends," Simmons said. "So we do tens of thousands or hundreds of thousands of simulations so it becomes necessary to have access to large-scale supercomputing resources." •

▶ Inset above: A polymer melt containing stiff oligomeric additives that tune its glass transition. The glass transition is how a material forms a glass, it's a process in which materials go from a melt or liquid to a solid without crystallizing. Unlike a metal or a diamond, glass doesn't have a lattice structure on the molecular side—they look disordered and yet seem solid.

Project Lead: David Simmons, Ph.D., University of Akron
Research Title: Tuning glass formation with molecular additives
Funding Source: Keck Foundation, National Science Foundation Division of Materials Research
Website: blogs.uakron.edu/simmonsgroup

Industrial Explosives

Ball estimates molecular energy to improve efficiency, greenness

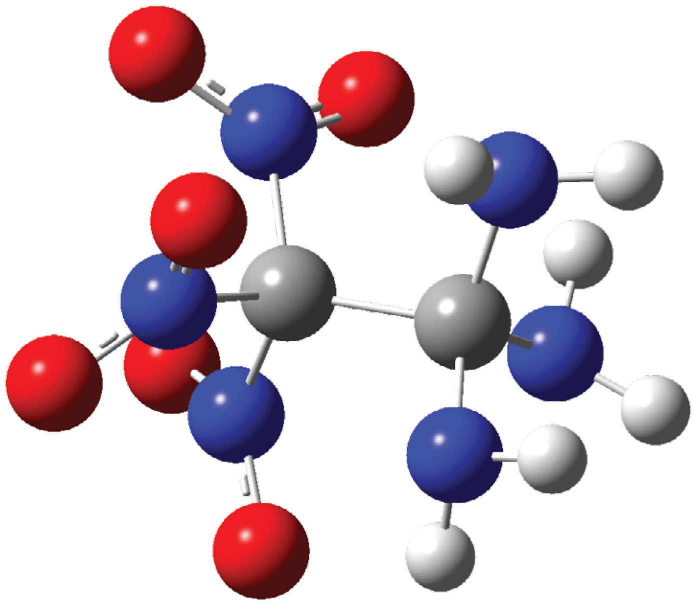
Alfred Nobel, namesake of the Nobel Prizes, was originally known for inventing dynamite, though not fondly, as he found out.

When his brother died, a newspaper erroneously reported Alfred's death. The obituary chided him for his invention that, especially at that time, often proved deadly. Afforded a rare glimpse of his potential legacy, the wealthy Nobel established the Prizes to ensure scholars are remembered for their positive contributions to society, as he wanted to be.

Over a century later, Cleveland State University's chair of the Department of Chemistry is working to ensure Nobel's invention is not only remembered, but continually improved. David Ball, Ph.D., is using OSC resources to calculate the thermodynamic properties of molecules for the application of new high energy density materials—or, put plainly, explosives.

"(OSC) is a great resource for the state of Ohio," Ball said. "It allows people who might normally not be able to have access to this kind of resource access to a modern computational facility where we can do cutting-edge work."

An explosion occurs when unstable molecules undergo a chemical reaction to create stable reaction products. In the case of high-nitrogen molecules, one reaction product is nitrogen gas, an energetically stable molecule. Other stable products include water and carbon dioxide. If a molecule has the right mix of carbon, hydrogen, oxygen and nitrogen, it can rearrange to create these stable products.



▶ Should it ever be synthesized, 1,1,1-triamino-2,2,2-trinitroethane (TTE) should give off 40 percent more energy than TNT, OSC-based calculations predict.

"In doing so, it gives off a lot of energy," Ball said. "That's where we get the energy from our fuels, that's where we get the energy from our explosives."

Explosives and similar fuels used for construction, military applications and as propellants give off huge amounts of energy when they decompose. Ball's group uses nodes on Oakley to estimate the energy of a given molecule and compare it to the energy of the decomposition products. The result is the amount of energy a molecule can potentially give off when it explodes.

The basic concepts of explosives are relatively simple; Ball and his students are evaluating the overall energy of these molecules in respect to possible reaction products to create more efficient, and possibly cleaner high energy density materials. Many products of these reactions are greenhouse gases. If the molecules can be rearranged into a product that's more efficient, not only will the fuels and explosives themselves be more useful in industry, but the environment as a whole will be better off as well—presumably what Nobel would have wanted. •

Project Lead: David Ball, Ph.D., Cleveland State University
Research Title: Investigations into high energy density materials, cage molecules and doped metal surfaces
Funding Source: Cleveland State University
Website: facultyprofile.csuohio.edu/csufacultyprofile/detail.cfm?FacultyID=D_BALL

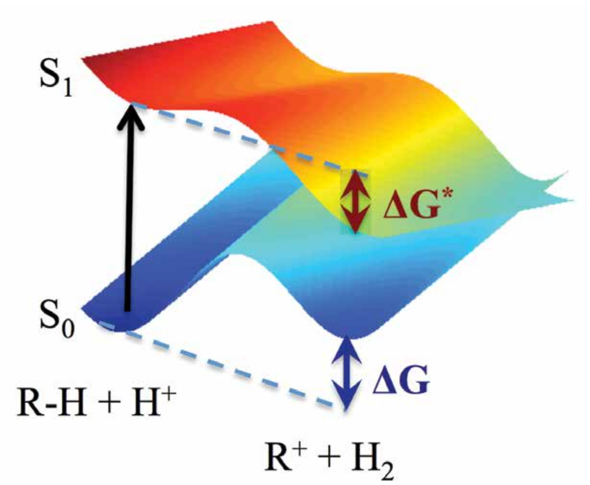
Energy

Today's world requires precision. It's not enough to build an electric car if nobody can find a charging station when they need one. For those who don't have an electric car, a sparkling engine under the hood is great, but how do we get it to run at an efficiency never thought possible? While we're on the subject of efficiently using petroleum, the fact is all fossil fuels will run out at some point, and solar fuel may just be the alternative. Researchers have turned to the Ohio Supercomputer Center to find smart ways to make for a better world tomorrow.

Solar Fuel

Glusac group considers sunnier alternative to petroleum-based energy

Consumption of energy is increasing worldwide due to the steady increase in the human population and the long-term growth of the international economy.



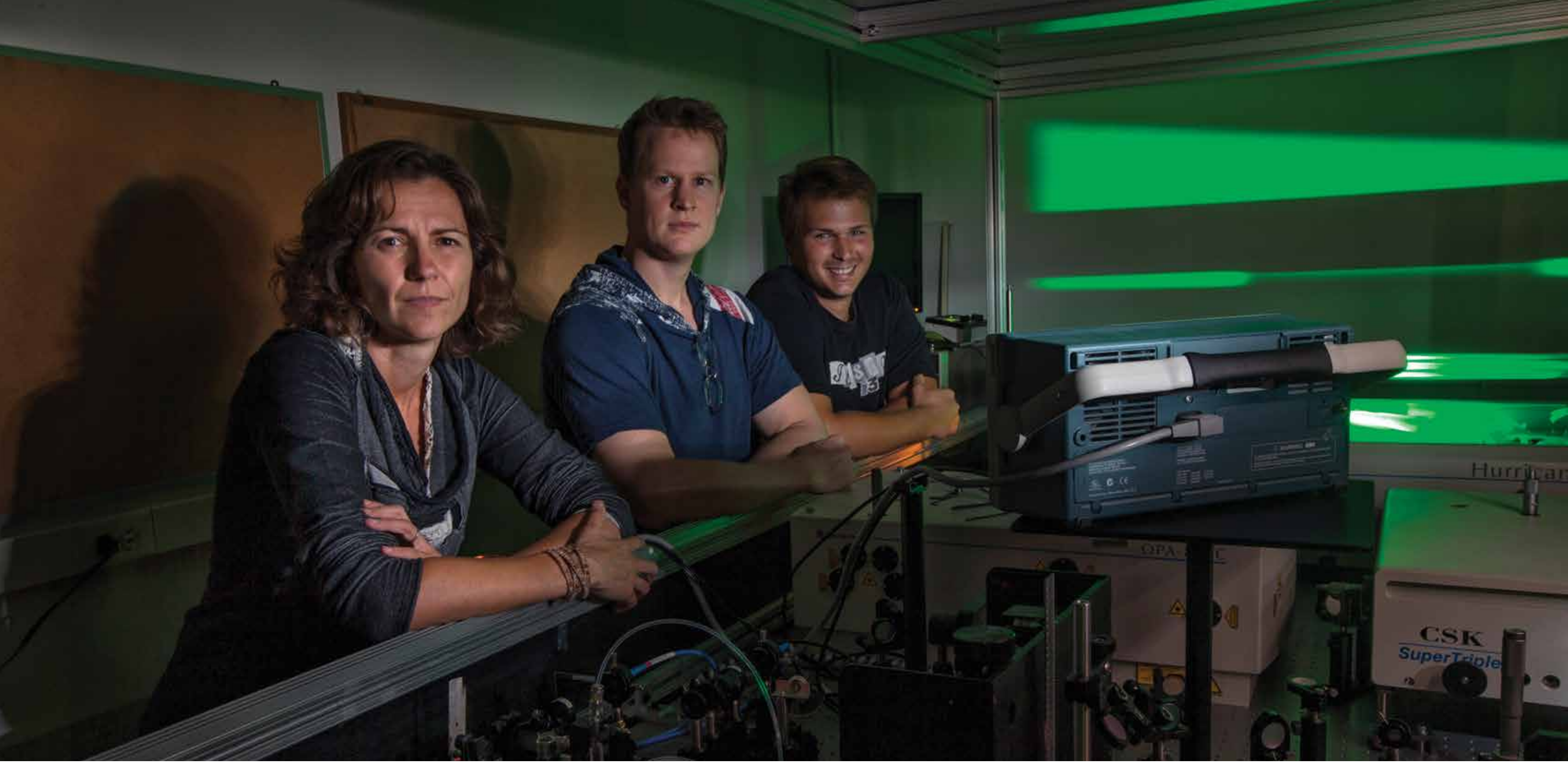
Above: In order to achieve a wider implementation of hydrogen-evolving catalysts in solar fuel production, Ksenija Glusac's research group is focusing on catalysts made of more earth-abundant elements. This graphic illustrates the calculated ground and excited-state thermodynamic driving forces for proton reduction by several organic hydride donors.

A group of researchers at a northwestern Ohio science lab have been leveraging Ohio Supercomputer Center services to investigate solar-based fuel production as a sustainable alternative to fossil fuels.

A solar fuel is an energy source produced from sunlight by way of artificial photosynthesis or thermochemical reaction. Solar fuel can be produced and stored for later use, providing energy in the evenings or on cloudy days when sunlight is not available, making it an attractive potential alternative to petroleum and other fossil fuels.

"The main energy sources used nowadays—fossil fuels—are not a good solution to our demands, because the fuel reserves are expected to dry out in several hundreds of years and the build-up of atmospheric carbon-dioxide produced from fuel causes serious environmental problems, such as global warming," said Ksenija Glusac, Ph.D., an associate professor of chemistry at Bowling Green State University. "One of the most promising alternative energy sources is light from the Sun, which we can use to split water molecules into hydrogen—a fuel—and oxygen."

Project Lead: Ksenija Glusac, Ph.D., Bowling Green State University
Research Title: Towards organic photohydrides: Excited-state hydride release in metal-free models
Funding Source: National Science Foundation, American Chemical Society, Bowling Green State University
Website: bgsu.edu/photo/glusac



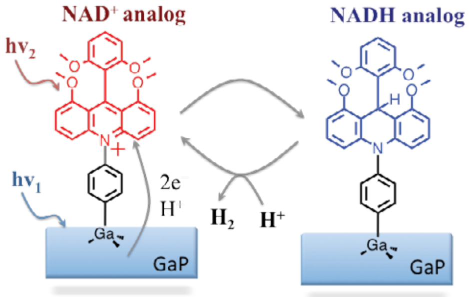
The process requires catalysts to initiate the oxygen and hydrogen-evolving chemical reactions, and the elements currently known for their water-splitting qualities are among the rare and costly transition metals. Some of the most commonly used transition metals for this process are iridium and ruthenium oxides for water oxidation and platinum for water reduction, because they bind the key catalytic intermediates in an optimal way, not too weakly yet not to strongly.

In order to achieve a wider implementation of hydrogen-evolving catalysts in solar fuel production, Glusac's group is focusing on catalysts made of more earth-abundant elements, such as carbon, hydrogen, nitrogen and oxygen. These catalysts are inspired by the naturally occurring cofactors, namely nicotinamide adenine dinucleotide (NAD^+) and its reduced variant (NADH), which perform similar reduction processes in our bodies.

"Our research is at the interface between organic and physical chemistry, and we accordingly use techniques common to both of these fields," said Glusac, whose research team is based at the university's Center for Photochemical Sciences. These techniques include a number of laboratory experiments, known as in-vitro studies, as well as computer simulation experiments, known as in-silico studies.

Computational screening of potential photohydrides is an important part of the study. Glusac's group employs a simple quantum mechanical modeling approach, known as the density functional theory (DFT) method, on OSC's HP/Intel Oakley Cluster to calculate the relevant thermodynamic parameters for the ground and excited-state hydride transfer reactions. An excellent match was obtained between the calculated and experimental values for several organic hydride donors; the researchers are now applying the methodology to a large series of model photohydrides and evaluating possible candidates for experimental studies.

If successful, this project will provide new guidance on the conversion of abundant energy from the Sun to sustainable fuels and value-added chemicals, thereby providing alternatives to the limited reserves of problematic petroleum-based sources. •



Above: Glusac's group is focusing on catalysts made of more earth-abundant elements, such as carbon, hydrogen, nitrogen and oxygen. These catalysts are inspired by the naturally occurring cofactors, namely nicotinamide adenine dinucleotide and its reduced variant.

Above: Glusac's group is seeking a more efficient conversion of abundant energy from the Sun to sustainable fuels and value-added chemicals. Here, she pauses for a moment in the lab with Stefan Ilic, a research assistant in chemistry, and George Hargenrader, a graduate assistant in chemistry.

Charging Stations

Sioshansi studying distribution of the electric car power system

When considering an electric vehicle, many motorists encounter a paradox: they would be willing to make the leap if there was more of a support infrastructure for them.

Conversely, investors might loosen the purse strings to fund electric vehicle infrastructure, such as charging stations, if more people drove them. To help both ends, Ramteen Sioshansi, Ph.D., associate professor of integrated systems engineering at The Ohio State University, is studying the efficiency and optimal locations of electric vehicle charging stations. He has developed a simulation technique using high performance computing at the Ohio Supercomputer Center to find control strategies for electric power system distribution.

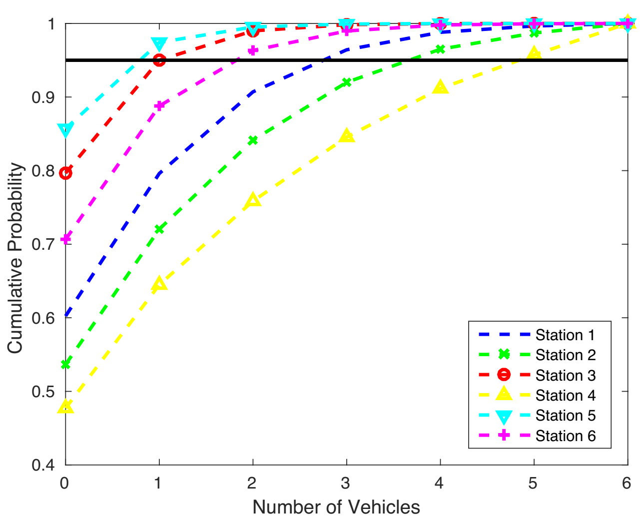
"Ultimately, in some sense, you have to start somewhere," Sioshansi said. "If you're just building a small handful of stations, and you're doing it to try to eliminate that barrier to people buying electric vehicles, you want to do a good job of deciding where to put them."

Luckily for Sioshansi, the Mid-Ohio Regional Planning Commission had data sets that modeled typical driving patterns in central Ohio. Sioshansi studied the location of vehicle concentrations at different times of day, assuming a random one percent sample of vehicles were electric.

"We did lots of scenario generation where we kept resampling the one percent out of there," Sioshansi said. "That made the model actually quite large, and so that's what having an HPC system was useful for."

With charging locations determined, the next question is: how much load can electric distributors handle? A fast-charging station for electric vehicles can put out 150 kilowatts (comparatively, a wall outlet is 1 to 2 kilowatts). To offset the energy drawn through the distribution feeder, one option is a rechargeable battery; another is solar panels. However, Sioshansi's group found that by effectively managing the charging load, simultaneously charging multiple vehicles is possible without overloading power circuits. For example, if a vehicle is parked at a charging station in a grocery store parking lot and only needs to charge for 15 minutes out of the 30 it will be parked, that load can be transferred to another vehicle that also needs to be charged.

"That's a nice finding," Sioshansi said. "As long as there is a small controller in the charging station, there's not all this added cost of having to put batteries or solar panels or things like that or do expensive upgrades on distribution transformers to manage the load." •



► Above: Ramteen Sioshansi, Ph.D., processes huge amounts of driving data through OSC to determine the optimal locations for electric vehicle charging stations, using central Ohio as a test market.

Left: A graph showing the cumulative probable number of vehicles near particular charging station locations.

Project Lead: Ramteen Sioshansi, Ph.D., The Ohio State University
Research Title: Electric vehicle fast-charging station with photovoltaic system
Funding Source: Department of Energy and National Science Foundation
Website: ise.osu.edu/isefaculty/sioshansi

Electron Processes

Dunietz lab researching charge-transfer mechanisms

A research group at Kent State University is investigating key processes in material science at a very fundamental level.

The computational group led by Barry Dunietz, Ph.D., provides molecular-level insight into charge-transfer processes through various molecular interfaces to understand the structure effects on the motion of electrons. Through computational simulations and the development of models using the Ohio Supercomputer Center's Oakley Cluster, the group investigates electron transport and transfer processes. This information can be used to focus experimental efforts to develop material and devices used for high efficiency photovoltaic and thermoelectric applications.

"My lab is solely computational," Dunietz said. "But definitely some of the work done on the supercomputer was done with very specific experiments in mind. Sometimes the calculations have provided a new molecular level understanding that inspired a different interpretation of the measurements than was offered originally."

While the charge-transfer process—the movement of electrons within and between molecules—is one of the most studied phenomenon in materials science, it can be unpredictable, as it is strongly affected by a wide range of parameters, including molecular structure, environment and temperature. To improve the efficiency of these reactions, the Dunietz group is gaining a molecular-level understanding of the charge transfer mechanisms and the rates at which they occur. By doing this, the group can provide insight into how the molecules can be designed and used in a way that enhances their key physical properties. Ultimately, optimal semiconducting materials for use in specific applications could be discovered.

"While our research is fundamental in nature, it can be used eventually to direct both the synthesis of the molecular material and their fabrication in optoelectronic devices," Dunietz said.

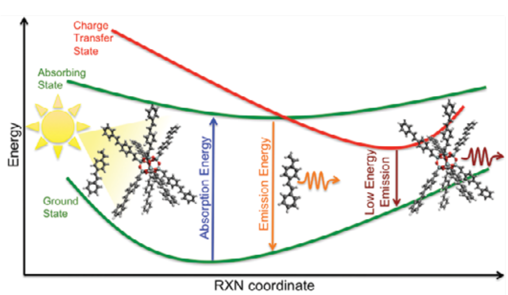
One main thrust of the group's work is related to the use of organic material in photovoltaic applications, such as solar panels. The traditional semiconducting materials used for solar panels are expensive and can have harmful environmental effects. The Dunietz group research on electron transfer and transport in organic semiconducting materials can contribute to replacing these with plastic-like materials in solar panels.

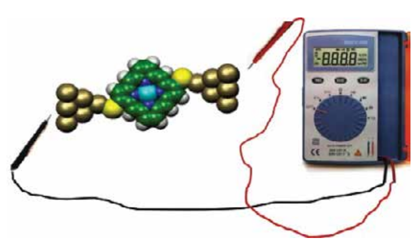
"Here we are looking into photo induced processes that are leading to charge separation and therefore to energy conversion," Dunietz said. "The extent of the cluster, its size, allows us to basically experiment on several ideas at the same time, therefore testing different approaches and being able to identify the correct one quicker."•

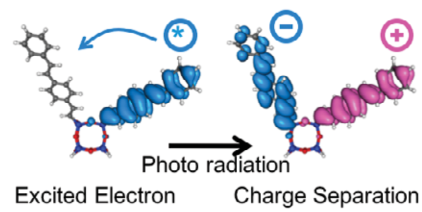
► Below left: A chart documenting how the relevant potential energy in a surface affects the absorption and emission spectral peak.

Below center: The Dunietz group research projects include the study of charge transport affected by potential bias across a molecular bridge.

Below right: The Dunietz group research projects include the study of charge transfer affected by photo radiation.







Project Lead: Barry Dunietz, Ph.D., Kent State University
Research Title: Modeling charge transfer and transport processes in organic semiconducting materials for energy conversion applications
Funding Source: Department of Energy, National Science Foundation
Website: personal.kent.edu/~bdunietz

Fuel Economy

Selamet seeks to improve efficiency of gasoline engines

In the summer of 2012, the federal government handed the auto industry a major technological challenge by setting a fuel-economy goal of 54.5 miles per gallon as the industry standard by 2025.

By comparison: In 2012, the standard was 29.7 mpg, which was raised to 35.5 mpg in 2016.

"It's a challenging target," said Ahmet Selamet, Ph.D., an Ohio State professor in the Mechanical and Aerospace Engineering Department. "In the last decade, there has been tremendous pressure to improve fuel economy. Well, it's no longer voluntary."

Selamet is working to understand and improve fuel economy in spark-ignition (SI), or gasoline, engines—which make up 98.7 percent of the 19.3 million new vehicles that hit the road each year. Selamet uses the computational fluid dynamics (CFD) software Star CCM+ on Ohio Supercomputer Center systems to perform detailed simulations of a turbocharger centrifugal compressor. These simulations deliver insight into characteristics, such as flow separation, surge instabilities and extending the low-flow compressor operating range, which could significantly help make engines more fuel efficient.

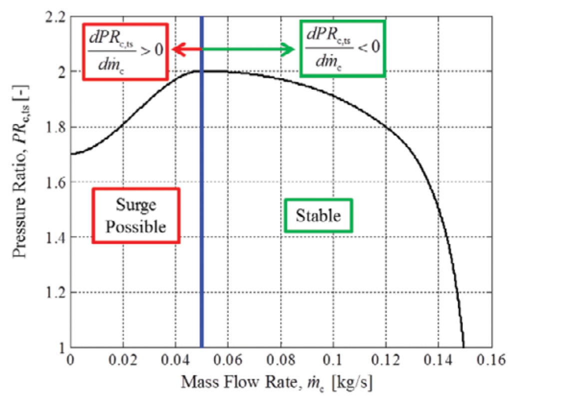
"While we keep improving, the vehicle mass goes up, so the engine has to work harder, and your improvements end up in another aspect of the car," Selamet said. "So one of the key enablers is to bring turbochargers into gasoline engines and integrate them."

Turbochargers achieve boost by using the exhaust flow from the engine to spin a turbine connected to the compressor. The turbine is connected to the exhaust and the compressor is connected to the intake side of the engine. The compressor takes the intake air and increases the pressure before it goes into the engine, boosting it.

"The end result is we are able to do more work and get more torque and power out of the engine for the same displacement," Selamet said. "We get more out of the engine by using otherwise wasted fuel energy."

The insight gained from the CFD simulations are taken to Selamet's turbocharger facilities at OSU's Center for Automotive Research (CAR) for physical testing. By accurately predicting compression system surge, the performance and fuel efficiency of SI engines can be improved.

"What we do is understand the basic physics, and that improved understanding goes into predictive tools automotive companies use," Selamet said. "It's a demanding task, and we would not be able to make significant progress without computational solutions." •



► Representative centrifugal compressor performance at constant rotational speed exhibiting progressive stall.

Project Lead: Ahmet Selamet, Ph.D., The Ohio State University
Research Title: Simulation of surge in centrifugal compression systems for improved stability and fuel efficiency
Funding Source: The Ohio State University
Website: engine.osu.edu

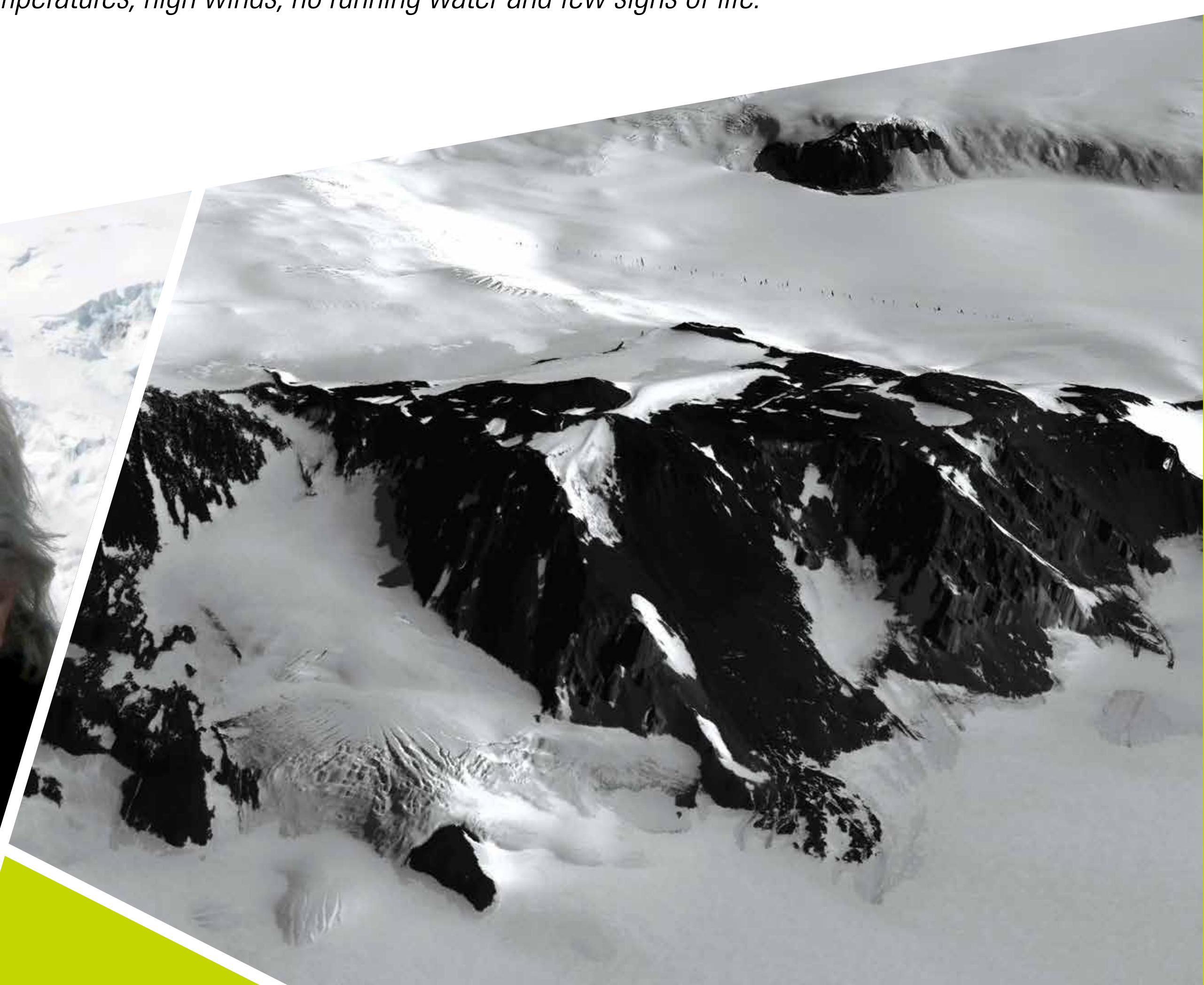
Environment

The answers to so many questions are literally all around us: above our heads, beneath our feet, in the air we breathe. The key is finding those answers, and in some cases, finding the tools we need to unlock the knowledge that is locked within and surrounding our planet. The researchers you're about to meet are leveraging high performance computing at the Ohio Supercomputer Center to better understand our environment and how we fit into it, where we've been and where we're going.

Landscape Evolution

Wilson research group examines size, shape of Antarctic cinder cones

Antarctica is more than five million square miles of vast, frozen ice and rock marked by bone-freezing temperatures, high winds, no running water and few signs of life.



But what it lacks in accommodations, it makes up for in something important to the rest of the world: Information.

While other parts of the world's landscape have evolved, Antarctica's polar temperatures and ice have stopped the ground in its tracks, offering researchers a goldmine of insight into the history of our planet, which might indicate what could happen in the future.

Terry Wilson, Ph.D., is an Ohio State University professor in the School of Earth Sciences whose research group investigates the structural architecture of the Earth. One of her recent projects harnessed the Ohio Supercomputer Center's (OSC) Oakley Cluster to use high-resolution Digital Elevation Modeling (DEM) data to perform morphometric analysis—an analysis of form, encompassing size and shape—of the Erebus Volcanic Province in Antarctica.

"Monitoring landscape change over time is integral to an understanding of Earth surface processes as they pertain both to society and to the natural world," Wilson said. "Rivers and glaciers are dominant agents of erosion, and much research is aimed at determining the rates of fluvial and glacial erosion and how these relate to landscape change. Polar glaciers, or cold-based glaciers frozen to their bed, are considered to be ineffective agents of erosion and, in Antarctica, it has been suggested that mountain landscapes have been preserved with little change over nearly 14 million years in the prevailing polar desert environment."

However, erosion rates in polar regimes have not been extensively studied. Wilson's group focused on cinder cones—small volcanoes that erupt around larger volcanoes or areas where the ground is undergoing stress.

"Cinder cones are helpful because they form as a structure consistently, not necessarily the same size but the same slope, the same height-to-width ratio," said Andrew Collins, a graduate student. "So if you're studying geomorphology, cinder cones in that nice controlled shape act as a control on your hypotheses."

Two questions the project sought to answer were: Do cinder cones show a slow, systematic change in a polar desert environment and whether cold-based glaciation actually affects the shape of cinder cones and other landforms over time.

Far left:Terry Wilson, Ph.D., The Ohio State University; Left: An oblique view of a Digital Elevation Modeling image, illustrating the high resolution. White areas are glaciers, black ones are volcanic rocks.

"The over-arching question is whether we can actually predict the age of cinder cones based on their shape, because they presumably degrade over time in a predictable way," Collins said.

Information about cinder cones will give insight into many different processes within Earth's crust. For example, under tectonic stress, cones can form in areas of crustal weakness near plate boundaries and actually be elongated on the surface by the powerful stresses below it. That indicates which plates were pushed together, how hard and from what direction.

"That helps us understand not only elements of the climate, but also shallow crust and potentially even deeper crust processes over time," Collins said.

Because the project location was Antarctica, there were many logistical challenges of field work, meaning much of the work was performed digitally. Collins used algorithms developed by other researchers to run high resolution imagery through the Oakley Cluster to create 3D models that help parameterize and compare cinder cones.

"OSC was huge, most of this work was done digitally through satellite stereo imagery to build these spectacular high resolution DEMs," Collins said. "The takeaway point is what happened in the past will continue to happen in the future. Also, it validates this particular method of remote sensing. This is a rapidly expanding field and this project demonstrates how viable this approach is and how valuable it can be." •

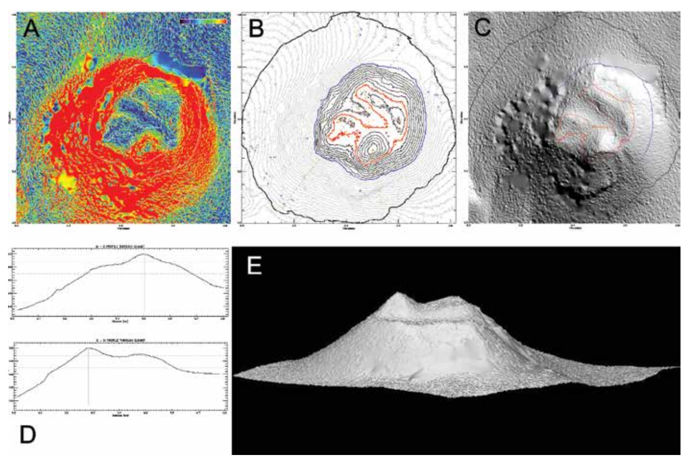


Image illustrates the actual measurement processes. A) Slope, where red indicates higher slope; B) contours generated to show delineation between different parts of the cone, termed summit, main flank, and lower flank; C) shaded relief image of the DEM with the same parts of the cone illustrated; D) profiles of the cone generated by the program; and E) image in 3D space showing the edifice.

Project Lead: Terry Wilson, Ph.D., The Ohio State University
Research Title: Morphometric analysis of Erebus volcanic province, Antarctica, using high-resolution DEM data
Funding Source: The Ohio State University
Website: earthsciences.osu.edu/people/wilson.43

Atmospheric Prediction

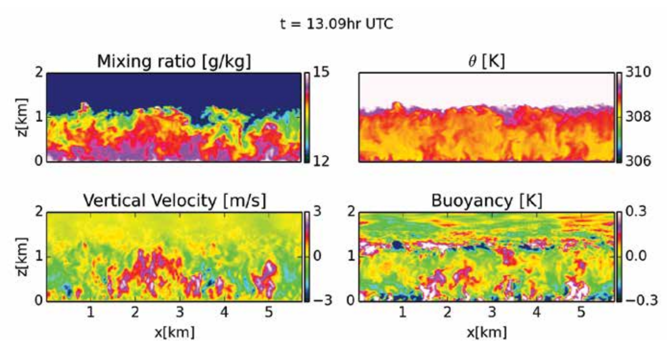
Heus studies boundary layer to improve weather, climate modeling

The clouds above our heads provide some of the biggest uncertainties in weather prediction, but a better understanding of their layers could unlock answers.

Thijs Heus, Ph.D., Cleveland State University, is using the Oakley Cluster at the Ohio Supercomputer Center to perform large eddy simulations—high-resolution computer simulations—to study the atmospheric boundary layer (ABL), which could result in better weather and climate modeling along with improved air quality.

"It starts with improved weather and climate models," Heus said, "not just for weather models but for climate prediction. What's going on in the boundary level is one of the bigger uncertainties. If we can get that right, then the overall weather and climate predictions would improve.

"The atmospheric boundary layer is the layer we are living in, so a good understanding of it impacts what goes on directly around us."



▶ Graphs show the humidity, temperature, buoyancy and vertical velocity in the atmospheric boundary layer throughout the day according to simulations done through OSC resources.

Above & below: Rendering of a generated cloud field.

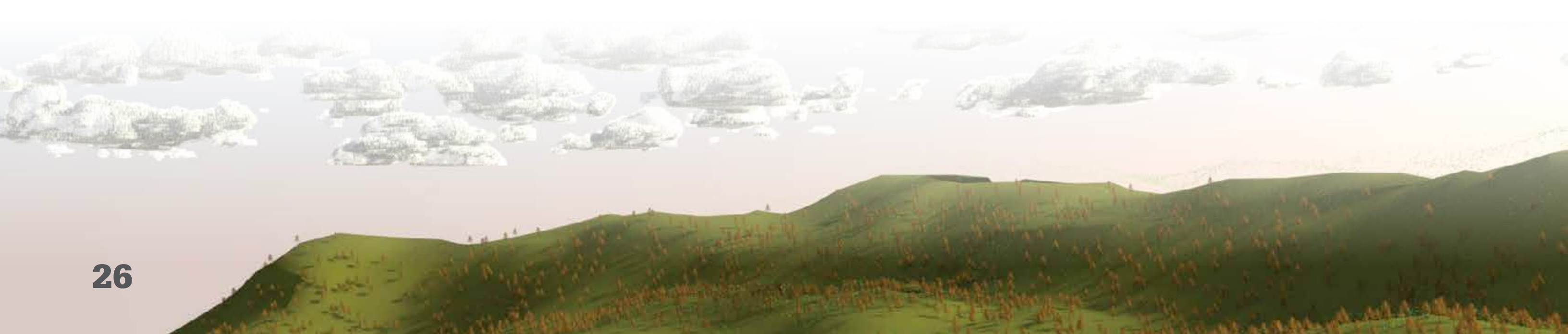
For example: Why is an urban environment warmer than outside the city? To accurately assess that you need a good understanding of the ABL.

The ABL is the lowest few kilometers of the atmosphere, and during the day the sun heats the ground and the lowest layers of air, making the ABL unstable and convective. This means warm surface air rises from just above the surface to right below the top of the ABL. This is key to meteorology because of its relevancy to air quality and pollution, and because the clouds directly above it hold that aforementioned source of uncertainty in weather and climate modeling.

Part of the uncertainty lies in the mixing between the top of the boundary layer and the atmosphere above, in a small-scale interfacial layer tens of meters high or less. Clouds are often rooted in this layer, and varying degrees of cloud cover control the amount of solar heating that fuels the CBL generation. Weather and climate models normally involve a larger scale, meaning sub-models need to be created. And in order to do that, it's important to have a strong understanding of the underlying processes.

The study is in collaboration with the National Oceanic and Atmospheric Administration (NOAA), and funded by the Department of Energy's Atmospheric Radiation Measurement facility at the Southern Great Plains site in Oklahoma. The NOAA team performs the meteorological observations. Heus' team takes those observations and performs the large-eddy simulations, and high performance computing is crucial to that process. •

Project Lead: Thijs Heus, Ph.D., Cleveland State University
Research Title: Characterizing the turbulent structure of the atmospheric boundary layer using large eddy simulations
Funding Source: Department of Energy
Website: facultyprofile.csuohio.edu/csufacultyprofile/detail.cfm?FacultyID=t_heus



Halogenated Hydrocarbons

Tarnovsky team leverages lasers to control chemical reactions

A research team at Bowling Green State University has been employing Ohio Supercomputer Center systems to better understand the photochemistry of halogenated hydrocarbons.

Their study will contribute to a general understanding of solvent environmental effects on chemical reactions and, perhaps, to the ability to control chemical reaction pathways using ultrafast laser techniques.

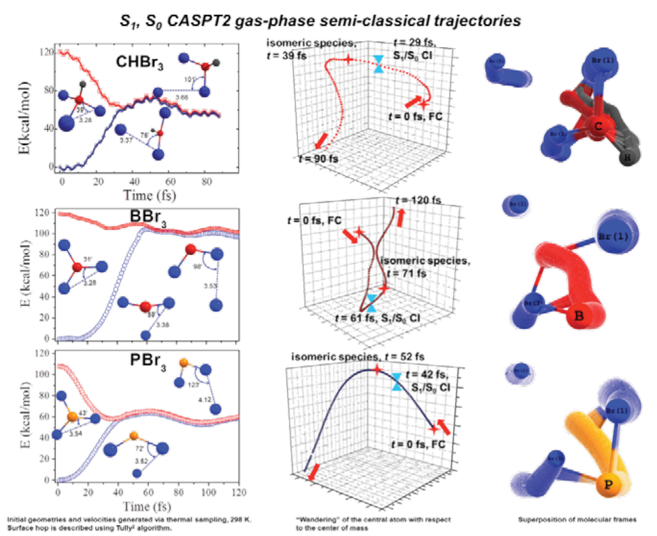
"The core of photochemistry is molecular dynamics in excited electronic states," said Alexander N. Tarnovsky, Ph.D., the leader of the research team, an associate professor of chemistry at Bowling Green and a member of the university's Center for Photochemical Sciences. "Understanding electronic and structural changes throughout the course of a photo-induced process in the liquid phase, where the most chemistry occurs, is of fundamental and practical importance."

Polyhalogenated alkanes are compounds with more than one halogen atom that replaces a hydrogen atom attached to the carbon in a hydrocarbon chain. These substances have characteristic physical and chemical properties unique to them, such as their ability to act as solvents able to nonpolar and slightly polar substances.

Apart from their importance to photosynthetic and environmental chemistry, polyhalogenated alkanes also serve well as model systems because of their relatively simple structure (five atoms at minimum) and easily altered carbon-halogen bonds. Their short-lived intermediates and photoproducts are detectable by several established time-resolved experimental methods, such as the ultrafast pump-probe methods used throughout this project. And, in a practical sense, several of these molecules are considered to be important sources of reactive halogens in the atmosphere, playing a role in ozone-depletion in the troposphere.

Tarnovsky's group leverages OSC's Oakley Cluster to generate calculations with an assortment of scientific applications, including Guassian, NAMD, Amber, Q-Chem and Molcas 07. Their results aid in explaining the team's ultrafast femtosecond pump-probe spectroscopy experiments, where the system response to excitation pulsed light ("the pump") is studied by examining the absorption/amplification of a monitoring pulse ("the probe") delayed in time from the initiating "pump" pulse.

"Small polyatomic solutes have density of states non-prohibitive for the tools of high-level computational photochemistry and detailed ultrafast time-resolved experimental studies," said Tarnovsky. "Gaining the atomic-level understanding of the photochemical reaction dynamics in these systems can be essential, per se, but it also provides the basis for a deeper understanding of photochemical reactions in more complex systems in condensed-phase environments." •



▶ Above: As a part of its study of halogenated hydrocarbons, members of the Tarnovsky group performed electronic structure calculations for phosphorus tribromide and boron tribromide.

Project Lead: Alexander Tarnovsky, Ph.D., Bowling Green State University
Research Title: Tracing ultrafast photoinduced rearrangement and energy flow in polyatomic molecules in solution
Funding Source: National Science Foundation
Website: bgsu.edu/departments/chem/faculty/alex_tarnovsky

Oceanic Viruses

Sullivan evaluates microbe health to gauge far-reaching impacts

Matthew Sullivan, Ph.D., gets priceless reactions when he shares a fun fact from his studies: There are over 50 million viruses in one mouthful of ocean water.

Before you cancel your beach trip, these viruses infect microbes, not humans. Sullivan's lab at The Ohio State University studies and catalogs these viruses, using data processing from the Ohio Supercomputer Center.

While the health of microbes may seem insignificant, these specimens are key in ecological processes, such as photosynthesizing light energy, creating sugars and, more importantly for humans, oxygen.

"Every other breath you take—that oxygen comes from the oceans," Sullivan said.

When a virus infects a microbe, it changes the microbe's biochemistry at a genetic level. Viruses move microbe genes around, changing the evolutionary trajectory of host cells. This has far-reaching impacts, from the spread of antibiotic resistance to the impact of climate change.

"We use measurements of currently existing viral populations with compute-intensive models to try to hindcast what those viral populations looked like back in time," Sullivan said. "Getting this right can help refine our predictive capability so we can make good management decisions in the future."

Until recently, less than one percent of ocean viruses were known. Sullivan was part of the Tara Oceans expedition, in which over 200 scientists circumnavigated the planet gathering ocean water samples. The group increased known viral genomes from approximately 2,000 to 30,000. The Tara Oceans dataset and findings were recently published in the journal Nature. From this data, the group created a reference map of viral communities.

"Imagine the global ocean virus atlas," Sullivan said. "You can use this new map that we've created with tools like the Ohio Supercomputer Center to be able to figure out where the organisms are that we want to study."

By tripling known ocean viral populations, Sullivan and the Tara group provide the scientific community with a critically needed catalog that could affect many fields of work.

"A lot of smart people are studying the sequence data associated with microbial communities in your body and the soils … but what they often ignore are virus sequence data," Sullivan said. "Our hope is that if we can generate the reference genomes through … the culture independent surveys of global oceans, people will start to see that virus data and recognize that maybe viruses are important in their microbial story." •

▶ Above: Sullivan was one of over 200 researchers that are part of the Tara Oceans expeditions that organizes voyages to study the ecology of the world's oceans.

Project Lead: Matthew Sullivan, Ph.D., The Ohio State University
Research Title: Ecological impacts and drivers of viral communities in the global oceans
Funding Source: The Ohio State University
Website: u.osu.edu/viruslab

Research Landscape

Supercomputers—like those at the Ohio Supercomputer Center—are simply the fastest, most powerful computers at a particular point in time. But what is it really? A tool: A super-fast, sleek tool designed to help researchers turn questions into answers. Those answers are applied to many wonderful purposes, such as making us healthier and smarter. From fighting off viruses to comprehending how we learn and to making our children safer on a drive to school, researchers are harnessing the tools at OSC to break ground on a wide swath of incredible knowledge.

Epidemic Forecasting

Rao seeks to proactively reduce the impacts of widespread disease

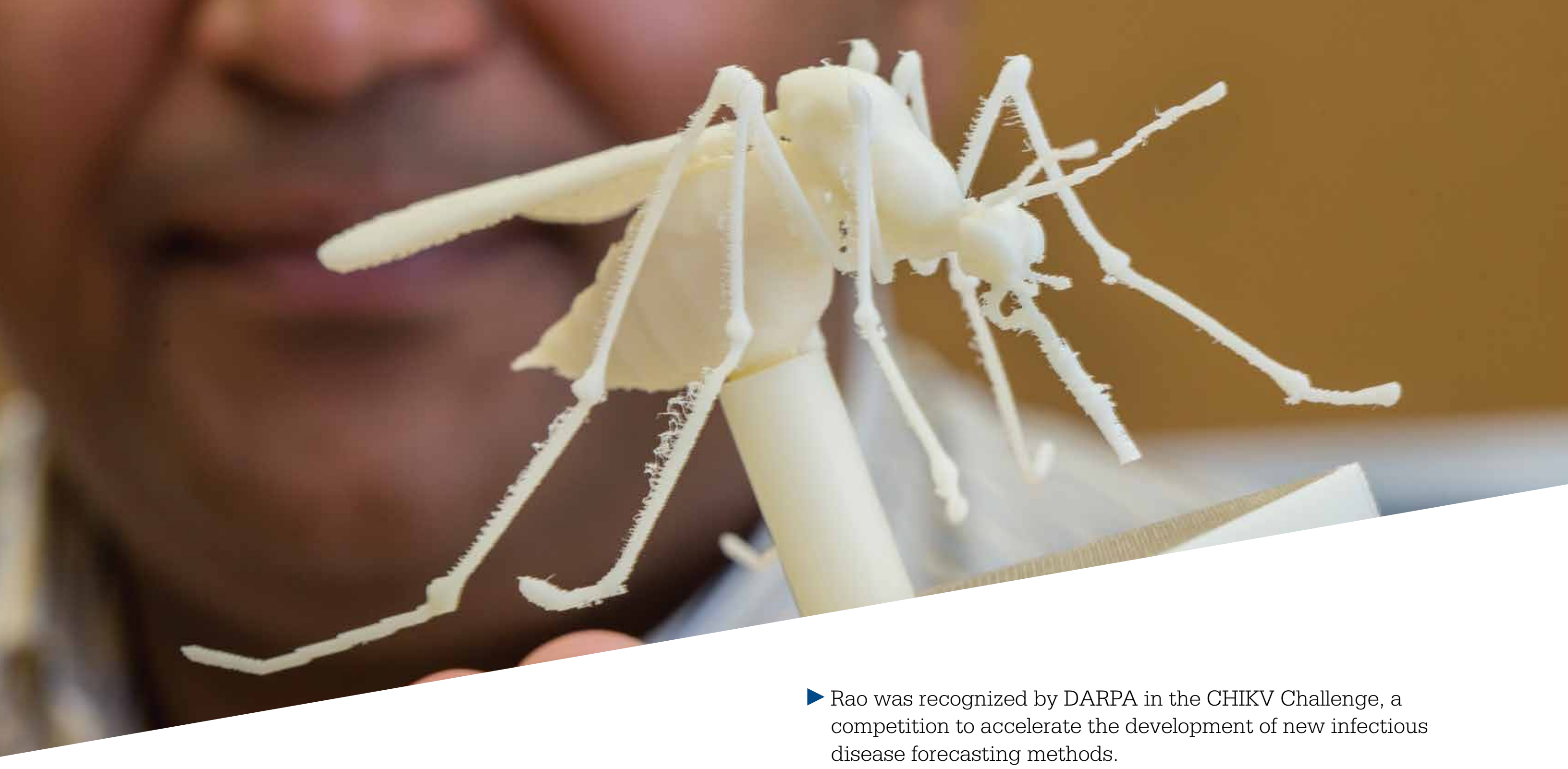
When life-threatening weather events loom, forecasters warn citizens days, even weeks, beforehand so they can take action.

It seems to work: We clear supermarket shelves, board up windows and even evacuate to higher ground ahead of the impending tempest to avoid danger. Blind to bias in its threat to human life is another force of nature—epidemics.

Unfortunately, we often do not know they are imminent until the disease has already infiltrated an area. Dhananjai Rao, Ph.D., an assistant professor in the department of computer science and software engineering at Miami University, is using machine learning and simulation through resources at the Ohio Supercomputer Center to apply the concepts of weather forecasting to epidemiology. He hopes this work will shift the paradigm for disease control from reactive to proactive.

"If we are able to forecast when, where and what an epidemic is going to be, then we can focus our energies and judiciously plan to mitigate the impact of those epidemics in those parts of the world so that the overall impact of the epidemic is significantly reduced," Rao said.

▶ D.J. Rao, Ph.D., has developed an award-winning disease forecasting model that could be used to take proactive steps to guard against infectious diseases.



► Rao was recognized by DARPA in the CHIKV Challenge, a competition to accelerate the development of new infectious disease forecasting methods.

Rao has recently been studying mosquito-borne diseases, particularly chikungunya and the Zika virus. While there have been some efforts to forecast other known diseases, these existing methods rely on historical data trends to project the next stages of the disease. Unfortunately, for newly discovered or recently spreading diseases, such as the Zika virus, there is no historical data on which to base these statistical models.

"The gotcha with that is the statistical regression models will not be able to tell you what are the ecological processes that are happening. It can only tell you what is the final outcome of the system," Rao said. "Statistical (regression) models you can think of as a black box. You don't really understand what is going on inside."

Rao's approach of fundamentally modeling the disease ecology provides a better idea of what these new diseases are, where they are going and, from there, how to effectively contain them. To create a disease forecast, Rao layers data from multiple fields that collectively create the "perfect storm" of an epidemic. These include weather patterns, mosquito population and life cycle, human population density, air travel and socioeconomic data.

There are also critical parameters for which there are no known data, such as the probability that a mosquito will bite a human. To account for unknown parameters, Rao uses machine learning and parallel simulation to estimate what these values should be. By looking at a combination of continuous and discrete event simulations, Rao uses OSC's Oakley Cluster to study the overall ecology of a disease and how the disease propagates.

This disease model analysis required 3.5 million simulations. This would take approximately 1,000 hours of CPU time, or about 90 days' work, on a single computer.

"Three months. In three months, the epidemic would have long passed through the Americas, or the region that we're looking at," Rao said. "On Oakley, we were able to pull it off in about 12 hours, even on peak load."

Rao was one of 11 teams or individuals recognized recently in a competition organized by the U.S. Department of Defense's Defense Advanced Research Projects Agency (DARPA). The competition, known as the CHIKV Challenge, seeks to accelerate the development of new infectious disease forecasting methods. The challenge identified gaps in current disease forecasting and, with help from Rao's groundbreaking model, DARPA as well as other government agencies can begin to look at how to mitigate the spread and affect of infections diseases.

The next step of the process will involve advising health interventions and public policies to help contain epidemics. Rao said these policies will differ depending on the region and timing of the disease spread.

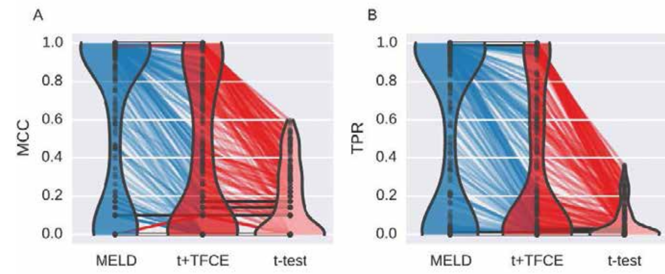
"There is not a day when we step out of the house without checking the weather, and that's where we want to go," Rao said. "For weather forecasting, it took about 100 years to come to where we are. With epidemic forecasting, we are hoping to be able to accelerate to where we want to be with supercomputing." •

Project Lead: Dhananjai Rao, Ph.D., University of Miami
Research Title: Accelerating parallel epidemiological simulations
Funding Source: Miami University
Website: users.miamioh.edu/raodm

Neural Datasets

Sederberg studies successes, failures of human memory

Within The Ohio State University's Computational Memory Lab, Per Sederberg, Ph.D., is developing computational models to link neural activity and behavior to guide experimental work.



▶ Results of simulations shows the performance of three different examination methods, including MELD, for each of 500 simulations performed.

Below: Scalp distribution of old/new effect assessed by MELD and another testing method used called t+TFCE.

Out of that work came the Mixed Effects for Large Datasets project, or MELD, a project that harnessed the powerful Oakley Cluster at the Ohio Supercomputer Center to benefit researchers who don't have similar access to high performance computing.

"In our initial evaluation of MELD, we focused on analysis of EEG (electroencephalography) data and found that it was much more sensitive than standard approaches," Sederberg said. "The work here allows us to show MELD provides greater flexibility and sensitivity for a broad swath of the large datasets increasingly frequent in biomedical research."

The problem with analyzing neural data sets, according to Dylan Nielson—a Ph.D. graduate student in neuroscience working for Sederberg—is it's currently limited by the fact they're too big.

"Generally speaking, you're trying to find which part of the brain shows some difference between two conditions," Nielson said. "So you might be trying to see which part of the brain is more active when someone is talking versus when they're reading. To do that you have to make some comparison at every point in the brain, so these statistical tests take a long time to run.

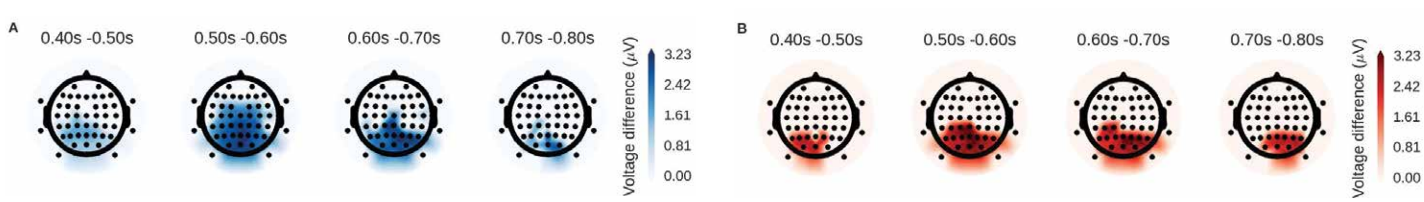
"Our goal with MELD was to come up with a way to run a more statistical test across an entire giant neural dataset."

These datasets are incredibly complex and validating the methods is time-consuming, meaning HPC capabilities were essential to developing MELD.

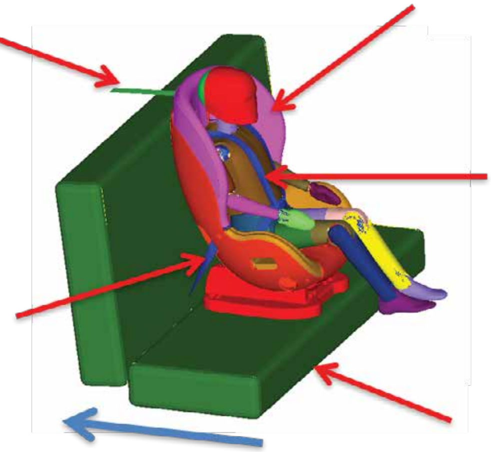
"Without HPC, it would have taken years and years to prove this method performs better than standard methods," Nielson said. "MELD is a way to do really sophisticated statistics in a feasible amount of time without violating a lot of the assumptions standard techniques might violate."

MELD is a technique that also could be beneficial to those outside neural science because of its ability to measure repeated behaviors over time.

"It's a technique that is potentially really powerful for certain types of large data problems," Nielson said. "So large populations of individuals over time—financial, housing, etc.—you could model at a market-by-market level across the country. So at every zip code, you could get a robust amount of estimates." •



Project Lead: Per Sederberg, Ph.D., The Ohio State University
Research Title: MELD—Mixed Effects for Large Datasets
Funding Source: The Ohio State University
Website: faculty.psy.ohio-state.edu/sederberg



Passenger Safety

Kang delves into modeling, simulation of automotive restraint systems

While it's a chore most parents dread, properly installing a car seat is one of the most important things they can do to protect their child.

Yun Seok Kang, Ph.D., a research scientist at the Injury Biomechanics Research Center (IBRC) at The Ohio State University, is working toward making child restraint systems (CRS) even safer. Kang's lab accesses Ohio Supercomputer Center (OSC) systems for modeling and simulation to understand occupant interaction with restraint systems and advise the most effective child restraint protocols.

Vehicles and CRS manufactured on and after Sept. 1, 2002, in the U.S. are federally mandated to include the Lower Anchors and Tethers for Children, or LATCH, system. This incorporates two lower anchors that secure to the vehicle's seat and a top tether that attaches to the vehicle roof, floor, shelf or seatback. Current safety standards test the strength of these anchors and tether by applying force for 24 to 30 seconds at a time. A weakness to this evaluation is the dynamic conditions of a crash are not taken into account.

"The thing about car accidents, it's not like quasi-static loading," Kang said. "It's dynamic loading and high energy with a large force in a very short duration applied to the LATCH."

Additionally, federal standards do not evaluate how much load the top tether can withstand independent of the lower anchors. To analyze this, Rakshit Ramachandra, a biomedical engineering Ph.D. candidate in IBRC, developed a computer model with a CRS and an anthropomorphic test device (ATD) placed on a foam bench. Kang's team then performed scenarios by running simulations of high-energy impacts replicating physical crash tests using OSC resources. The team investigated the effects of two different CRS models, three levels of foam stiffness and four top tether locations.

"Each of these simulations required at least 36 to 48 hours to run on our single standalone workstation," Ramachandra said. "These simulations when run on OSC were significantly shorter in duration, I would say more like 4 to 5 hours."

After 180-plus simulations, they found that the tether experienced the largest load, or greatest force, when secured to the roof of the vehicle and the smallest load when secured to the vehicle seatback. This information can help vehicle and CRS manufacturers optimally design safety systems.

"That's why we love using OSC computational power," Kang said. "And that helps our children." •

▶ Inset above: Kang's lab created a computer model for testing LATCH locations using Altair HyperMesh software.

Project Lead: Yun Seok Kang, Ph.D., The Ohio State University
Research Title: Dynamic top tether loads in various anchor locations in side impacts
Funding Source: Center for Child Injury Prevention Studies (CChIPS)
Website: ibrc.osu.edu/research/cchips

Social Networks

Minai, Shekfeh simulate how we learn from those around us

How do we as individuals learn from the people with whom we interact on a daily basis?

From whom within our communities is it best to learn? And what makes some communities more innovative than others?

These are some of the questions Ali Minai, Ph.D., a University of Cincinnati professor in the Department of Electrical Engineering and Computing Systems, is trying to answer. Using a multi-agent systems model on the Oakley Cluster at the Ohio Supercomputer Center (OSC), Minai and his Ph.D. student, Marwa Shekfeh, are performing simulations that will help us understand how individuals build knowledge and generate ideas through their social networks.

"There are two ways we can answer these questions," said Minai, who has a background in complex systems and computational neuroscience. "One is field work, in which we go out and try to find real-world social networks where this process is going on; that is incredibly difficult to do in a controlled way. The alternative is to do it through simulation, and that's why we need high performance computing.

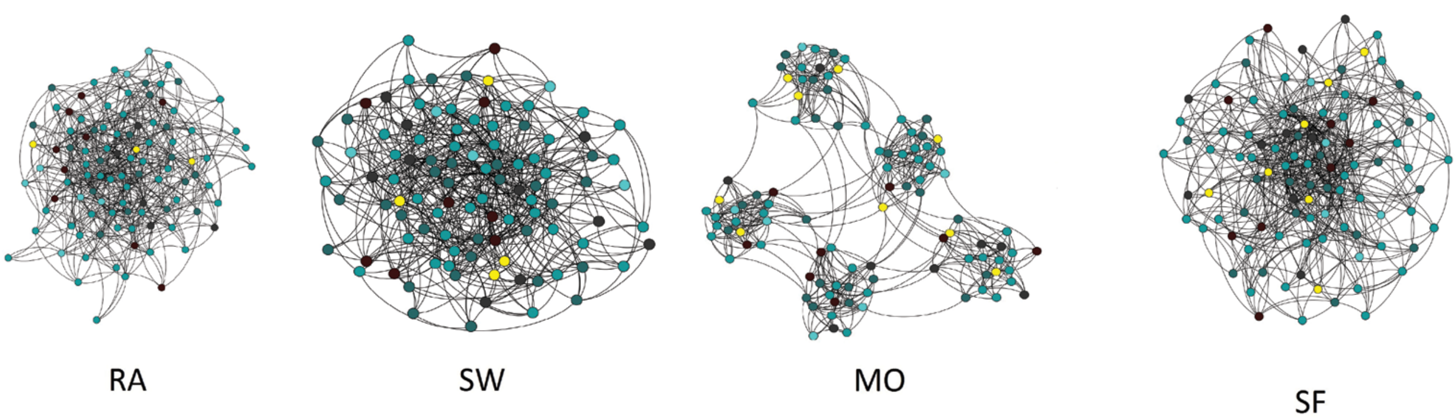
"In our model, each individual has their own knowledge, which consists of many facts associated with each other. We want to simulate hundreds, thousands, even tens of thousands of individuals. For this to be even somewhat meaningful, we have to model the mental processes of each individual in a simple but plausible way. We look at how patterns of social connectivity and whom agents attend to influence collective learning and creativity."

To gain insight for the multi-agent systems model, Minai collaborates with a group, including psychologists at the University of Texas at Arlington who study individuals in group settings. Minai and other group researchers at Stony Brook University and Hofstra University also look at data such as scientific publications where researchers cite the work of other researchers systematically.

"If you look at the work of hundreds or thousands of researchers within a field, you can often find out who was influenced by whom and to what extent," he said.

"The implications are huge depending on what we find. The results could be relevant for education and public policy, and even for situations such as teams working on projects within corporations or research labs. Though creativity is often seen as a solitary activity, in fact it depends strongly on social factors. We hope our models can help clarify this and enhance prospects for systematic innovation." •

► The figures show the state of knowledge at the end of a learning episode in four types of simulated multi-agent social networks: RA—randomly connected; SW—small world; MO—modular communities; SF—scale-free. Each node represents an agent, and the links show who talks to whom. The colors of the nodes indicate how knowledgeable each agent is after learning, with lighter colors indicating greater knowledge.



Project Lead: Ali Minai, Ph.D., University of Cincinnati
Research Title: Multi-agent system model of collective learning and creativity
Funding Source: National Science Foundation (INSPIRE Award)
Website: www.ece.uc.edu/~aminai

Services & Systems

What's the value of a powerful supercomputer if researchers don't have access to it? … if they have no licensed software to use on it? … if they're having trouble writing their code to run on parallel systems? … if their results are output in a list of code that can only be understood in a more visual medium? These questions drive many of the plans and efforts of the Ohio Supercomputer Center, where the staff continually seeks answers to these questions and more. The services and systems of OSC lead most clients to the conclusion that its powerful supercomputers are of extraordinarily high value.

Statewide Users Group

A melting pot of eye-opening scientific research projects immersed attendees of the December 2015 Statewide Users Group (SUG) meeting at the Ohio Supercomputer Center (OSC). Research on topics—virtual welding simulation, evolutionary modeling and water absorption, just to name a few—were on full display during the Flash Talk and Poster competitions.

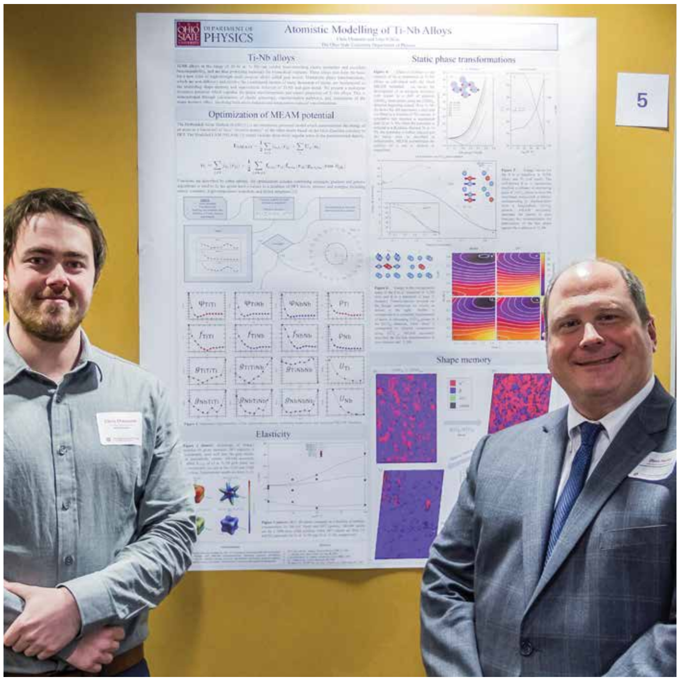
The general aims of SUG meetings is to highlight new scientific developments produced through the use of OSC resources, foster connections between OSC staff and SUG members, and gain feedback as to the future of OSC and its role in supporting science across Ohio. Since the first meeting of SUG in November 1986—almost a full year before the official 1987 establishment of OSC by the Ohio Board of Regents (now the Ohio Department of Higher Education)—Ohio research practitioner-advisors have provided OSC's leadership with expert program and policy advice. To that end, SUG meets twice a year (October and April) to provide a forum for discussing issues, trends and developments in research and maintains several standing committees to consider vital issues.

The SUG Allocations Committee oversees a peer review grant process that allocates system resources to all academic users of the center. The Hardware and Operations Committee advises leadership on user needs and priorities for hardware configuration and acquisitions, as well as policy, procurement and operational issues. The Software and Activities Committee reviews software supported by the center for availability, clarity of documentation, quality of user interface, ease of use, logical development of the presentation, effectiveness, contribution to OSC resources and degree of restrictions.

In recent years, SUG meetings have featured well-attended poster and flash talk competitions.

"This format has reinvigorated SUG and the next challenge for us is to continue that growth," said Brian Guilfoos, HPC client services manager at OSC. "I'm very happy with the turnout we've had and the exceptional number of people from around Ohio coming out to show what they're using the services we provide."

Guest speakers are also a regular aspect of SUG meetings. The December 2015 meeting featured two keynotes. Dr. Daniel Lacks, professor of Chemical Engineering at Case Western Reserve University, delivered a presentation titled "Solvophobicity," in which he discussed what makes a surfactant effective when the solvent is not just water. Suzy Tichenor, director of the Industrial Partnerships Program at Oak Ridge National Laboratory, followed with a presentation titled, "Oak Ridge Leadership Computing Facility and Industry: Partnering for Success."



Poster Winner December 2015 SUG Meeting

Project Lead: Chris Ehemann, The Ohio State University

Research Title: Atomistic modeling of Ti-Nb alloys

Funding Source: The Ohio State University

Chris Ehemann, a graduate research associate within The Ohio State University's Department of Physics, claimed first place in December's poster competition for his work on a project that used OSC resources for atomistic modelling of niobium-titanium (Ti-Nb) alloys.

"Ti-Nb alloys have been found to exhibit bone-matching elastic properties and excellent biocompatibility, making them a promising material for biomedical implants," Ehemann explained. "These alloys also form the basis for a new class of high-strength multi-purpose alloys called gum metals. We presented a molecular dynamics potential that captures the phase transformations and elastic properties of Ti-Nb alloys … involving both stress-induced and temperature-induced transformations."

The research team Ehemann belongs to developed a Modified Embedded-Atom Method (MEAM) potential for the Ti-Nb system, fitted to first-principles data using a genetic algorithm. Accuracy of the MEAM potential was tested by predicting the measured elastic anisotropy and phase transformation dynamics. OSC's computational resources to the project included Density Functional Theory (DFT) calculations performed with the Vienna Ab-initio Simulation Package with PAW-PBE pseudopotentials. Molecular dynamics simulations were performed using the LAMMPS package.

The research project was credited to Ehemann and Ohio State Professor John Wilkins, Ph.D.

Flash Talk Winner December 2015 SUG Meeting

Project Lead: Aaron Wilson, The Ohio State University

Research Title: Improving the regional arctic system reanalysis with high performance computing

Funding Sources: The Ohio State University, the National Science Foundation, NASA, the National Center for Atmospheric Research

Aaron Wilson, a research associate within the Byrd Polar and Climate Research Center at The Ohio State University, was the flash talk winner for his presentation on Arctic System Reanalysis (ASR), a high-resolution regional assimilation of model output, observations and satellite data.

"What we're attempting to do is create a regional reanalysis that's really high resolution in space and time," Wilson said. "It's a blend of model observations to get a cohesive picture through space and time of the climate of the (arctic) region, and so we can take a model for the past and team that up with the observations and be able to look back and find out whether the climate changed over time."

ASR has been refined to ASRv2, a far superior tool for analyzing Arctic climate change over the observation period of 2000-2012. Wilson leveraged the power of 2,048 cores of OSC systems for ASRv2 analysis.

Wilson was part of a research team that included David H. Bromwich, Lesheng Bai, Keith Hines, Sheng-Hung Wang, Ziquan Liu, Hui-Chuan Lin, Michael Barlage and Ying-Hwa Kuo.

▶ Above: OSC Interim Executive Director David Hudak, Ph.D., poses with winners.

Education & Training

High performance computing (HPC) and networking resources come together at the Ohio Supercomputer Center (OSC) to create an exciting and innovative teaching and research environment. And, through the integration of increased training and education leadership over the past year, OSC is working toward deeper engagement with our users. OSC staff members assist faculty and student researchers by providing workshops, one-on-one classes, web-based training and materials. Also, classroom accounts are available for teachers who want to incorporate HPC resources into courses.

On-site instruction

Our on-site instruction workshop provides users an engagement opportunity to learn how to begin leveraging our supercomputing resources while answering users' questions face-to-face. OSC client services has worked to identify the core competencies of a basic, intermediate or advanced HPC client in order to create a curriculum for each skill level. This way, if someone wants to begin using supercomputing resources but knows nothing about how to use them, we can explain everything our new users need to know so they can log on and be productive.

Taking training on the road

Because it is not always easy to have our academic users travel all the way to Columbus for instruction, OSC staff work to visit campuses around the state several times per year to facilitate classroom projects, train students on the basics of supercomputing and demonstrate the broad service offerings OSC can provide. This takes an instructional load off faculty members, so their time is maximized to focus on content and solving problems.

OSC also held a statewide curriculum meeting for users to discuss ways to improve the OSC classroom experience. Participants representing 12 universities received direct support from OSC, shared materials and received instruction on OnDemand and AweSim interfaces, as well as for several software packages. OSC also offers training and consultation for individual clients to build core competencies for effective HPC use.

Classroom accounts

Instructors running courses can leverage OSC services in their classroom for computational science. OSC provides accounts for students and a limited amount of resource units for a semester. OSC leads also will go to classes and talk with students about supercomputing, what it is and why it might be of interest.

XSEDE training

We are often a remote site for XSEDE training and can help clients connect to that and other training opportunities as well. XSEDE—the Extreme Science and Engineering Discovery Environment—is the most advanced, powerful and robust collection of integrated digital resources and services in the world. It is a single virtual system that scientists and researchers can use to interactively share computing resources, data, and expertise. XSEDE integrates the resources and services, makes them easier to use, and helps more people use them.

Faculty recruitment

OSC can serve as a resource available to faculty leadership that can be very helpful in recruiting talented candidates interested in HPC. We can participate in the conversations that are ongoing with faculty candidates and talk about the services OSC provides as Ohio's shared-supercomputing model, which is different than what is found at institutions in other states. Our services are largely paid for through a state subsidy; we can highlight what we provide and offer to help in the recruitment process.

Help Desk

Our 24x7 Help Desk, with Level 2 and 3 support during the day, features an expert staff that can help identify what your problem is and connect internally and externally to experts who can help you be more productive.

Summer Institute

Participants experience the dynamic fields of high performance computing and network firsthand at our two-week summer camp for Ohio high school freshmen, sophomores and juniors. The center employs a staff of experts in HPC, networking, engineering and the sciences to teach students computing fundamentals, such as programming language, parallel processing techniques and visualization toolkits. Students live in dormitories at The Ohio State University and participate in field trips to sophisticated laboratories.

Young Women's Summer Institute

Young Women's Summer Institute (YWSI) is a week-long program for middle-school girls in Ohio sponsored by the Ohio Supercomputer Center. The camp is designed to promote computer, math, science and engineering skills, as well as provide hands-on experiences. YWSI helps girls develop an interest in these subjects by allowing them to work on a practical, interesting scientific problem using the latest in computer technology.

Educational Innovation

FSAE app helps student racing teams gain 'wind tunnel' access

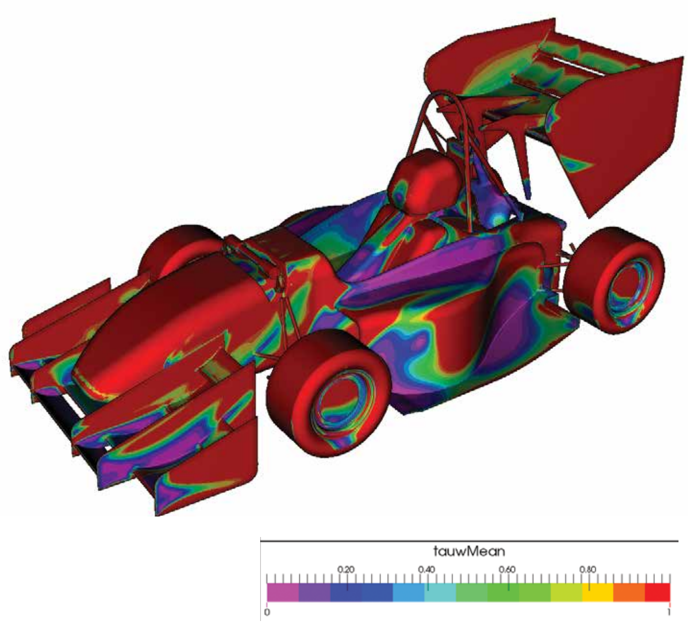
In late 2015, an engineering services provider developed a computational fluid dynamics (CFD) app that allows college students on Formula SAE (Society of Automotive Engineers) teams to perform aerodynamics simulations on Ohio Supercomputer Center systems and get wind tunnel-like data for development of their race cars.

"The idea with this whole AweSim app eco-structure is to get modeling and simulation in the hands of people who normally couldn't afford it, or don't have the time to become an expert," said Ray Leto, president of TotalSim USA—a charter AweSim partner located in Dublin, Ohio. "There's another avenue you can go down to get information and this app is a great example of that."

Formula SAE is a competition amongst student-run college teams in which a fictional manufacturing company has contracted a design team to develop a small Formula-style race car. The teams design, build and test a prototype based on a series of rules aimed at promoting safety and problem solving. The app itself meshes geometry, configures solver settings, generates output visualizations and organizes results so students can focus on designing and improving their Formula SAE cars without being forced to become CFD experts.

Six Formula SAE teams, hailing from The Ohio State University, the University of Akron, Indiana University–Purdue University Indianapolis (IUPUI), University of North Carolina–Charlotte and the University of Southern California, use the app.

"It's invaluable because we don't have access to a wind tunnel or anything of that nature," said Andrew Borme, senior lecturer of Motorsports Engineering at IUPUI.



▶ The app renders geometric shapes into a mesh, configures solver settings, generates output visualizations and organizes results so students can focus on designing and improving their Formula SAE cars without first being forced to become CFD experts.

Services

The Ohio Supercomputer Center (OSC) is much more than a dark room full of glittering, powerful hardware, a fact that our clients discover the moment they request an account to perform whatever research they need done. Our clients resoundingly agree the characteristics they enjoy most are the services and assistance they receive from our staff, which brings down any perceived barriers to high performance computing and delivers the ability to gain incredible insights into their respective projects.

The OSC staff provides subject-matter experts from around the center to assist with individual client requests. For any issues that arise, OSC's 24/7 support desk, which includes daytime Level 2 engineering support, offers clients technical expertise and consulting services at any hour of any day.

Industrial engagement

Under OSC's AweSim program, engineers, simulation and engineering experts and industry leaders collaborate to provide small- to mid-sized manufacturers with simulation-driven design that enhances innovation and strengthens economic competitiveness. AweSim provides affordable, accessible and scalable modeling and simulation on high performance computers via:

- online modeling and simulation apps
- educational resources
- industry-specific expertise and consultants

From research involving Formula-style racing to food processing, AweSim continues to grow, with over 30 projects and 150 AweSim developers/clients, helping each to reduce prototyping time and costs while improving products and streamlining operations. A number of prominent studies indicate that modeling and simulation based on high performance computing is critical to competitiveness within most industries, and those who have harnessed this powerful tool see the benefits immediately. On average, for every $1 invested in modeling and simulation, companies receive at least $7 in return on investment. OSC has been a leader in the field of HPC industrial engagement since the center's creation in 1987.

Web software development

In Summer 2016, OSC launched OnDemand 3.0, a vastly upgraded version of its "one-stop shop" for acess to its high performance computing services. This latest version of OSC's custom-built OnDemand web portal is the first to be based on Open OnDemand, an NSF-funded OSC endeavor to develop an open-source web portal that can provide advanced web and graphical interfaces for HPC centers.

With OnDemand 3.0, OSC clients can upload and download files, and create, edit, submit and monitor jobs, among its many features. Some of the features of OnDemand 3.0 include a new and faster file browser app, system status and job apps; remote graphical desktops on OSC clusters; as well as an in-browser terminal app for shell access and support for federated authentication.

In addition to these user features, the OnDemand 3.0 platform also enables developers to create and even share their own web apps with other users, a feature first demonstrated through the AweSim program.

Scientific software development

As professionals in high performance computing and software engineering, OSC staff have deep expertise in

25
Ohio-based universities

33
companies

1,267
clients

developing and deploying software that runs efficiently and correctly on large-scale cluster computing platforms.

OSC experts are available for consulting or collaboration with research computing teams that require such expertise to increase the size and/or complexity of problems that they can tackle or to reduce the runtime for their analyses. Our staff have experience with several computing languages, programming models, numerical libraries and development tools for parallel/threaded computing and data analysis. The types of services we provide are outlined below.

Services/Expertise

- Performance analysis and optimization
- Parallel algorithm development
- Software development for accelerators
- Workflow and I/O tuning
- Software engineering for scientific codes
- Software debugging

Visualization & virtual environments

OSC's award-winning Interface Lab translates technology into effective training and assessment tools for use by various sectors, such as the health care, automotive and manufacturing industries. Currently, the lab is developing new shared virtual environments, where individuals can move around freely without tethered devices.

The Interface Lab is dedicated to the study of advanced human computer interfaces and user assessment. In addition to providing high performance graphic displays for both interactive and recorded presentations, the Interface Lab offers dexterous devices to precisely localize and track 3D digitization, user movements, morphometrics and haptic (force reflecting) interaction with complex data. The Interface Lab also provides equipment for recording and generating various types of audio for both interactive sessions and presentations. Finally, the lab provides various methods for obtaining quantified physiological assessment during interactive study sessions.

Specialized equipment includes:

- Stereo Displays
    - High resolution projector and large screen (22' x 11') display
    - High resolution monitors
    - Oculus Rift head mounted displays
- Motion tracking
    - 8 camera Optitrack (OPTICAL) reconfigurable system, currently 20' x 20' space
- Haptic devices
- Physiological Assessment
    - Biopac MP150U-W monitoring system with wireless modules for Galvanic Skin Response (GSR finger electrode), Respiratory effort transducer, a SS4A ear clip and Pulse Plethysmograph
    - fNIR PRO system for monitoring frontal lobe activity

124
trainees

10
training opportunities

451
awards made

459
projects served

19
academic courses used OSC supercomputers

Systems

In 2016, OSC brought on board the largest supercomputer in its history. Its name pays tribute to renowned Olympic sprinter, beacon for racial equality and youth advocate James C. "Jesse" Owens. Owens set or tied four collegiate world records in a single afternoon, sprinted to four gold medals and two Olympic records at the 1936 Berlin Games and dedicated much of his later life to helping youths overcome obstacles to their future success.

The Owens Cluster increases the center's total computing capacity by a factor of four and its storage capacity by three, with aggregate throughput performance of approximately 200 gigabits per second. With $12 million in capital funds, the center not only brought in the new Dell/Intel Xeon cluster, but also upgraded disk storage and revamped infrastructure services to improve reliability and serviceability.

The new system will be powered by Dell PowerEdge servers featuring the latest family of Intel Xeon processors, include storage components manufactured by DDN and utilize interconnects provided by Mellanox.

Additionally, the center provides more than 140 different software packages to researchers, with about 20 of them licensed packages. Researchers can bring their own licensed software, open source packages or in-house developed applications, as well. Among the most-used software codes this past year were VASP for atomic scale materials modeling, OpenFOAM for computational fluid dynamics, LAMMPS for molecular dynamics simulation and MATLAB for numeric computation and visualization.

High performance computing & storage

In 2015, approximately 1,300 researchers across Ohio depended on several key OSC systems:

Dell Intel Xeon Owens Cluster

23,392 cores provide a total peak performance of 750 teraflops

HP Intel Xeon Phi Ruby Cluster

4,800 cores provide a total peak performance of 144 teraflops

HP Intel Xeon Oakley Cluster

8,304 cores provide a total peak performance of 154 teraflops

DataDirect Storage System

3.4 petabytes of high-performance spinning disk with 40 GBps bandwidth

IBM Tape Library System

More than 5 petabytes of tape backup

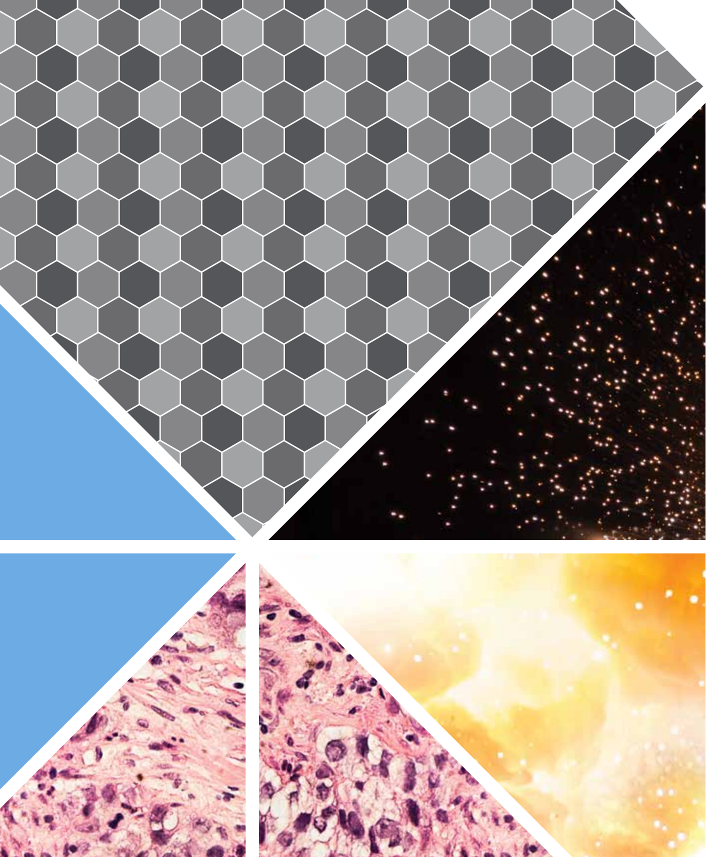
161M+
core hours consumed

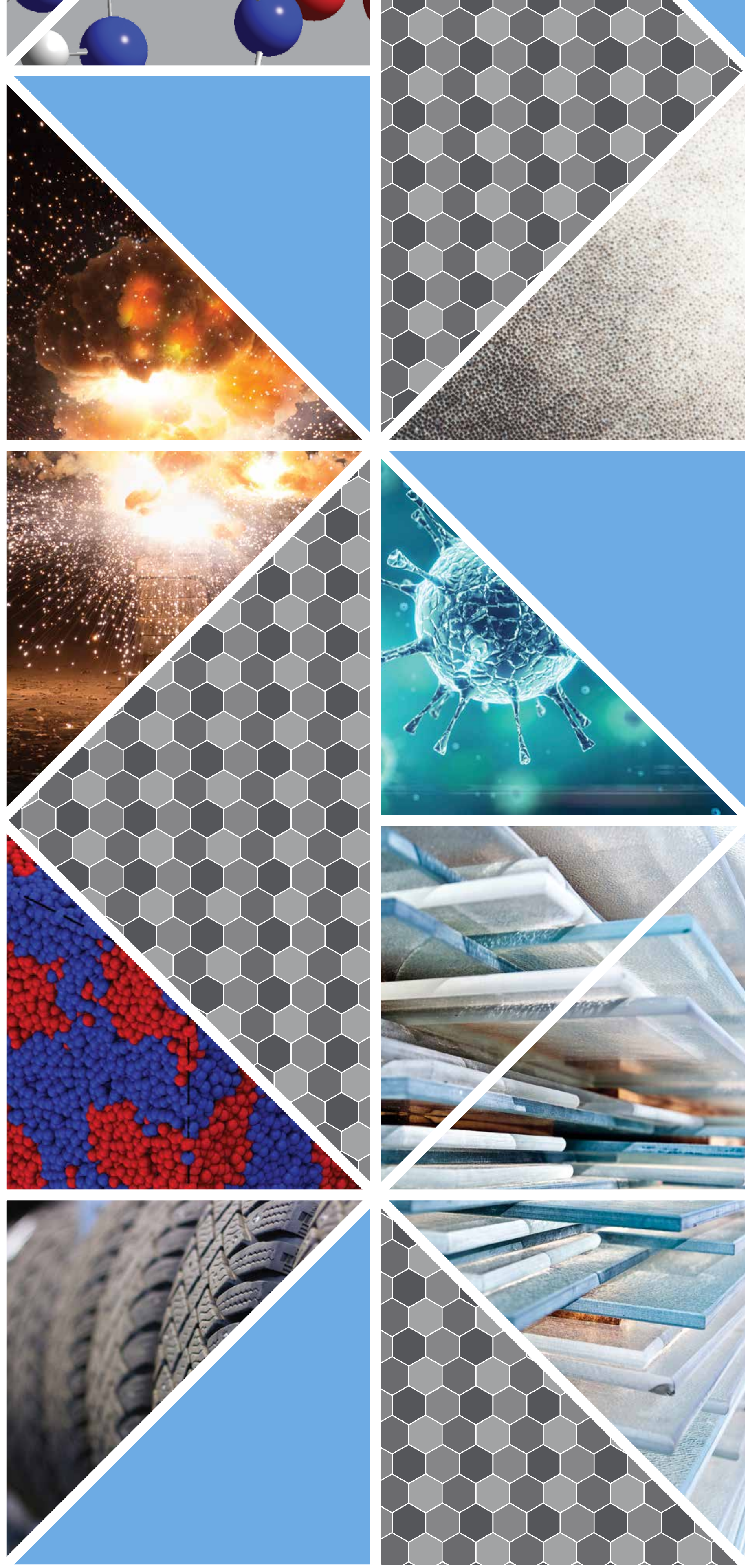
4M+
computational jobs

842 TB
data stored

99.7%
up-time (target: 96%)


39
38
EXIT
42
Networks
Networks
Networks





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