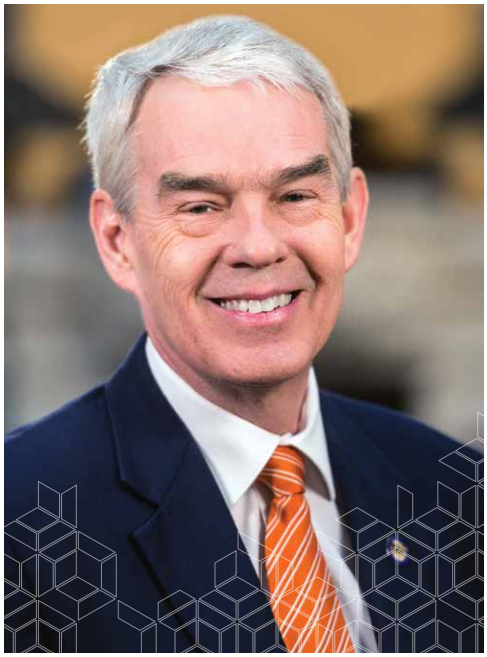
RESEARCH REPORT 2021

Ohio Supercomputer Center



"RESEARCHERS AND INNOVATORS ACROSS THE STATE IN ACADEMIC, COMMERCIAL AND NONPROFIT FIELDS ARE BLAZING A TRAIL TO A BETTER AND STRONGER OHIO THANKS TO THE OHIO SUPERCOMPUTER CENTER. THE OSC'S ADVANCED RESEARCH AND GROUNDBREAKING DISCOVERIES ARE HELPING PREPARE THE HIGH-TECH WORKFORCE OF TOMORROW."

— RANDY GARDNER,
CHANCELLOR,
OHIO DEPARTMENT OF
HIGHER EDUCATION

Photo: Chancellor Randy Gardner directs ODHE and oversees the strategic initiatives of OH-TECH and its member organizations in support of the state's technology infrastructure needs.

Leadership

David Hudak, Ph.D.
Executive Director
(614) 247-8670 | dhudak@osc.edu

Doug Johnson
Associate Director
(614) 292-6286 | djohnson@osc.edu

Karen Tomko, Ph.D.
Director, Research Software Applications
(614) 292-1091 | ktomko@osc.edu

Alan Chalker, Ph.D.
Director, Strategic Programs
(614) 247-8672 | alanc@osc.edu

Brian Guilfoos
Manager, HPC Client Services
(614) 292-2846 | guilfoos@osc.edu

Jeff Triplett
HPC Operations Manager
(614) 688-0320 | jtriplett@osc.edu

Ohio Supercomputer Center

By centralizing Ohio's supercomputing services at the Ohio Supercomputer Center (OSC), the state's higher education and industry communities gain cutting-edge capabilities at unmatchable value. OSC delivers flexible, secure and reliable computational power and comprehensive client support at a fraction of the cost of similar commercial services or smaller standalone systems. Ohio's academic and industrial communities alike benefit from OSC's affordable, on-demand supercomputing that enables groundbreaking research and innovation throughout the state.

Governed by the Chancellor of the Ohio Department of Higher Education (ODHE), the Ohio Technology Consortium (OH-TECH) serves as the technology and information division of ODHE. The consortium comprises a suite of widely respected member organizations collectively unsurpassed in any other state: OSC, OARnet and OhioLINK. The consortium drives efficiencies through common services provided to member organizations through the Shared Infrastructure and Consortia Services divisions.

Table of Contents

OSC Overview

Case Studies

Services

Tags

■ Area of Science

Advanced Materials
Biological Sciences
Environment
Industrial Engagement
Research Landscape

▲ InnovateOhio Sectors

Aerospace
Agribusiness
Automotive
Aviation
Energy/Chemical
Invention/Discovery*
Manufacturing

InnovateOhio—the DeWine Administration's commitment to leading an aggressive, innovative path towards a better and stronger Ohio—has outlined these traditional areas of innovation strength throughout the state's history.

**Invention/Discovery describes InnovateOhio's Edison category.*

Director's Letter

While the COVID-19 pandemic is not yet in the rearview mirror, the lasting effects get a little clearer each day. For OSC, the disruptions of the pandemic clarified one of the most important aspects of our work: community. Nearly overnight, our definition of togetherness fundamentally changed and, subsequently, we have reforged our connections and found new ways to gather.

OSC is no stranger to bringing distant communities together. The support we regularly provide to our clients all over the state of Ohio and the world had our staff prepared for virtual interaction even before the pandemic. Even so, the sudden displacement from our physical workspaces revealed the importance of cultivating our communities.

In response, we are intentionally reshaping how we gather together with our clients. Our Campus Champions program continues to grow as we engage campus IT support staff at Ohio's colleges and universities to serve as local advocates for supercomputing and resources for their faculty and students. Our new Researcher Recognition program enables anyone to nominate the deserving work of oneself or one's peers for spotlighting on our website and in the Research Report. And we are redeveloping our biannual Statewide Users Group meeting to make it just as engaging online as in person.

We are also reflecting on the ways in which our client community helps us grow stronger as a service provider. Our clients hail from across Ohio's diverse and thriving research and innovation ecosystem and present us with a fascinating range of high performance computing (HPC), data storage and support needs. To meet these demands, our machines are tooled with a broader range of capabilities than comparable academic supercomputer centers; our data storage is secure, reliable and backed up; and our software applications and client support teams are cross-trained, qualified and capable of helping in any situation.

We are so proud to be a part of making possible the grand and consequential work you will read about in the following pages. While we call this the "Research Report," I hope you will see how the impact of work enabled by OSC extends far beyond the laboratory and into the lives of Ohioans every day.

Whether you are a current or prospective client, a scientist, artist, engineer or teacher, if you are interested in learning more about how OSC's high performance computing and storage could benefit your work, please reach out—we would love to help.

David Hudak, Ph.D.
Executive Director

2020–21 Highlights

ICICLE AI Institute

OSC will serve as a core collaborator in the new NSF AI Institute for Intelligent Cyberinfrastructure with Computational Learning in the Environment (ICICLE), one of 11 new Artificial Intelligence (AI) Research Institutes. The $20 million institute is led by The Ohio State University.

National and Local Engagement

Our staff participated in a variety of workshops and sessions at the Supercomputing Conference, hosted a virtual version of its Young Women's Summer Institute and multiple "What's So Super About Supercomputing?" youth webinars, and adapted our biannual Statewide Users Group conference to a virtual format.

Classroom Support

Classroom utilization of OSC resources accelerated dramatically, with a 232% increase in the number of Ohio higher education courses employing our tailored class.osc.edu user portal for virtual computer labs and hands-on experiences with data-intensive platforms such as R Studio and Jupyter.

OSC Clients

5,756
Clients

32
Higher Education

39
Commercial

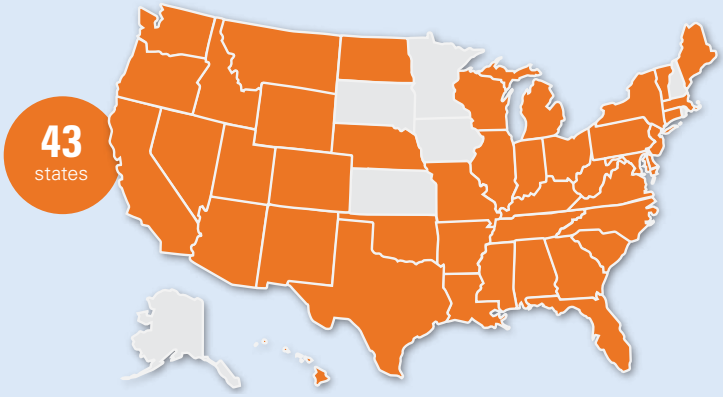
39
Nonprofit & Government

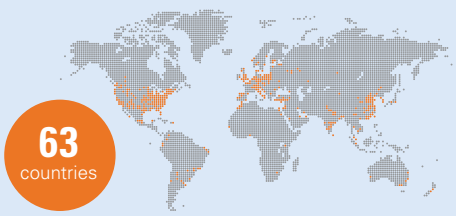
97
Other Educational Institutions

Catalyzing Discovery Across Disciplines

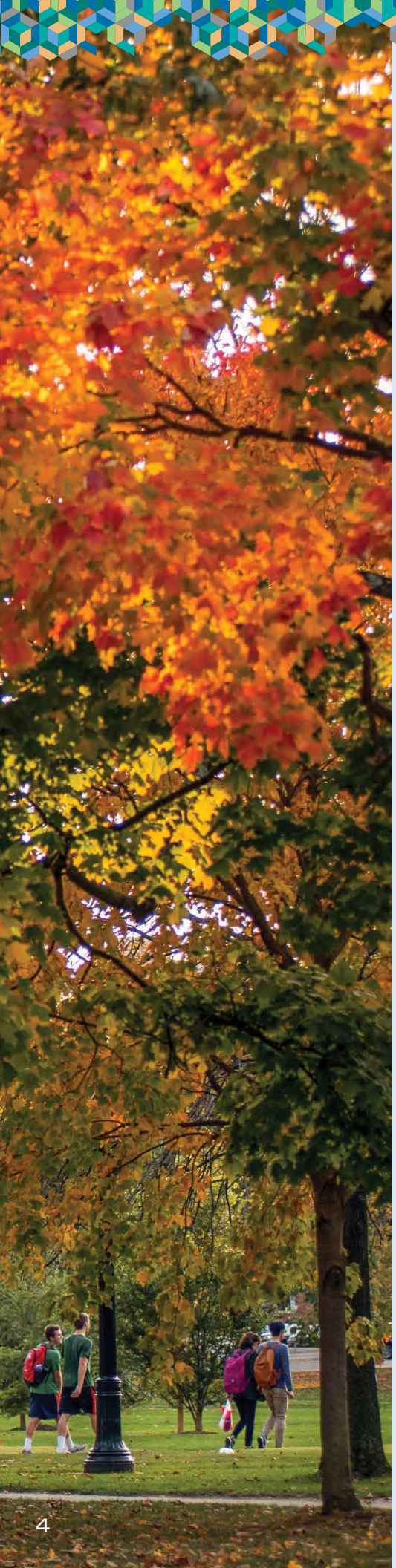
Natural Sciences | Engineering & Technology | Medical & Health Sciences
Agricultural & Veterinary Sciences | Social Sciences | Humanities & the Arts

Serving Ohio & Beyond





All data from July 2020 through June 2021.



Campus Champions

The Ohio Supercomputer Center's (OSC) Campus Champions program is composed of high performance computing (HPC) advocates at academic institutions across the state. Campus Champions serve as local proponents for access and utilization of OSC resources on their campuses. They also receive their own project accounts with no-cost access to a range of OSC services, giving them an additional resource in their own toolkits.

Campus Champions help OSC by:

- Promoting the availability of OSC resources to researchers at their institutions
- Onboarding new researchers to project accounts to test out OSC resources
- Identifying researchers' specific needs to help OSC create personalized training sessions

Current Campus Champion Institutions

Miami University

The Ohio State University

Kent State University

Ohio University

The University of Akron

Becoming a Campus Champion is Simple

If you utilize OSC resources at your institution and want to help your colleagues get connected with HPC resources, please contact us at oschelp@osc.edu.

ARCHITECTURE SIMULATIONS

Classroom architecture programs amplified by OSC

RESEARCH LANDSCAPE

Rendering models is a key part of the modern architectural design process. Brendan Ho, a professor in the College of Architecture and Environmental Design at Kent State University, helps students analyze the spaces in which they live and work. Rendering has been an essential component in his studio Encapsulated Episodes, co-taught with Director Ivan Bernal.

Students in Ho's studio simulate elements such as light, movement and materiality in their interior renderings. The average personal computer is not well equipped to handle the complexity of these simulations, so renderings lack sufficient detail. With help from the Ohio Supercomputer Center (OSC), students in Ho's class have been able to run their simulations at full resolution with ease.

"Being able to work with OSC really enables the students to explore ideas to their full potential," Ho said. "They are able to see what their designs look like fully rendered out, without noise or pixelation."

Utilizing OSC's high performance computing capabilities, Ho's students are able to adjust aspects of their simulations and continually test them. Ho teaches an iterative approach to architectural design through creation, testing and evaluation. The ability to edit simulations and test them repeatedly helps familiarize students with that process.

Thanks to OSC's reliable performance and on-demand access, students gain the additional benefit of more time to actively work on their designs during class without having to leave extra time at the end to account for slow rendering speeds.

"Students would typically end up with fewer iterations of their projects with lower resolution renderings," Ho said. "OSC enables students to have more time to push their design ideas by spending less time on production."

The experience gained by interacting with high performance computing resources not only enhances students' architectural studies but prepares them for future experiences and careers.

"We're pushing students to think about large-scale concepts, to enable them to be agents of change worldwide," Ho said. "They need to be able to understand how to interact with supercomputers in order to evaluate and understand the complex systems that make up our environments." •

Biography: osc.edu/r21/bho

EXPERIENTIAL LEARNING

University of Dayton students gain hands-on experience with computing, research

■ RESEARCH LANDSCAPE | ▲ INVENTION/DISCOVERY

Although many college students have access to a personal computer for their studies, it can be challenging for them to learn about how modern, complex computing systems are used in the science, engineering and technology fields without working with the systems directly.

Faculty members at the University of Dayton solve this problem by using the Ohio Supercomputer Center (OSC) in several courses and teaching clinics.

"OSC was an obvious choice because it is a parallel system and we are teaching about parallel computing," said Tarek Taha, a professor in the Department of Electrical and Computer Engineering. "They have software set up so students have the exact same environment—it makes teaching simpler and more effective. Students are getting access to cutting-edge technologies."

While computers previously processed one task at a time, today's systems have multiple processors that require programmers to split and coordinate tasks that can be processed in parallel, Taha noted. It is a common issue that students will encounter in science and technology fields, with applications ranging from artificial intelligence to gaming.

"There's a lot of demand for this in industry," he said.

Not only does the parallel computing course give students first-hand experience programming with multiple processors, but it also helps them build confidence working in a supercomputer environment, said Tanvir Atahary, a research engineer in the School of Engineering. By working with OSC, students are exposed to the most current hardware and software in the field.

"I've taught this two semesters, and I got feedback from my students that they got a good job based on this class," Atahary said.

Yangjie Qi is one University of Dayton student who has benefitted from OSC's resources. Qi is working on designing next-generation computer chips that can be used in the artificial intelligence field. He has relied on OSC's resources to simulate how different chip designs will perform. Taha estimates that work which would take months to complete in the school's computer lab can be finished in one or two days by drawing on OSC's parallel computing capabilities.

"If I use my own computer to run something it will be stuck there—it's hard to do anything else during that time," Qi said. By using OSC, "I can get 10 times the results—that really accelerates my research."

Photo (far left): Students at the University of Dayton benefit from access to the resources of the Ohio Supercomputer Center.

Photo: OSC's high performance computing helps accelerate research at UD.

Photo (left): Muhammad Usman, professor of mathematics

Photo (center): Tanvir Atahary, research engineer in the School of Engineering

Photo (right): Tarek Taha, professor in the Department of Electrical and Computer Engineering

Photos courtesy University of Dayton.

Muhammad Usman, a professor of mathematics at the University of Dayton, also has used OSC in the classroom to help graduate students advance research projects. As Usman's focus is on applied mathematics, students have tackled issues ranging from developing complex financial models to understanding patterns in biology.

One graduate student, Abigail Rodenburgh, used OSC for a math clinic project that compared various numerical methods for understanding how animals develop spots and stripes. She recalls that the analysis was so computationally intensive that she crashed a personal computer attempting to perform the work.

Usman set up the student with an OSC account so she could draw on the massive computer power of the Owens cluster to conduct the research. Rodenburgh, who had gained high performance computing (HPC) experience previously through a National Science Foundation program for college students, was comfortable using the terminal interface to submit basic jobs to OSC. As the project spanned a semester, she was grateful to be able to access the Center's resources.

Rodenburgh earned a master's degree in applied mathematics from the University of Dayton in 2019 and today works in the private sector conducting research with HPC. She recommends that other students consider gaining experience in this field.

"Having computational resources allows students to do work that is valuable to industry and provides the experience they need to get jobs where they can have a high impact," Rodenburgh said.

Usman appreciates his students' ability to access OSC, as well as the Center's responsive customer service and its workshops that advance users' skills in parallel computing.

"It's very quick to get the account and to start the projects immediately," Usman said.

The University of Dayton faculty members will continue to draw on OSC's power for upcoming student projects in mathematics and engineering, with plans to include both undergraduate students and graduate students in the experience. •

Muhammad Usman biography: osc.edu/r21/musman

Tanvir Atahary biography: osc.edu/r21/tatahary

Tarek Taha biography: osc.edu/r21/ttaha

PLANT BIOLOGY

Scientists simulate how plants communicate through chemicals

■ BIOLOGICAL SCIENCES | ■ ENVIRONMENT | ▲ AGRIBUSINESS

Scientists know that plants emit chemicals into the soil to communicate information to other plants. These chemical messages, sent through fungal networks, may warn plants to defend against threats in their environment or to stop encroaching on another plant's space.

Jonathan Morris and Kathryn Morris of Xavier University are investigating how fungal networks function as communication channels. In addition to conducting experiments with plants at the Oak Ridge National Laboratory, the married researchers are using the Ohio Supercomputer Center (OSC) to develop simulations of how the chemicals move through the soil.

The research findings will be of interest to other scientists studying plant ecology and will be applicable to agricultural management.

"This research offers us a better understanding of how herbicides move around when applied to agricultural crops and a better understanding of chemical interaction in ecology," said Kathyrn Morris, an associate professor of biology.

The project also has provided critical hands-on experience in computer modeling to Xavier undergraduate students involved in the research, said Jonathan Morris, an associate professor of physics.

Although computer modeling is a skill that physics, mathematics or computer science majors expect to learn and use, biology students may not initially see the connection to their discipline, Jonathan Morris noted. But the biology majors in the plant communication project quickly learned how to work with MATLAB code and computer modeling through their work with OSC, he said. One student confirmed that the experience was opening the doors to new internship opportunities.

Using OSC also allowed the professors and students to access computer servers and work on code together remotely in real time during the pandemic, Jonathan Morris said.

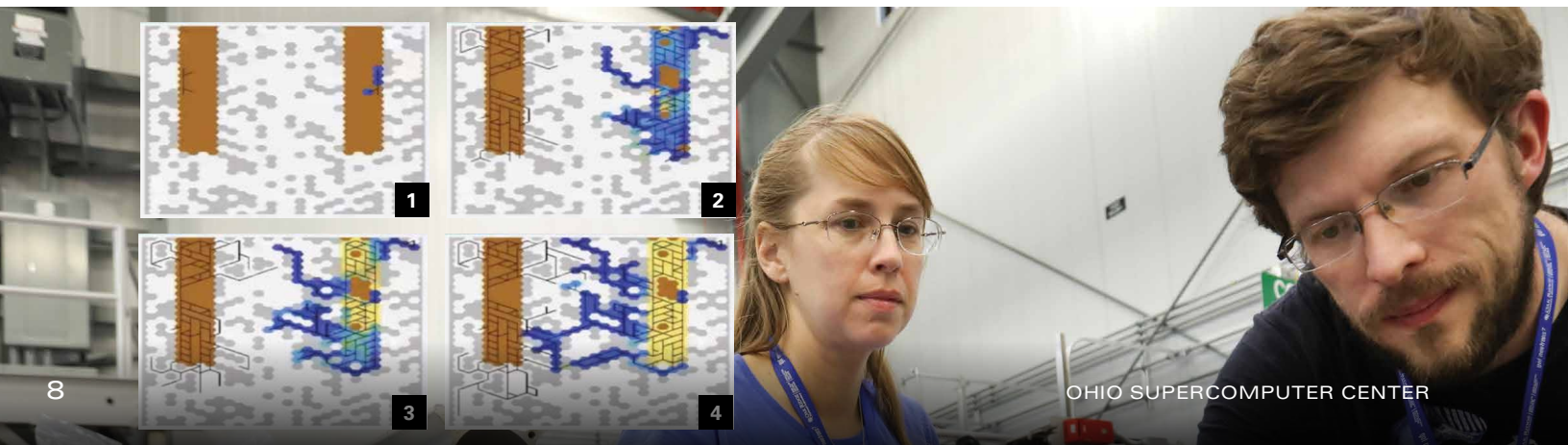
"It's a well-packaged resource that allows easy collaboration that is beyond the scope of what a small undergraduate research university like Xavier could dream of having," he said.

As the plant communication research continues, Xavier University plans to expand its use of OSC resources in the classroom, Jonathan Morris said. He already uses OSC in his introductory computing course, in which students use MATLAB software and the OnDemand web portal to complete assignments. As part of a new data science major at Xavier, undergraduates also will use OSC resources in courses in machine learning and high performance computing. •

Jonathan Morris biography: osc.edu/r21/jmorris

Kathryn Morris biography: osc.edu/r21/kmorris

Jonathan and Kathryn Morris working at the Oak Ridge National Laboratory. Photo Credit: ORNL/Genevieve Martin. Inset: This image shows the simulated movement of a chemical along the fungal network, eventually connecting the two plants. Image credit: Jonathan and Kathryn Morris.



ECOLOGICAL NETWORKS

Preserving pollinator communities through simulations

BIOLOGICAL SCIENCES | ENVIRONMENT

With a focus on plant and pollinator species, Colin Campbell, associate professor of physics at the University of Mount Union, studies how these groups interact with one another. Some interactions are mutualistic, where both species benefit, but other interactions are beneficial for only one species. The net effect of many interactions can result in stable or unstable communities, which can be modeled as networks.

Calling on the Ohio Supercomputer Center (OSC) for computational assistance, Campbell wanted to investigate these unstable networks and how established communities are impacted by invasions of whole other communities of species.

The types of simulations that Campbell runs at OSC are critical to understanding how to manage ecological issues impacting plant-pollinator communities, such as colony collapse disorder, and are also relevant for issues that arise in other ecological communities, including microbes in the human gut.

"No community is really stable. There are always factors pushing a community; things like climate change or the unintentional transport of species across continents," Campbell said. "In some cases, we observe a collapse of pollination services. One approach to restore or bolster crop pollination is to introduce new species to the community. However, predicting effective strategies where the new species don't immediately die out or negatively affect the rest of the community can be challenging. Computational modeling is particularly appealing in this situation because it's hard to do empirical experiments that are well controlled."

Campbell is part of a team that runs simulations that model what would happen if a random collection of species invaded a population, as well as what would happen if a controlled set of species were introduced. Understanding how native species react to different types of invasions reveals what can be done to help ensure more stable communities long term.

"It's nothing that I could run in any reasonable period of time on just a local desktop, or even a powerful local server," Campbell said. "You really need to have some high-powered computational firepower to do this."

Campbell noted that these intensive simulations would be hard to manage among other daily tasks without the help of OSC and its short wait times.

"If I'm able to write a script, submit it to the supercomputer center, come back an hour later and I'm still in that headspace and I have the results from that analysis—you can't really put a price on that," he said. •

Citations: osc.edu/r21/ccampbell

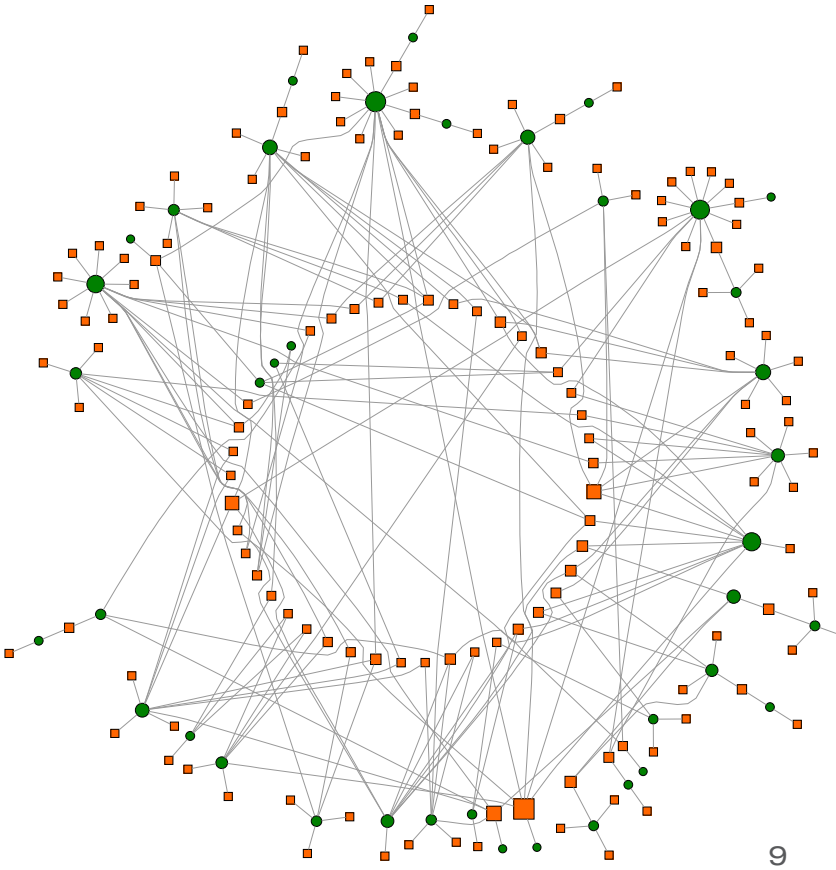
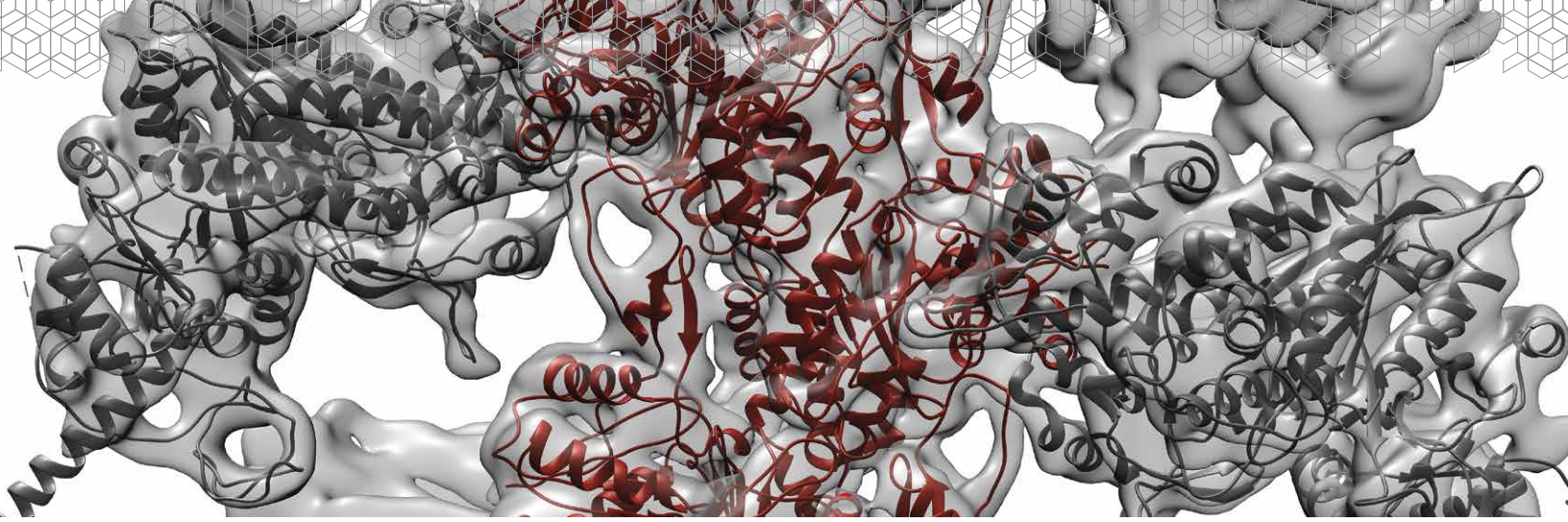


Figure: A regional species pool consists of plant species (green circles) and pollinator species (orange squares). If two species interact when both are present in a community, they are connected by a gray edge.



STRUCTURAL BIOLOGY

Capturing molecular motors in action

■ BIOLOGICAL SCIENCES | ▲ INVENTION/DISCOVERY

After Krishna Chinthalapudi joined The Ohio State University College of Medicine as an assistant professor, the college notified him that he could make use of the computational power of the Ohio Supercomputer Center (OSC) for his research program. Chinthalapudi, who is the principal investigator of a structural biology research group that works with large data sets, was enthusiastic about the opportunity.

"The resources are very helpful because they are on a much bigger scale than what members of my research team can run on our local workstations," he said.

Chinthalapudi's group is focused on understanding how different molecular motors—which he describes as nanomachines in the body—work efficiently and what functions they perform. The researchers use cryo-electron microscopy, X-ray crystallography and high-resolution fluorescence microscopy to magnify the tiny proteins, identify hotspots in them and study how the enzymes work.

"Our studies on molecular motors will provide a deeper knowledge of the structure, function and regulation of molecular motors," Chinthalapudi said. "This knowledge will advance our understanding of emergent molecular motor functions in cells and lay the foundation for future development of precision therapeutics."

Using OSC's high performance computing resources on the Pitzer cluster, Chinthalapudi and colleagues were able to process and analyze images of the molecular motors and how they move along their biological tracks.

Figure: This image was captured using the cryo-EM technique. The image illustrates how myosin motors (dark gray) walk on the filamentous actin tracks (red colored).

One of the benefits of using OSC is that scientists can make rapid advances in research in a shorter window of time, Chinthalapudi noted. With six members of the research team working with large amounts of data, it could take months to process the data necessary to solve a single structure.

"Losing time is not an option—we can increase the use of computational resources at OSC and maximize our productivity," Chinthalapudi said about working with OSC.

OSC staff provided assistance with installing the software required for the research. The structural biology team also uses OSC for storing and backing up their large data sets—which is a requirement for federally funded work, Chinthalapudi explained. The team's research is supported by a grant from the National Institutes of Health.

Chinthalapudi noted that many researchers in the structural biology field struggle to process large data. He encourages colleagues and large research teams in this discipline—whether at Ohio State or elsewhere—to explore the resources and capabilities of OSC.

"It saves time; it saves resources," he said. •

Biography: osc.edu/r21/kchinthalapudi

TRANSPORTATION STUDIES

Using computational simulations to test greener tractor-trailers

■ INDUSTRIAL ENGAGEMENT | ▲ AUTOMOTIVE | ▲ MANUFACTURING

TotalSim US, a computational fluid dynamics (CFD) consulting and solutions firm based in Dublin, Ohio, is helping the state of California certify fuel-efficient and environmentally friendly tractor-trailers using resources provided by the Ohio Supercomputer Center (OSC).

For the past decade, Technical Director Naethan Eagles has been involved with CFD testing for heavy commercial vehicles, a method that is efficient in determining aerodynamic performance, drag levels and fuel efficiency. The California Air Resources Board (CARB) is interested in understanding these variables for their Tractor-Trailer Greenhouse Gas Interim Aero Device Approval Program.

This program contributes to California's reduction of greenhouse gas emissions by requiring tractor-trailers and their devices to meet a certain standard of efficiency to be permitted to drive within the state. In 2019, changes to the program allowed for the use of CFD testing in the certification process instead of physical wind tunnel or coast down testing, which can be more costly and less accurate than computational simulations.

"In order to have a tractor-trailer and certain devices on the trailer, those devices and the tractor-trailers must meet a certain standard laid out by California law," Eagles said. "Manufacturers have to demonstrate that they comply with these regulations. In opening the computational fluid dynamics method as a way to evaluate those devices, it actually allows for a pretty efficient testing approach."

TotalSim follows testing protocols and procedures outlined by CARB. If the tractor-trailer and devices meet a certain level of aerodynamic efficiency, the firm incorporates the data into the approval request form required by CARB, which is then processed by the board.

Eagles noted that OSC has been critical in allowing TotalSim to run its CFD simulations and for being able to accommodate its large workloads.

"Over the course of the last several years, we probably have run hundreds of thousands, if not millions, of core hours at OSC, building up that understanding of how these models work," Eagles said.

Eagles mentioned that the accessibility and cost effectiveness of OSC has allowed this project to run smoothly.

"OSC has enabled us to do our work much more cost effectively and take on these larger projects without having to worry about the risk of investing in infrastructure that would enable us to do this in-house. We are able to use OSC as and when we need to, and it makes life so much easier," Eagles said. "It is just a fantastic resource to have at our doorstep here in Ohio." •

Website: totalsim.us

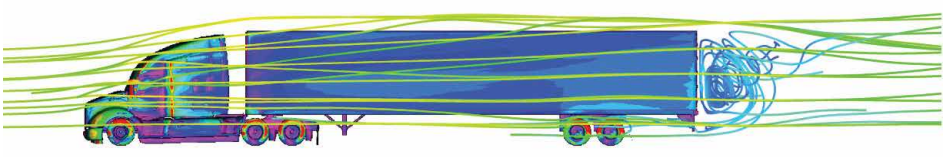


Figure: Computational fluid dynamics (CFD) testing can reveal a tractor-trailer's level of aerodynamic efficiency.

ARTIFICIAL INTELLIGENCE

Accelerating drug discovery with AI

■ BIOLOGICAL SCIENCES | ▲ INVENTION/DISCOVERY

Xia Ning has a large portfolio of research projects at The Ohio State University that focus on understanding how artificial intelligence can be used to solve issues in health care.

Discovering new drugs to treat disease is one of Ning's goals. Traditional research methods, which call for lengthy trials with animal models, have disadvantages.

"To find a single drug is costly and time consuming," said Ning, an associate professor who holds joint appointments in Ohio State's College of Medicine and College of Engineering.

Ning is drawing on her expertise in computer science and biomedical informatics to create a new path to drug discovery. Her lab examines millions of small molecules and uses that information to create novel models that could be strong candidates for drugs.

"In order to learn from millions and millions of chemical structures, we need a lot of computational power," Ning said.

The Ohio Supercomputer Center (OSC) is integral to the project. Each model requires the use of one graphical processing unit (GPU) and 96 GB of RAM for the data generated, Ning noted.

Compared to the conventional central processing units (CPUs) researchers may use in their labs, GPUs offer a significant boost in computing power. OSC features GPUs across its systems to allow clients to efficiently process large amounts of data, and consistently upgrades its hardware to ensure access to the most cutting-edge technologies.

Those computing resources have helped Ning reach important milestones in her drug discovery work. Research findings from the project have been accepted for publication in the prestigious journal Nature Machine Intelligence and also have attracted new grant funding to the lab.

Ning has been a heavy user of high performance computing centers since her days as a faculty member at Indiana University. She joined Ohio State in 2018.

"The first thing I did here was look for similar resources," Ning recalled. "I didn't think about having my own cluster—that would have taken me a lot of effort."

In addition to OSC's capabilities and technical support, Ning appreciates its availability to her lab members. OSC offers Open OnDemand, an interface funded by the National Science Foundation that allows users to remotely access the Center resources online from any device.

"(OSC) provides a very nice Open OnDemand tool that we can access through the web," Ning said. "I believe all of my students are using it. It's very easy for us to use, and we don't need to worry about maintenance or software installation."

Ning also employs OSC for teaching Python programming in her biomedical course. The Center creates a class project through which her students can quickly access computational resources and see results immediately through the OSC web portal, she said.

Over the next year, Ning will continue to work with OSC on the drug discovery project, as well as on research on predicting peptides that could be used for vaccine development.

"As long as we're doing research," Ning said, "we'll rely on OSC." •

Website: u.osu.edu/ning.104

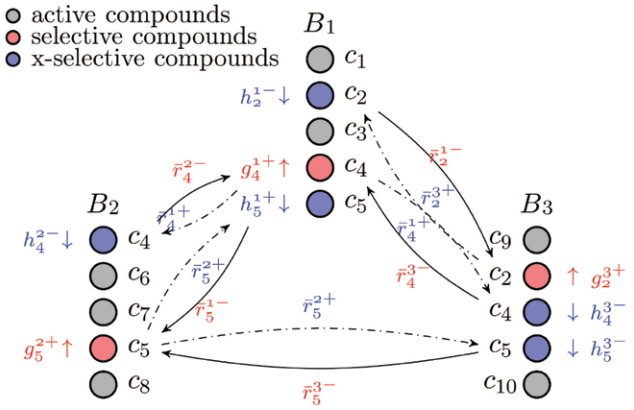


Figure: Advanced AI and large-scale computing enabling multi-purpose drug discovery.

COMPUTATIONAL CHEMISTRY

Nanoparticle research yields education in data science

■ BIOLOGICAL SCIENCES | ▲ ENERGY/CHEMICAL

Luiz Oliveira teaches the foundations of chemistry to undergraduate students at Mount Vernon Nazarene University. By participating in Oliveira's research, which draws on the resources of the Ohio Supercomputer Center (OSC), students gain experience equivalent to completing an extra course in computational chemistry.

Oliveira, an associate professor of chemistry, has a background in physics, chemistry and biophysics. His research explores the interface between biophysics and materials science. The professor and his undergraduate researchers examine how biomolecules and nanomaterials interact, which has implications for nanomedicine, biosensing, nanobioelectronics and bioelectrochemistry.

When he joined the faculty of Mount Vernon Nazarene, Oliveira discovered that he was eligible to use $1,000 of OSC resources each year. The researcher quickly learned the benefits of working with the Center, such as the opportunity to use a wide range of software that would be difficult for him to access otherwise, as well as high-level technical support from staff members.

"I've been very surprised at the number of tools that are available and the help provided," Oliveira said.

OSC also provides a unique educational experience for his undergraduate student researchers, which include two chemistry majors and one biology major. Using OSC's Open OnDemand software interface, the students can access a virtual Linux terminal directly from their web browsers. They are learning the Python programming language to analyze research results.

The students are gaining valuable skills, regardless of whether they pursue careers in research or in other fields, according to Oliveira.

"Data science is everywhere," he said. "My hope is that what they are learning can be applied to whatever path they choose."

The faculty member is now interested in bringing OSC resources into his classroom so that more students may gain such experience.

Oliveira also is enthusiastic about encouraging more of his colleagues at Mount Vernon Nazarene University to use OSC. He is the first faculty member from the higher education institution to work with the supercomputer center, and he hopes that others will take advantage of OSC's resources for research and teaching.

"If it was not for OSC," Oliveira said, "I would not be doing research at Mount Vernon Nazarene University." •

Biography: mvnu.edu/employees/luizoliveira

PIPELINE PRESERVATION

CRES research findings promote infrastructure integrity

■ ADVANCED MATERIALS | ■ INDUSTRIAL ENGAGEMENT | ▲ ENERGY/CHEMICAL | ▲ INVENTION/DISCOVERY

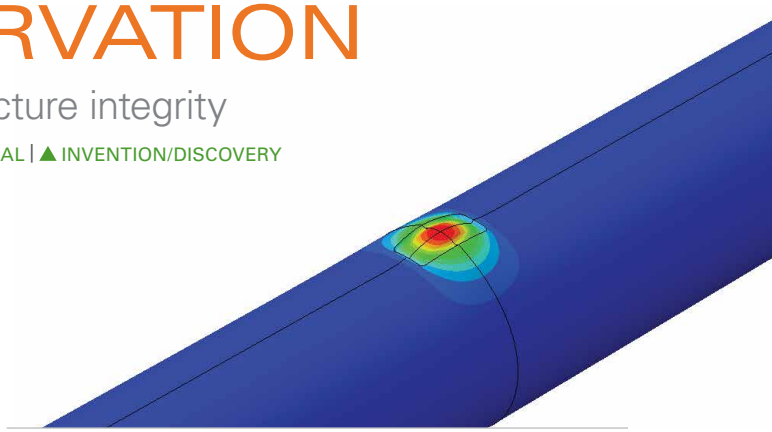
Across the United States, 2.6 million miles of pipeline transports goods such as petroleum and natural gas, according to the U.S. Department of Transportation. This critical infrastructure is regularly threatened by ground movements, landslides, mining operations and corrosion.

Paul Pianca, operations manager at the Center for Reliable Energy Systems (CRES) in Dublin, Ohio, works with his team to mitigate these threats and maintain pipelines' structural integrity.

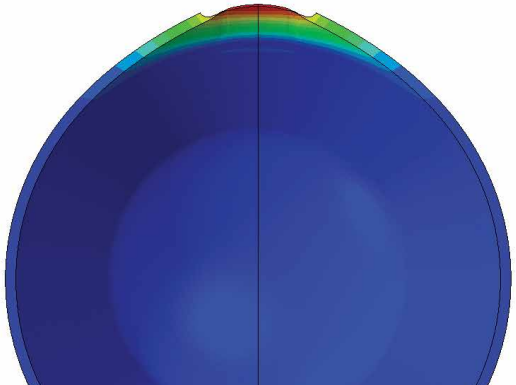
CRES provides technical solutions for the energy industry. Bringing together mechanical and materials expertise, engineers at CRES simulate the conditions affecting specific pipelines to determine optimal remediations for problem spots. This can be challenging when thousands of data points and calculations must run simultaneously to create an accurate simulation.

Corrosion, despite being one of the most significant threats to pipelines, is not fully understood. While engineers can identify corrosion, determining the threat level and appropriate fixes can be a challenge. This is where the Ohio Supercomputer Center (OSC) comes into play.

"On this project, we are studying when and how several nearby corrosion defects can interact with each other to be as harmful as one larger defect. This requires running thousands or even tens of thousands of different finite element analysis (FEA) cases," Pianca said. "That's a lot of computation that needs to happen. So, after getting the results, we can combine the data points for each case, and analyze them together to create a behavior model of how those interacting corrosion defects would affect the safe operation of a pipeline. We can provide that research to all operators across the U.S. to help increase the safety of the pipelines."



Figures: Burst pressure simulation of a corroded pipe.



Findings from CRES' research are often used by large pipeline consortiums, such as the Pipeline Research Council International (PRCI).

CRES' computational needs fluctuate based on its contracts and time of year, but OSC accommodates the variable workload by offering flexible, on-demand access that eliminates the need to maintain expensive supercomputing systems in house.

'OSC helps us modulate our computational needs as it changes week to week," Pianca said. "On those big jobs that we accept, we can have a lot of computation, and they really help us find the answer that the industry needs." •

Website: cres-americas.com

Statewide Users Group

Ohio Supercomputer Center (OSC) clients across the state utilize the Center's high performance computing (HPC) resources to conduct complex and innovative research in a variety of disciplines. The Statewide Users Group (SUG) conference is an opportunity for the user community to come together and learn more about OSC's vision and direction, as well as hear about other users' research projects.

Prioritizing health and safety for OSC users and staff alike, the fall 2020 and fall 2021 SUG conferences took place virtually over Zoom. Each conference featured updates from various staff members at OSC on topics such as the Center's response to COVID-19, new hardware in service and updates to the client portal.

These conferences emphasized the many ways attendees can engage with OSC beyond SUG meetings. OSC staff highlighted how researchers can make use of available services, learn more about OSC's impact and help shape future plans. To learn more about these opportunities, visit osc.edu/fallsug21.

The most recent SUG conference concluded with a combined flash talk and poster presentation competition. Seven presenters were given five minutes to discuss their research projects that utilized OSC's HPC resources.

The winner of the competition was Theresia Yazbeck of The Ohio State University for her presentation titled "Modeling Fluxes, Fate And Transport Of Ammonia Emission From Egg Production And Manure Management Facilities." Second place resulted in a tie between Youngstown State University's Alina Lazar and Ohio University's Himanshu Singh, who presented "Accelerating the Inference Time of Machine Learning-based Track Finding Pipeline" and "Predicting the Equilibrium Adsorption Morphologies of Surfactant Molecules on Metal Surfaces via Advanced MD Simulations," respectively.

Photo: Natalia Vassilieva of Cerebras Systems was a guest speaker at the fall 2020 SUG conference.

Photo: OSC Director of Strategic Programs Alan Chalker gave updates about the Center during the SUG conferences.

Photo: During the fall 2021 SUG conference, OSC highlighted the many ways researchers can interact with OSC.

Photo: Ohio State's Theresia Yazbeck claimed the top spot in the fall 2021 poster competition, conducted virtually.

Education and Training

Education

Research that utilizes the Ohio Supercomputer Center's (OSC) resources spans a variety of disciplines, including medicine, anthropology, business, architecture, computer science, economics, horticulture and crop sciences, engineering, chemistry, environmental sciences, mathematics and physics. For students at numerous institutions, these research programs play an integral role in their education.

Summer K–12 Programs

OSC has hosted the annual Summer Institute (SI) since 1989 and the Young Women's Summer Institute (YWSI) since 2000. These programs encourage Ohio high school students and middle school girls to engage with high performance computing (HPC) and STEM education through first-hand experience.

SI is a two-week residential summer program for high school students entering their sophomore, junior or senior year. Participants learn programming language, parallel processing techniques and visualization toolkits. YWSI is a weeklong program for middle school girls centered on developing computing, math, science and engineering skills through hands-on projects. In 2021, OSC offered SI and YWSI in a virtual format to ensure the safety of students and staff. SI focused on computer science and supercomputing, and YWSI explored the topics of water quality and stream health. The virtual events attracted strong participation and engagement, and OSC will incorporate them into its planned in-person programming for 2022.

Virtual Computer Labs

OSC staff regularly make classroom accounts available to assist faculty and student researchers as they utilize HPC in their courses. In FY 2021, more than 5,500 students from 20 different Ohio universities gained hands-on experience with supercomputing in 249 courses.

During the COVID-19 pandemic, many classes went to a remote format, putting up a barrier to completing work in the lab environment. OSC responded by providing access to cloud computing resources at no charge to numerous classes to ensure students can access lab environments from home. Students at a wide variety of colleges and universities in Ohio—including Kenyon College, Bluffton University, Kent State University, Mount Vernon Nazarene University and Wittenberg University—have used OSC's virtual computer labs.

Workshops

To promote the continued adoption of HPC, OSC staff members offer workshops, one-on-one classes, web-based training and consulting services to users and potential users. Topics covered include getting started using OSC, containers for research computing and performance tuning. During the COVID-19 pandemic, these trainings and workshops moved to a remote setting, a development that has expanded access to these resources. Twenty-two training opportunities were offered with over 400 participants in attendance during FY 2021.

User Services

Office Hours

For answers to specific questions about research done on Ohio Supercomputer Center (OSC) systems or simply for advice on getting started, clients can speak directly with OSC experts.

In-person consultations have shifted to a virtual environment until further notice. Visit osc.edu/events to see the full schedule of office hours and sign up for a time.

Technical Support

OSC provides clients with various ways to get support for training, onboarding for new users, system status updates and resolution of issues such as debugging, software installation and workflow improvements.

- Getting Started Guide: osc.edu/resources/getting_started
- Technical Support: osc.edu/resources/technical_support
- OSC Help desk:
  - Level-1 basic support and Level-2 advanced support
  - Monday through Friday, 9 a.m. to 5 p.m.
  - Contact oschelp@osu.edu or 1-800-686-6472
- @HPCNotices on Twitter (real-time system status updates)

Consulting

As professionals in high performance computing (HPC) and software engineering, OSC's staff has deep expertise in developing and deploying software that runs efficiently and correctly on large-scale cluster computing platforms. They are available to advise on advanced approaches to debug or optimize code.

Research Collaboration

Staff members at OSC often collaborate with researchers around the state on various research and education projects. This year, OSC became a core collaborator in the new National Science Foundation AI Institute for Intelligent Cyberinfrastructure with Computational Learning in the Environment (ICICLE). Led by The Ohio State University, the project will build the next generation of cyberinfrastructure and make AI easy for scientists and non-experts to use. OSC is one of three major supercomputer centers that will supply ICICLE with high performance computing and large-scale data storage.

Software

To ensure an increasing number of user communities can seamlessly carry out their research, OSC maintains a broad selection of applications, including over 200 software packages. Getting started guides can be found on OSC's website for most supported software, and OSC staff update and test these software packages regularly.

Gateways Development

The Ohio Supercomputer Center's (OSC) gateways development team helps streamline access to high performance computing (HPC) resources by assisting clients in the creation and maintenance of custom web interfaces. By simplifying workflows, users can direct their focus to their ongoing research and innovations.

OSC OnDemand

ondemand.osc.edu

OSC OnDemand serves as a central, web-based portal that provides efficient access to OSC's HPC and storage services. Users can upload and download files and create, edit and submit jobs without the need for software installation. A simplified classroom version of OSC OnDemand, available at class.osu.edu, has opened up HPC resources for classroom projects.

In fiscal year 2021, more than 1,000 users accessed OSC OnDemand each month, with almost 3,000 unique users in total.

Open OnDemand

openondemand.org

In 2015, OSC was awarded a National Science Foundation Grant (NSF #1534949) to make an open-source version of OnDemand available to other HPC facilities. Open OnDemand officially launched in 2017, followed by version 2.0 in 2021 supported by an additional NSF project award (NSF #1835725).

This interface equips HPC users at any level of expertise to efficiently utilize remote computing resources by making them easy to access from any device. Features of Open OnDemand include file management, command-line shell access, job management and monitoring across multiple batch servers and resource managers, and graphical desktop environments and applications.

Open OnDemand has been deployed by over 200 HPC centers around the world, more than half of which are located in the United States.

MyOSC

my.osc.edu

OSC's client portal, MyOSC, serves as the account management platform for OSC users. Clients can adjust passwords and contact information, manage project access, report funding and publications and run custom usage reports. The OSC team is continually working on updates to MyOSC to enhance the user experience and make the portal as useful and effective as possible.

Hardware Services

Cluster Computing

A leader in high performance computing and networking, the Ohio Supercomputer Center (OSC) serves as a vital resource for Ohio's researchers. With flexible and scalable clusters rivaling those found at National Science Foundation centers and other national labs, OSC supercomputers provide a peak computing performance of 5.5 petaflops. OSC routinely upgrades its clusters to ensure that researchers can access top-of-the-line supercomputing resources.

During FY 2021, OSC engineers deployed a new service to complement the Slurm HPC resource managers on the Owens and Pitzer clusters. The new service is based on the popular Kubernetes container open-source project. Like Slurm, this software helps manage distributed systems but complements the HPC resource manager.

OSC is supporting virtual computer labs for an initial group of 12 classes with nearly 400 students using this new service along with the OSC Open OnDemand software. Future use of the Kubernetes service will be focused on improving OSC's ability to support science gateways, data services and other workflow management software.

Research Data Storage

In autumn 2021, OSC worked with NetApp to upgrade storage and servers for OSC user home directories. The upgrade doubles the capacity and more than doubles the performance. Engineers are working to finalize the remote data backup site for the home and project directories at a location geographically distant from the Center to ensure data security and availability.

This project will provide a significant increase in the level of protection and resiliency OSC provides for its clients' data. It will also form the foundation of the long-planned research data archive.

In addition to the upgraded storage service, OSC has tape backup infrastructure capable of redundantly storing up to 23.5 PB of data.

OSC also provides Protected Data Service (PDS), which is designed to address the most common security control requirements encountered by researchers while also reducing the workload on individual PIs and research teams to satisfy these requirements. OSC currently supports protected data types including International Traffic in Arms Regulations (ITAR), Export Administration Regulations (EAR), Health Insurance Portability and Accountability Act of 1996 (HIPAA), personally identifiable information (PII) and proprietary data.

Photo: The IBM 3584 tape robot at OSC's data center provides more than 23.5 petabytes of highly reliable and secure backup storage.

Statistics

Client Scholarship & Savings

39% of Articles in Top 10% of Journals*

151 Funding Agencies Acknowledged*

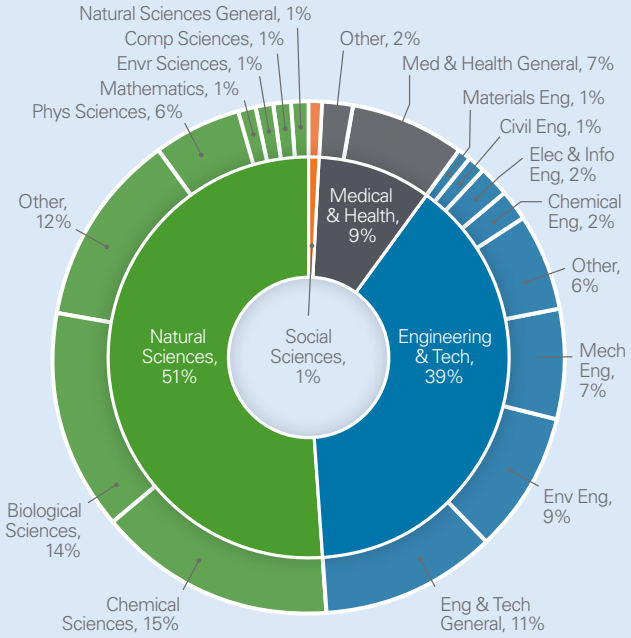
Est. Annual Cost Savings**

- $5.2M Ohio Higher Ed
- $1.6M Non-academic
  (includes Other Education, Non-profit/gov, Commercial)

$23.1M in Leveraged Capital Investments**

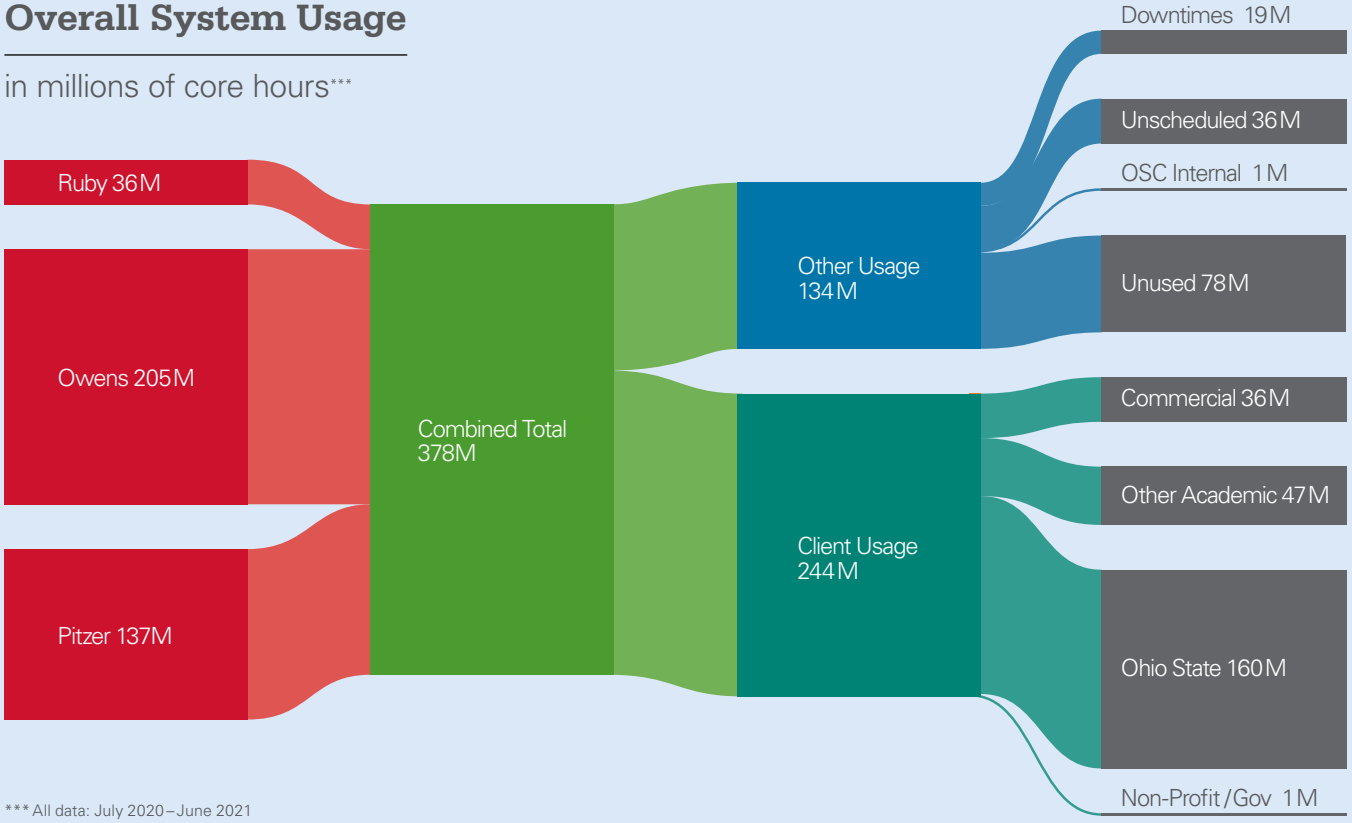
*Scholarship data 2016–2020
** Financial data FY2021

Usage by Field of Science



Overall System Usage

in millions of core hours***

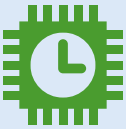


*** All data: July 2020–June 2021

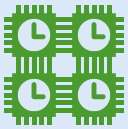
Supercomputers

OSC's current supercomputers include the Owens cluster, named for American Olympic hero and Ohio State graduate Jesse Owens, and the Pitzer cluster, whose namesake, Russell M. Pitzer, co-founded OSC and taught as a professor of chemistry at Ohio State.

233 M+
Cluster CPU Core Hours



1.5M+
GPU Hours



4.5 M+
Huge-Memory Core Hours

87%
Average System Utilization

75%
of Jobs Started Within 30 minutes

99.7%
Availability*

5.7 PB
Stored on Disk

65%
Average Storage Utilization

3.4 PB
Data Transferred

200+
Software Packages

*includes planned outages

Compute	Owens 2016	Pitzer 2018	Pitzer Expansion 2020	TOTALS
Cost	$7 million	$3.4 million	$4.3 million	$14.7 million
Theoretical Performance	~1.6 PF	~1.3 PF	~2.6 PF	~5.5 PF
Nodes	824	260	398	1,482
CPU Cores	23,392 Intel Broadwell	10,560 Intel Skylake	19,104 Intel Cascade Lake	53,056
RAM	~120 TB	~70.6 TB	~93.7 TB	~284 TB
GPUs	160 NVIDIA Pascal P100	64 NVIDIA Volta V100	102 NVIDIA Volta V100	326

twitter.com/osc
facebook.com/ohiosupercomputercenter
linkedin.com/company/ohio-supercomputer-center
osc.edu

Ohio Supercomputer Center
An OH·TECH Consortium Member

OH-TECH is the technology and information division of the Ohio Department of Higher Education.
1224 Kinnear Road | Columbus, OH 43212 | 614-292-9248