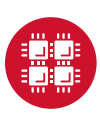
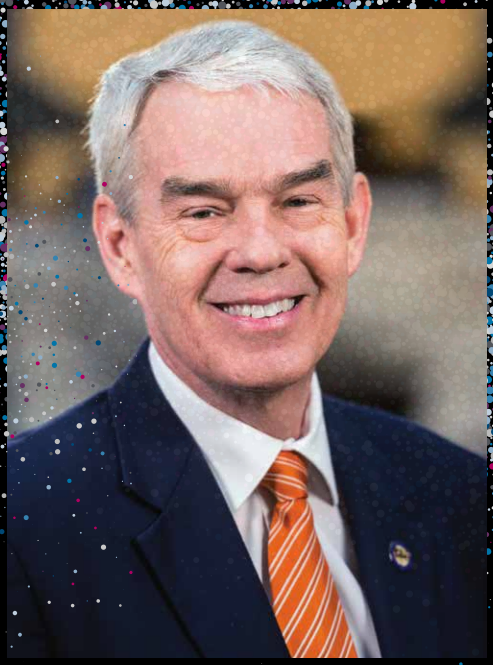
RESEARCH REPORT

2021–2022



Ohio Supercomputer Center



"With the new computing cluster Ascend and enhanced storage and backup services, the Ohio Supercomputer Center is well positioned to serve the needs of its academic, commercial and nonprofit clients and support workforce development initiatives such as Intel's manufacturing endeavors in the state."

— 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.

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Ohio Supercomputer Center

The Ohio Supercomputer Center (OSC) empowers Ohio higher educational institutions and private industry by providing capable, accessible, reliable and secure computational services enhanced by training, consulting and research partnership. Through OSC's high performance computational resources, the State of Ohio leverages significant economies of scale resulting in better services and cost savings. OSC can help position Ohio's higher educational institutions and companies as world leaders with a computationally enabled workforce and research endeavors.

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.

osc.edu

TABLE OF CONTENTS

TAGS

■ Area of Study

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.*

2021–22 HIGHLIGHTS

AI Bootcamps

With support from the NSF, OSC began hosting a series of free workshops to better prepare cyberinfrastructure professionals to provide computing and data services to a growing number of artificial intelligence research users. The 2022 bootcamps covered topics such as data science, machine learning, neural networks, Bayesian modeling, software and data.

Storage and Disaster Recovery

OSC has updated its project and global scratch service storage system to increase total capacity and performance. The Center also completed the development of a new disaster recovery location in Cleveland for data storage, which is a physical twin of the Columbus tape library.

Creating ACCESS to Cyberinfrastructure

OSC is collaborating on a five-year, $10 million NSF-funded initiative, led by the University of Colorado Boulder, to reimagine cyberinfrastructure user support services and delivery to keep pace with the evolving needs of academic scientific researchers. The initiative is part of the NSF's Advanced Cyberinfrastructure Coordination Ecosystem: Services and Support (ACCESS) program.

DIRECTOR'S LETTER

When the Ohio Supercomputer Center (OSC) contemplated the name for its newest high performance computing (HPC) cluster, we chose a word that reflected not only Ohio's history of innovation, but its future aspirations. "Ascend" references the state's track record of aviation and space breakthroughs while also capturing the optimism and ambition of the researchers, inventors and educators making advancements in the Buckeye State.

Launched in fall 2022, Ascend is OSC's first computing cluster devoted entirely to intensive graphics processing unit (GPU) work. The Dell Technologies-based HPC cluster with advanced NVIDIA GPUs can support the growing research fields of artificial intelligence (AI), machine learning, big data and data analytics in Ohio and beyond. We are pleased to offer this cutting-edge resource to our academic communities and commercial clients and look forward to watching your successes with it.

As the OSC staff initiated the new computing cluster, we also were excited to learn about Intel's $20 billion commitment to build one of the world's largest microchip manufacturing complexes in nearby Licking County, Ohio. We have been working with Intel closely for years to advance HPC.

Intel processors have been used in 13 supercomputer clusters, including 3,020 processors actively in use in the Owens and Pitzer clusters. The two organizations conducted joint case studies on Open OnDemand, the Center's open-source HPC web portal employed around the world. OSC also has worked with Intel on multiple test and pilot projects and has welcomed keynote speakers from the company at OSC Statewide User Group (SUG) conferences.

As workforce development is a core principle for OSC, we are well positioned to support the training of Ohioans in the semiconductor technologies that will be the focus of Intel's manufacturing complex, which is expected to employ 3,000 workers.

In addition to the Ascend and Intel projects, there are many other reasons why 2022 has been a productive and dynamic year for OSC. As you will learn from this year's Research Report, OSC has attracted National Science Foundation (NSF) funding to support more cyberinfrastructure services and artificial intelligence training. We have bolstered our data archive and disaster recovery offerings. And researchers and innovators across the state and nation—from small companies to public and private universities—are continuing to make great discoveries and product developments with the aid of OSC's supercomputing resources.

Whether you are a prospective, new or existing client, OSC has many services and resources that can help you advance your work. We invite you to read more about our offerings in this year's Research Report, and you are always welcome to reach out to us directly to learn more about how we can collaborate.

David E. Hudak, Ph.D.
Executive Director

IMPACT

OSC serves higher education, nonprofit, government, education and commercial communities in Ohio, with services available to clients across the nation and globe. From hardware and software offerings, computing resources and data storage, training and educational opportunities, OSC continued to make a measurable impact on clients' discovery, learning and innovation in the last year.

8,494
Clients

735
Trainees

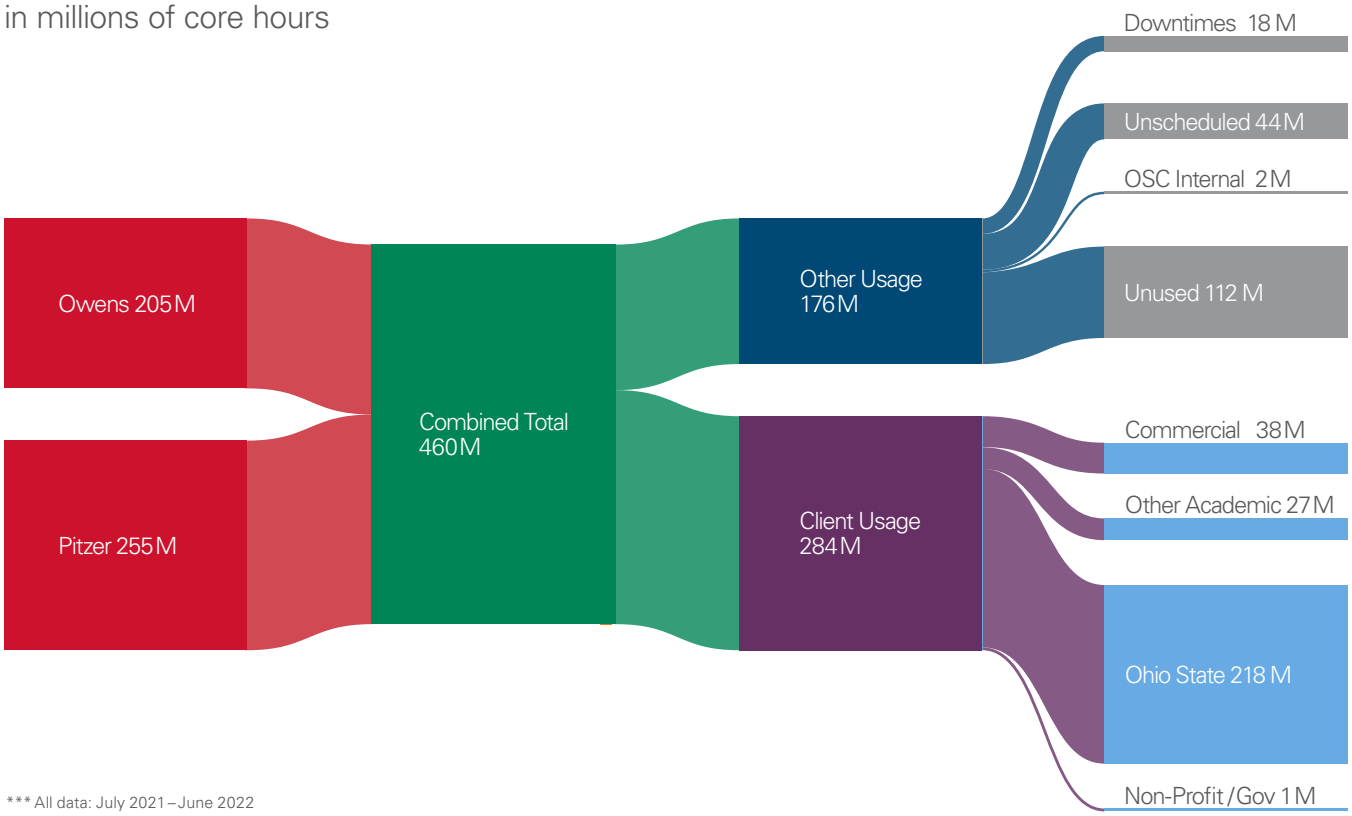
127
College Courses Used OSC Resources

29
Training Opportunities

$9.3+ MILLION
Estimated annual cost savings compared to commercial cloud

OVERALL SYSTEM USAGE

in millions of core hours



*** All data: July 2021 – June 2022

NEW GPU CLUSTER ASCEND

The Ohio Supercomputer Center (OSC) has launched Ascend, a new Dell Technologies-based high performance computing cluster with advanced NVIDIA graphics processing units (GPUs) to support artificial intelligence (AI), machine learning, big data and data analytics work.

Ascend is OSC's first computing cluster devoted entirely to intensive GPU processing, helping Ohio academia and industry elevate their research endeavors. The name Ascend evokes the state of Ohio's long history of advancements in the aviation and aeronautics fields.

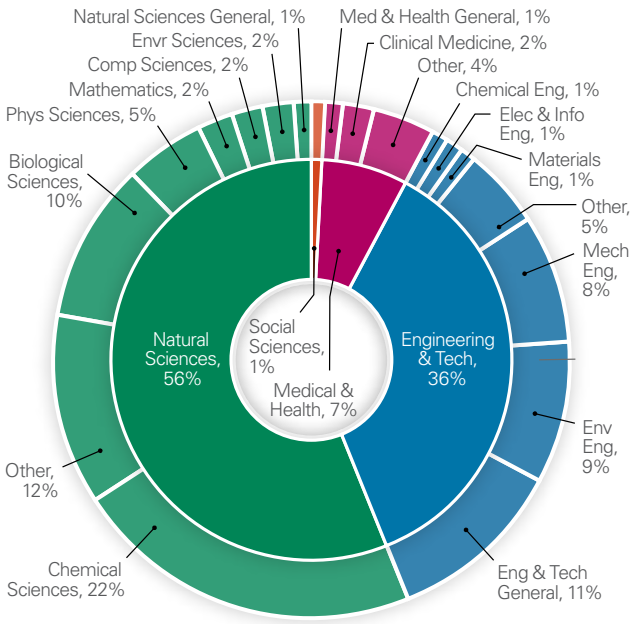
Dell Technologies designed and constructed the new system while AMD provided CPUs and NVIDIA supplied GPUs and InfiniBand networking. Ascend triples OSC's capacity for AI, modeling and simulation. The new system joins OSC's Pitzer and Owens clusters' current capabilities of 5.5 petaflops, more than 18 petabytes (PB) of disk storage capacity and more than 23.5 PB of expandable backup storage.

NEW HARDWARE SERVICES

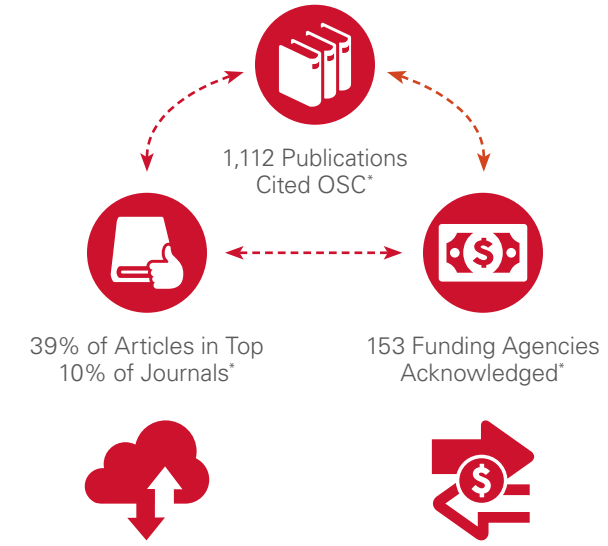
In October 2022, OSC retired the Data Direct Networks (DDN) GRIDScaler system and expanded the IBM Elastic Storage System (ESS) for both project and global scratch services. This initiative, which involved migrating over 6 PiB of data and over 500 million files, has significantly improved the performance of OSC's project and scratch storage.

A new disaster recovery location for data storage in Cleveland came online in early 2022. This initiative provided a physical twin of the Center's Columbus tape library, which currently backs up nearly 3 billion files with an aggregate size of over 8 PB. The tape backup infrastructure is capable of redundantly storing up to 23.5 PB of data and is anticipated to be scalable to more than 141 PB of capacity in the coming years.

USAGE BY FIELD OF STUDY



CLIENT SCHOLARSHIP & SAVINGS



*Scholarship data 2017–2021
** Financial data FY2022

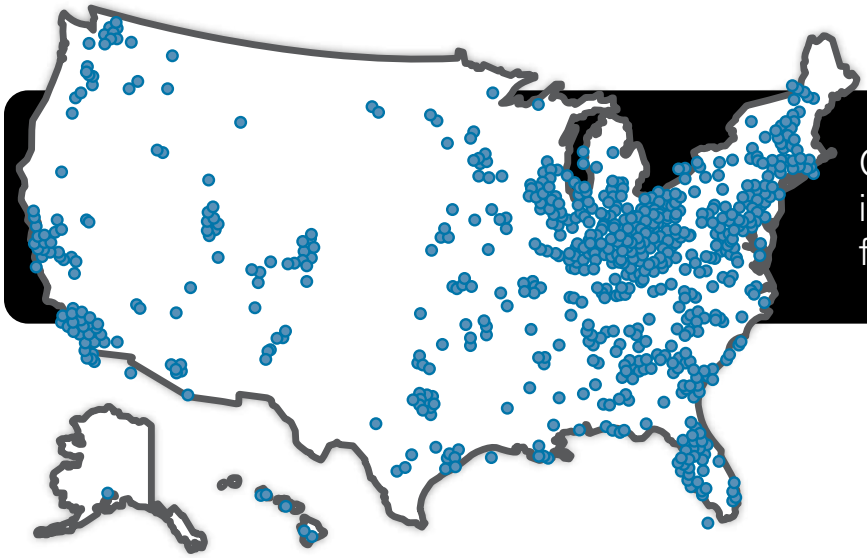
INTEL COLLABORATIONS

OSC and Intel have been working closely for years to advance the development of high performance computing. Intel's recent $20 billion commitment to construct one of the world's largest microchip manufacturing complexes or "fabs" in Licking County, Ohio, will open up new opportunities for this collaboration. The Center is well positioned to support the training of Ohioans in the semiconductor technologies produced by the manufacturing complex, which is expected to employ 3,000 workers.

Intel processors have been used in 13 supercomputer clusters at OSC, including 3,020 processors actively in use in the Owens and Pitzer clusters. The two organizations conducted joint case studies on Open OnDemand, the Center's homegrown, open-source HPC web portal now in use around the world, and OSC Director of Strategic Programs Alan Chalker sits on Intel's HPC Advisory Board. OSC has also worked with Intel on multiple test and pilot projects, as well as the modernization of WARP3D solid modeling software. Additionally, keynote speakers from Intel have appeared at multiple OSC Statewide User Group (SUG) conferences.

AI BOOTCAMP

With funding from the National Science Foundation, OSC has developed a series of free workshops to help cyberinfrastructure professionals gain expertise in burgeoning artificial intelligence (AI) technologies. The pilot program "AI Bootcamp for Cyberinfrastructure (CI) Professionals" launched in spring 2022 and will continue through 2023. The inaugural six-week bootcamp, taught by experts from The Ohio State University's Department of Computer Science and Engineering, attracted strong interest from cyberinfrastructure professionals at higher education and government research institutions across the county. OSC enrolled 62 professionals from 50 organizations in 28 states.



OSC served 8,494 clients in FY 2022, a 48% increase from the previous year

NATIONAL CYBERINFRASTRUCTURE INITIATIVE

OSC is collaborating on a five-year, $10 million National Science Foundation-funded initiative, led by the University of Colorado Boulder, to reimagine cyberinfrastructure user support services and delivery to keep pace with the evolving needs of academic scientific researchers. The initiative—part of a larger NSF program called Advanced Cyberinfrastructure Coordination Ecosystem: Services and Support (ACCESS)—will feature the use, design and development of OSC's Open OnDemand.

PRIORITY ACCESS FOR COVID RESEARCH

During the pandemic, OSC granted high priority computing access to COVID-19 research projects at no cost to clients. In 2020, 8.5 million core hours representing 59,258 jobs were dedicated to this work, which was led by researchers from institutions across Ohio. Projects included the development of an app that simulated the impact of public health policy decisions on infection spread; the identification of possible drug targets, interventions and therapies; an examination of the impact of disease misinformation; a study on the effect of stay-at-home orders; and development of a method to understand vaccine efficacy.

VIRTUAL TOUR

osc.edu/visit

A new virtual tour of the OSC data center allows visitors to explore our resources remotely. The interactive guide offers prospective and current users of our supercomputing clusters, as well as others interested in our program, an opportunity to look inside OSC's operations at the State of Ohio Computer Center in Columbus. To experience the virtual tour or learn about in-person tour options, explore the visit page of the OSC website.

STATEWIDE USERS GROUP CONFERENCE

The Statewide Users Group (SUG) conference provides a venue for the client community to learn more about OSC's vision, direction, services and resources, as well as provide input on the Center's plans.

The conference features keynote speakers such as **Jeff McVeigh of the Intel Corporation**, which plans to build a major new manufacturing facility in the Columbus area. McVeigh talked about Intel's overall technology development strategy, new products it will launch in the near future and plans for upcoming years.

SUG, which is held each fall and spring, also featured poster presentations and flash talks that highlighted new research findings from around the state of Ohio.

The award winners of the spring 2022 competition are:

- First place: **Dan Spakowicz,** The Ohio State University, "Exogenous sequences in unmapped tumor transcriptome data"
- Second place (tie): **Eric Hantz**, The Ohio State University, "Actives-Based Receptor Selection Strongly Increases Success Rate in Structure-

Based Drug Design;" **Caroline Wheeler**, The Ohio State University Wexner Medical Center, "The tumor microbiome correlates with response to immune checkpoint inhibitors in renal cell carcinoma."

The award winners of the 2021 fall competition are:

- First place: **Theresia Yazbeck**, The Ohio State University, "Modeling Fluxes, Fate And Transport Of Ammonia Emission From Egg Production And Manure Management Facilities."
- Second place (tie): **Alina Lazar**, Youngstown State University, "Accelerating the Inference Time of Machine Learning-based Track Finding Pipeline;" **Himanshu Singh**, Ohio University, "Predicting the Equilibrium Adsorption Morphologies of Surfactant Molecules on Metal Surfaces via Advanced MD Simulations."

SUMMER YOUTH EDUCATION PROGRAMS

OSC's signature youth education programs, the Summer Institute (SI) and Young Women's Summer Institute (YWSI), returned to in-person formats in 2022. Both programs are focused on introducing Ohio teens to STEM topics and helping them understand educational and career pathways.

3,490+ STUDENTS
FROM **23 OHIO UNIVERSITIES**
PARTICIPATED IN COURSES
USING OSC RESOURCES

Fifteen Ohio high school students toured research facilities at The Ohio State University and participated in interactive STEM projects that taught them how to use HPC resources during the two-week SI program. YWSI welcomed 15 middle school girls who studied a central Ohio watershed, learning how to analyze data, use new software programs and visualize results.

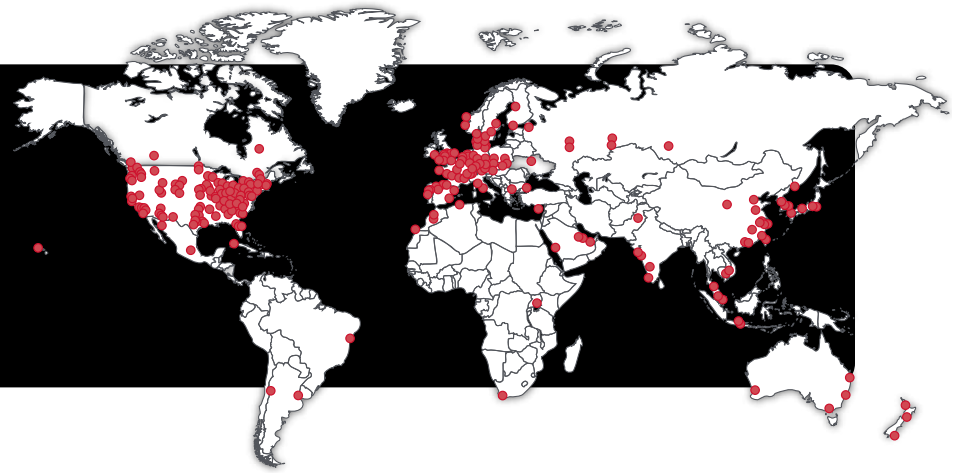
LEADERSHIP ROLE AT PEARC

Alan Chalker, OSC director of strategic programs, served as general co-chair of the 2022 Practice and Experience in Advanced Research Computing (PEARC) Conference Series, which was established in 2017 to address the changing needs of the advanced cyberinfrastructure community. PEARC22 attracted more than 660 registrations and 24 exhibitors. The agenda featured 141 distinct sessions, and 92 papers and posters were published in the proceedings. OSC also drew more than 150 participants to conference sessions and tutorials focused on use of its Open OnDemand product.

CONTINUOUS SERVICE DURING WEATHER EVENTS

Despite extreme weather events that have occurred in the last few years, the Center has been able to provide uninterrupted client access to its high performance computing clusters and data storage service. OSC is protected by a generator and backup system that provide resiliency and redundancy in its computing and storage equipment in the event of a power outage—even those that may persist for several days.

Open OnDemand has been deployed by nearly 400 HPC centers around the world



RESEARCH

Researchers and innovators from a wide range of entities—public and private higher education institutions, pharmaceutical and design companies—use OSC resources such as the Owens and Pitzer computing clusters and Open OnDemand portal to advance their research and product development and support student education experiences.

55
Ohio Colleges & Universities

68
Companies

54
Nonprofits & Govt. Agencies

200
Other Educational Institutions

CLASSROOM LEARNING

Professor builds Ohio State course around research using the Ohio Supercomputer Center

■ **Research Landscape** ▲ **Energy/Chemical**

Chris Hadad has been a client of the Ohio Supercomputer Center (OSC) for over two decades and leads one of the most active accounts. A professor of organic chemistry at The Ohio State University, Hadad is currently developing medical countermeasures against organophosphorus chemical nerve agents used in chemical warfare and as pesticides in agriculture.

More than 20 years ago, Hadad was inspired by the impact of OSC on his research to help others in the scientific community learn about and access high performance computing (HPC) resources.

"The idea I've always had was essentially to help develop expertise in different research groups on how they can use computational methods as a benefit to their experimental studies," he said.

To accomplish this goal, in 1996 Hadad developed a course at Ohio State, "Computational Chemistry," that teaches graduate-level students how to use HPC within their various fields of research.

Today Hadad has taught the course 16 times and has made a significant impact on students' education and careers. "Computational Chemistry" introduces students to real-world research using the HPC resources provided by OSC. The students choose their projects based on what interests them, and Hadad helps them tailor their use of OSC to find the answers they are seeking.

When Hadad began teaching this course, some students encountered difficulty using OSC, as they first needed to learn Unix commands to interface with the systems, the professor recalled. With the development of OSC's online portal Open OnDemand, much of this complexity has been eliminated, as OnDemand integrates software familiar to the students.

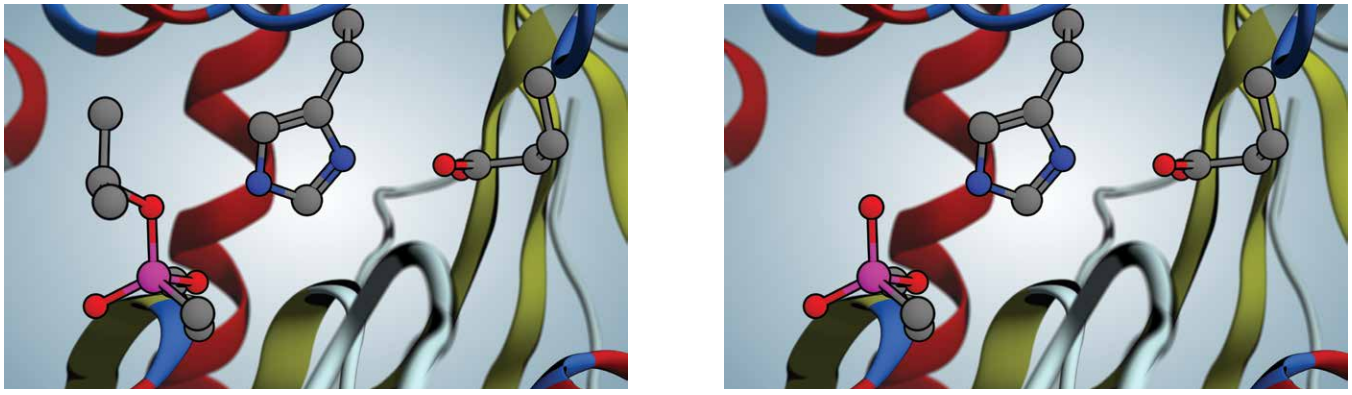
Not only are Hadad's students highly engaged in the classroom, but they also complete research that later may become the basis for their theses.

"Over 40 student projects have actually been published in different journals, many of them in some of the best journals in chemistry," Hadad said.

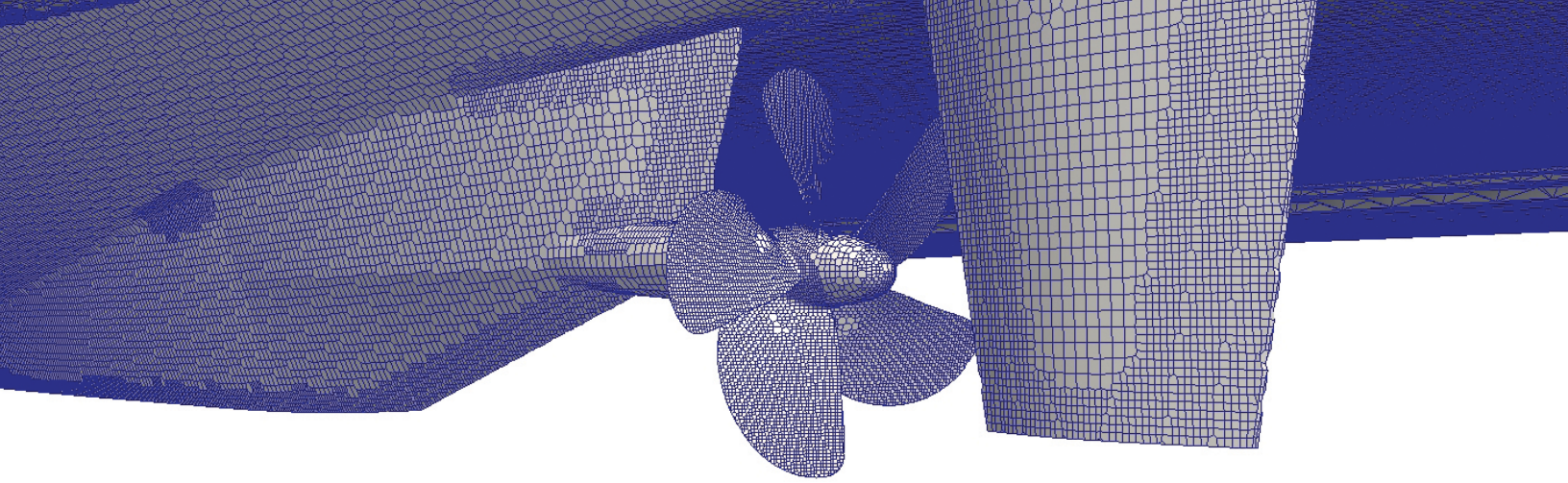
Hadad's integration of OSC within the classroom has helped disseminate HPC skills throughout educational and research communities.

"I've even had faculty take my class, including some faculty who have then gone on to other institutions to teach a computational chemistry class there," Hadad said.

Read and share online: osc.edu/r22/hadad



Left: Catalytic active site of OP-inhibited acetylcholinesterase by the nerve agent Sarin as generated in silico from the 5FPQ crystal structure. Right: Catalytic active site of OP-aged acetylcholinesterase by the nerve agent Sarin as generated in silico from the 5FPQ crystal structure.



PRODUCT DESIGN

Cotty Fay Marine Design uses HPC resources to study product performance, impact

■ Industrial Engagement **▲ Manufacturing**

Cotty Fay Marine Design is a small firm in Washington state that uses its engineering expertise to improve the design and performance of products, ranging from the mechanical parts on watercraft to the manufacturing equipment used by various industries.

Company owner Endicott (Cotty) M. Fay employs computational fluid dynamics to simulate how product designs may behave in—and impact—the environments in which they are intended to operate.

One example is a recent study he conducted for the National Marine Manufacturers Association, which asked him to evaluate the effect of wake surfing on lakeshore erosion and turbidity. Some lakes in the Midwest are prohibiting the water sport, in which surfers ride the waves created by a specially designed or outfitted motorboat, due to concerns about its possible environmental impact, Fay said.

To simulate the waves generated by the boats, Fay required significant computing resources. He used the Ohio Supercomputer Center's (OSC) Pitzer cluster and OpenFOAM software to run the calculations. By harnessing about 200 cores of processing power, the run took only about 48 hours to complete. Although Fay has his own advanced computer workstation, at 12 cores the same calculations "would have taken weeks—it wouldn't have worked," he said.

After reviewing the data and conducting further analyses, Fay and his colleagues determined that the sport did not have a significant detrimental impact on the shoreline or lake, according to their recent study published in the Journal of Water Resource and Protection.

In addition to the wake surfing work, Cotty Fay Marine Design has been hired by commercial and federal government clients to design mechanical components—such as propellers, rudders and nozzles—that can reduce watercraft noise and its environmental impacts. The noise from large ship propellers, for example, can disturb the feeding routines of whales, Fay said.

Although the marine industry has long been a focus for Fay, the company also has tackled design work for other fields. Fay has studied the wind loads on a conveyer system that transports wood chips over long distances for the production of paper products. The firm also has analyzed designs for hamburger patty manufacturing equipment, home air purifier systems, and a washing machine that can effectively clean plastic used for manufacturing plastic containers.

The common theme to the work is hydrodynamics, or the study of how water or air may flow and impact efficiency and noise of these various mechanical systems.

Cotty Fay Marine Design plans to continue to work with OSC on these projects, as Fay appreciates the flexibility, reliability and affordability of its resources.

"Using OSC helps from a business standpoint, as it allows me to afford to do the work. It helps American businesses become more competitive—it's a great service."

Read and share online: osc.edu/r22/cottyfay

Above: Cotty Fay Marine Design uses the OpenFOAM software for projects such as modeling noise levels from a ship propeller.

DATA ARCHIVES

Finding solutions for long-term research data storage needs

■ **Research Landscape** ▲ **Invention/Discovery**

Case Western Reserve University is one of the most research-intensive higher education institutions in the state of Ohio. Ranked R1 by the Carnegie Classification of Institutions of Higher Education, during fiscal year 2021 it attracted more than $390 million in competitive sponsored research projects.

With such high research activity, Case Western Reserve needs to manage and store a large amount of data. Researchers often must meet requirements set by their funding agencies, academic publishers and home institution to retain study data for several years, in case that data needs to be audited or reproduced.

Case Western Reserve had been storing archival research data in a tape-based system hosted by the institution, but recently began exploring alternative options that would shift the maintenance and administration to an outside service, said Mike Warfe, director of research computing. After evaluating several national information technology vendors, Case Western Reserve chose to work with the Ohio Supercomputer Center (OSC).

"We decided to use OSC primarily because of network capacity—we're both on the 100 Gigabits per second (Gbps) OARnet network," Warfe said. "Not having to worry about network bandwidth or any hidden fees made the storage option at OSC very attractive to us."

Another draw was Case Western Reserve's ability to use OSC's Globus Connect subscription to transfer its data across networks at very high speeds, Warfe said. Once OSC created a Globus resource for the university to use, Case Western Reserve could administer it directly and autonomously.

Warfe also cited the affordable cost of using OSC as a benefit to Case Western Reserve and its researchers. With reasonable fees and adequate data storage capacity, OSC is an attractive alternative to other options on the market that recently have become more expensive or more limited in capacity, he said.

"It's a service that the campus community values, and it helps researchers with some of the challenges they have with data management," Warfe said.

Case Western Reserve began its data transfer to OSC in late 2021 and is continuing the project through 2022. The institution plans to store over 1 Petabyte of data, Warfe said.

Although the data archive partnership is new, the two institutions have collaborated previously. Warfe and his colleagues also are actively involved with OSC through their participation in the Statewide Users Group (SUG) and other working committees. Case Western Reserve and OSC mutually benefit from this engagement, as Warfe can inform OSC about the latest needs of his university's researchers while also learning about the newest OSC resources and services that may benefit his institution.

Read and share online: osc.edu/r22/cwru

ARTIFICIAL INTELLIGENCE

Natural language processing makes sense of vast volume of content

■ **Research Landscape** ▲ **Invention/Discovery**

While natural language processing may not have much name recognition among the general public, many people rely on it every day. Using Google to find information online? The search engine employs natural language processing to comb through and analyze massive numbers of webpages and return the most relevant answers.

Huan Sun, an associate professor in the Department of Computer Science and Engineering at The Ohio State University, is fascinated by natural language processing, a subfield of artificial intelligence, and its many applications. With the aid of the high performance computing (HPC) power of the Ohio Supercomputer Center (OSC), Sun and her students have garnered scientific awards for their findings on the subject.

In one recent project, the Sun group created deep learning models that can review the content contained within tables commonly used on websites and understand the relationship between the pieces of information. While conventional search engines refer the user only to the table itself, the deep learning models take a step further and extract and analyze information from the tables, Sun explained.

In a separate study, the Ohio State researchers collaborated with Nationwide Children's Hospital to create a system that makes the wealth of information buried in clinical texts more accessible. In addition to helping clinicians save time reviewing and drawing conclusions from individual clinical notes, the system also allows them to submit specific questions for analysis, Sun said.

Through her participation in Ohio State's new AI Institute for Intelligent Cyberinfrastructure with Computational Learning in the Environment (ICICLE), which is a National Science Foundation (NSF) AI Institute, Sun is expanding her natural language processing work to other domains. The initiative, in which OSC serves as a key HPC resource, has allowed Sun to create additional partnerships with researchers in bioinformatics, biomedical sciences, public health and environmental sciences.

Within ICICLE, Sun is focused on applying conversational artificial intelligence, which is concerned with building natural language interfaces, to various problems. Her group currently is helping ICICLE's foodshed research team use the technology in a study of the impact of grocery store closures on residents' food access.

Regardless of the research project, Sun and her students rely on OSC resources, using both Pitzer and Owens clusters.

"We use OSC for almost every single project that we're doing," Sun said. "We've been very happy to acknowledge them in almost every single paper we publish."

Sun appreciates the $1,000 annual faculty credit that she can use towards OSC services, as well as the fast technical support that keeps her studies moving forward. OSC has helped Sun meet project goals, which in turn has attracted additional support—such as NSF funding—to advance her natural language processing research.

Read and share online: osc.edu/r22/sun

PRECISION MEDICINE

Karyopharm Therapeutics scientists search for biomarkers to yield targeted patient treatments

■ **Industrial Engagement** ▲ **Invention/Discovery**

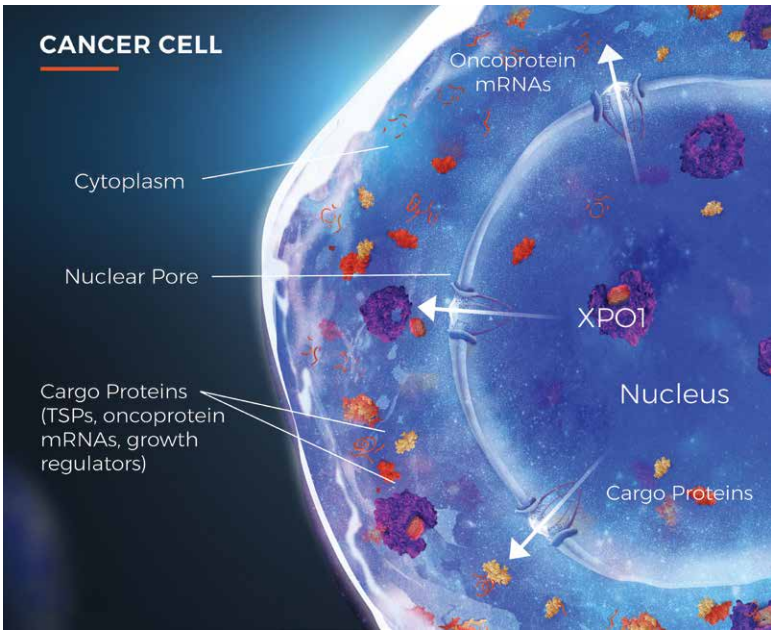
A drug designed to treat a certain type of cancerous tumor might work well in some patients but not others. To determine why, scientists can study whether specific genetic mutations may impact the therapy's effectiveness.

Karyopharm Therapeutics, a commercial-stage pharmaceutical company pioneering novel cancer therapies, is taking a closer look at these unique molecular characteristics of different cancers with the help of the Ohio Supercomputer Center (OSC).

Karyopharm's lead selective inhibitor of nuclear export (SINE) compound and first-in-class, oral exportin 1 (XPO1) inhibitor, XPOVIO® (selinexor), is approved in the U.S. Selinexor is marketed by the company in three oncology indications and has received regulatory approvals in various indications in a growing number of ex-U.S. territories and countries, including Europe and the United Kingdom (as NEXPOVIO®), China and Singapore.

Christopher Walker, an alumnus of The Ohio State University, serves as the company's director of bioinformatics. Walker conducts genetic sequencing of cancerous tumors and analyzes data to help Karyopharm predict potential responsiveness and whether or not selinexor may be effective in a certain population. The work requires high performance computing power and relevant software programs that can manage a large volume of raw DNA and RNA sequencing data.

During his time as a postdoctoral and research fellow at Ohio State, Walker conducted oncology research using OSC resources. After joining Karyopharm Therapeutics, Walker sought to establish a bioinformatics infrastructure for the company and determined that OSC would be a valuable asset. Working with OSC to enhance the pharmaceutical company's bioinformatics capabilities has been preferable to trying to build or maintain such resources in-house, he said.



The karyopherin protein exportin 1 (XPO1) facilitates the shuttling of hundreds of its cargo proteins from the nucleus to the cytoplasm. XPO1 is over-expressed by many types of cancer cells.

"The infrastructure is there—it's set up to be really easy to use—and the software we use for processing next-generation sequencing data is preloaded and well-maintained at OSC," Walker said.

The research partnership is yielding useful results for Karyopharm Therapeutics. In a published study of patients with advanced, refractory dedifferentiated liposarcoma, for which selinexor is being investigated, Walker and colleagues found that selinexor treatment may be effective against tumors that did not express a gene called CALB1. Additionally, at the 2022 American Society of Clinical Oncology conference, results from Karyopharm's Phase III SIENDO study were presented, showing that TP53 mutation status may be associated with response to selinexor. Further investigation is needed.

Walker is excited about a new era in science in which bioinformatics may be used to predict the patients most likely to benefit from new therapies.

"You'll find more and more drugs being approved for specific malignancies with a specific mutation type and maybe even with a specific expression profile at the RNA level in the near future," Walker said. "That's what I envision in the field."

Read and share online: osc.edu/r22/karyopharm

WEB PORTALS

Open OnDemand aids engineering school's supercomputing curriculum

■ **Research Landscape** ▲ **Invention/Discovery**

In 2019, the Milwaukee School of Engineering (MSOE) unveiled a major addition to its campus: the Dwight and Dian Diercks Computational Science Hall, featuring Rosie the supercomputer. The facility opened in the wake of the launch of MSOE's bachelor's degree in computer science, with a curriculum focused on the growing field of artificial intelligence.

Alumnus Dwight Diercks, who along with his wife Dian donated $34 million for the facility, has worked for the technology company NVIDIA since 1994 and today serves as its senior vice president of software engineering. MSOE worked closely with the company on assembling the necessary hardware and software for the supercomputer, which features NVIDIA graphics processing units (GPUs).

NVIDIA recommended that MSOE adopt Open OnDemand, an open-source high performance computing portal developed by the Ohio Supercomputer Center (OSC). Open OnDemand is used by researchers and college students around the world to access supercomputing resources anywhere from any device.

Derek Riley, a professor and program director for electrical engineering and computer science at MSOE, reports that most of the jobs run on Rosie use the Open OnDemand portal. MSOE established the supercomputer primarily as a teaching tool for undergraduates studying machine learning and data science, and Open OnDemand has made it easy for them to directly access Rosie, Riley said. Students can avoid time-consuming technical setups and instead gain more experience using the supercomputer to answer a variety of scientific and engineering questions.

"It can't be overstated how important it is for students to focus on the problems we want them to learn," he said.

MSOE's approach to supercomputing also reflects the work environment that many students will find themselves in after graduation, as most employers have engineering teams that handle the more technical aspects of supercomputer setup and maintenance while the data scientists conduct analyses, Riley said.

Not only has Open OnDemand been beneficial for undergraduates to use, but MSOE's own system administrators have found it easy to learn and manage, Riley said.

"We've had a really great experience using it—we've been really happy with it," he said. "We've been able to use it primarily out of the box, and it's the main entry point for students and faculty to the cluster."

Read and share online: osc.edu/r22/msoe

Above: Rosie the supercomputer supports the Milwaukee School of Engineering's computer science program.
Image courtesy of Milwaukee School of Engineering.

IMMUNE-ENGINEERING

Researchers use deep neural networks to predict transcription factor binding

■ **Biological Sciences** ▲ **Invention/Discovery**

Emily Miraldi, assistant professor in the Divisions of Immunobiology and Biomedical Informatics at Cincinnati Children's Hospital, Department of Pediatrics at University of Cincinnati School of Medicine, leads an "immune-engineering" research group that uses mathematical modeling of the immune system to predict immune responses and understand disease.

The Ohio Supercomputer Center (OSC) plays an important role in the research, as Miraldi has needed high performance computing resources to solve computationally demanding mathematical problems.

"The biological question motivating my work at OSC is a very famous one: Cells in the human body share a common DNA blueprint but have a great diversity of functions and behaviors," Miraldi said.

The diversity of cell types in the human body are driven by unique patterns of gene expression, which are controlled by proteins called transcription factors. Aberrant gene expression patterns are a hallmark of many diseases and can be traced to altered gene regulation by transcription factors, Miraldi explained.

"Discovering the transcription factors that control disease-associated gene expression provides an opportunity to develop therapies that might target those transcription factors to improve disease outcomes in the 'poorly behaving' cell types," Miraldi said.

In an article published in the journal Genome Research, Miraldi's team recently showed that a new data type called "Assay for Transposase Accessible Chromatin" (ATAC-seq), could identify transcription factor regulators of gene expression across cell types (Miraldi et al. (2019) Genome Research, Pokrovskii et al. (2019) Immunity).

Before having access to OSC's high performance computing resources, the team's studies used simple mathematical models to predict the transcription factor binding from ATAC-seq. With more computational capability, Miraldi began using deep neural network models, which enabled her to improve the accuracy of the transcription factor binding predictions.

"We initially used ATAC-seq data in a crude way to infer transcription factor binding sites, but, taking advantage of the high performance computing resources at OSC, were able to use the latest advances in deep neural network modeling to more accurately predict transcription factor binding events from ATAC-seq."

The resulting collection of open-source, user-friendly deep neural network models is called "maxATAC." The maxATAC models can be used by other research groups to predict transcription factor binding from ATAC-seq in any human cell type—including single-cell (sc) ATAC-seq, which is now a standard technology at many research institutions.

"Transcription factor binding prediction scATAC-seq is especially valuable at Cincinnati Children's Hospital, where there is great desire to understand gene regulation and disease mechanisms from scarce patient samples (e.g., cancer tumor biopsies, transplant rejection) that can only be analyzed by single-cell technologies," she said.

Read and share online: osc.edu/r22/miraldi

Dr. Emily Miraldi (center) along with graduate students Tareian Cazares (left) and Faiz Rizvi (right) lead the multi-lab maxATAC modeling collaboration at Cincinnati Children's Hospital.

ENGINEERING INNOVATIONS

Researchers examine pipeline corrosion at the molecular level

■ **Industrial Engagement** ▲ **Energy/Chemical**

When he joined the Ohio University faculty in 2015, Sumit Sharma found a new application for his expertise in molecular modeling and simulations: understanding pipeline corrosion.

The university's Institute for Corrosion and Multiphase Technology investigates the causes of—and solutions for—this costly problem for the oil and gas industry. Although energy companies had been adding corrosion inhibitors to pipelines, the industry wanted to learn more about how the inhibitors work at the molecular level, Sharma said.

Corrosion inhibitors are surfactants, or substances that adhere to the interfaces of oil and water or metal and water. Drawing on his expertise with modeling surfactant behavior, Sharma's research group developed new tools that can predict how these molecules will adhere to the surface of the metal pipelines. The models help pipeline engineers understand how changing the chemical makeup of the corrosion inhibitors leads to changes in their effectiveness in the field. Understanding the workings of corrosion inhibitors will help reduce unforeseen corrosion-related failures of pipelines, which previously have been linked to numerous accidents that have resulted in the loss of lives, injuries and significant damage to the environment, Sharma said.

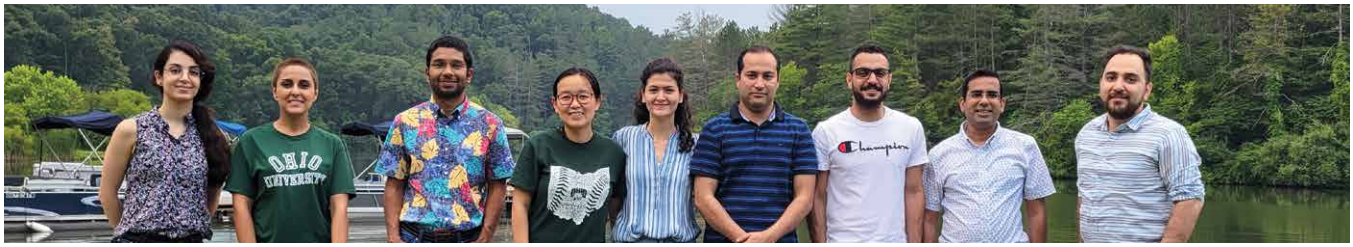
"We are working on solving practical engineering problems by studying the underlying basic science that various industries can use, and the use goes beyond the systems that we are studying," Sharma said about the broad applications of their research approaches.

Because molecules can very densely pack themselves on surfaces, the researchers needed high performance computing power to obtain a close, detailed look at their behavior. Ohio University pointed Sharma to the Ohio Supercomputer Center (OSC), which he now uses for molecular simulations. These high-performance simulations consume more than a million CPU hours at OSC in a typical year.

Sharma has two grants from the National Science Foundation (NSF), and so he also makes use of the federal agency's Extreme Science and Engineering Discovery Environment (XSEDE) computing services to advance his work.

The researcher will continue to harness these various supercomputing resources to tackle other molecular modeling and simulation challenges. Sharma currently is studying how surfactants interface with metallic nanoparticles, which may be used in bioimaging and drug delivery in the human body. Adding surfactants to the nanoparticles can prompt them to form certain shapes that make them useful for applications such as invading and killing cancer cells. The NSF awarded Sharma a prestigious five-year Faculty Early Career Development (CAREER) grant to support the metallic nanoparticles work in 2021.

Read and share online: osc.edu/r22/sharma



Sumit Sharma (second from right) and his research group at Ohio University utilize expertise in molecular modeling and simulations to study issues such as pipeline corrosion and drug delivery.

COMPUTATIONAL CHEMISTRY

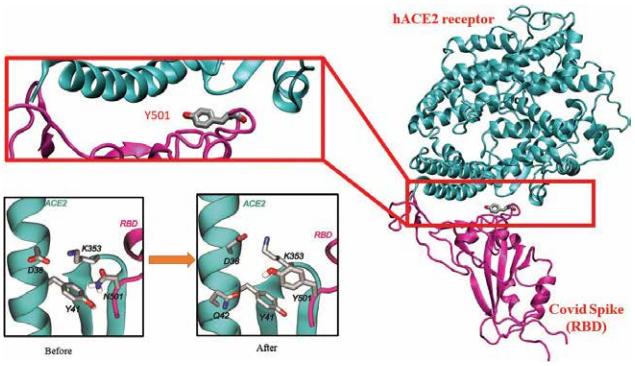
Scientists discover why some molecular mutations make COVID-19 more contagious

■ **Research Landscape** ▲ **Energy/Chemical**

With the COVID-19 pandemic presenting an ongoing global challenge, Xiche Hu's lab at the University of Toledo is taking a closer look at the mutations of the coronavirus.

For more than 20 years, Hu's lab has been researching an issue known as molecular recognition, which is how two molecules locate each other and bind together to perform a biological function. When the COVID-19 pandemic started, Hu wondered if his molecular recognition expertise could help scientists understand how the coronavirus identifies the right receptors to bind to in the human body to trigger infection.

"We immediately realized that there were many molecular recognition issues, so we felt duty bound to study this," he said. "The Ohio Supercomputer Center (OSC) had called for researchers studying the coronavirus, offering a special grant. We applied and were granted priority access and an unlimited budget for 18 months."



Right panel: A figure displaying the binding of the receptor binding domain (RBD, colored in magenta) of the mutated SARS-CoV-2 spike protein with the human cell surface receptor ACE2 (hACE2, colored in cyan). Lower left panel: the binding interactions for the 501th residue of SARs-CoV2 before and after the N501Y mutation.

Hu and two doctoral students at University of Toledo, Pawan Bhatta and Majed Aljohani, began by studying the atomic-level differences between the original SARS-CoV-2 and the new variants of concern.

Using high-level quantum mechanics calculations, Hu's group can determine the binding energy between COVID-19's spike proteins and the human receptors within the cell. A greater binding energy can make the virus more contagious.

Making an accurate calculation of binding energy requires highly complex computational algorithms and vast computational resources.

"If we did one of these calculations in our lab, we are talking about weeks or months, but when we do it at OSC we can finish it within days," Hu said. "We often need to do multiple calculations in parallel, so the OSC resources are instrumental to this research."

In four out of five variants of concern, researchers found that a common mutation, N501Y, increased the binding energy between parts of the human cell and the virus. In addition, the scientists discovered that the mutation enables the virus to form a network of water molecules that boosts the variant's ability to infect cells.

These discoveries may allow the scientific community to further develop methods to fight the COVID-19 pandemic.

"With this research we can move to the next step, screening a library of compounds to find which molecules can block out this site, preventing infection," Hu said.

Read and share online: osc.edu/r22/hu

RESOURCES

Current and prospective clients can take advantage of OSC's many technical resources, from computing clusters and hardware services to software packages and web portals. OSC also supports clients by providing easy access to technical expertise, workshops and training sessions, and educational and networking events.

233 M+
Cluster CPU Core Hours

1.5 M+
GPU Hours

4.5 M+
Huge-Memory Core Hours

87%
Average System Utilization

75%
of Jobs Started Within 30 Minutes

EDUCATION AND TRAINING

Workshops and Training

Clients and potential users can register for workshops, one-on-one classes, web-based training and consulting services. Topics include getting started using OSC, containers for research computing and performance tuning.

Virtual Computer Labs

Faculty can request classroom accounts for students to use HPC resources in research or coursework at no cost.

SUG Poster Competition

College student users can sign up to present their HPC research at the Statewide Users Group conference, held every spring and fall, and receive awards for their work.

Youth STEM Programs

Middle school and high school teens in Ohio can apply to participate in the Summer Institute (SI) or Young Women's Summer Institute (YWSI) to gain experience with STEM research that can help them choose educational and career paths.

CLIENT SUPPORT

Office Hours

Speak directly with OSC experts through virtual consultations. Visit osc.edu/events to see the full schedule of office hours and sign up for a time.

Technical Support

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/start
- Technical Support: osc.edu/support
- OSC Help Desk: Basic and advanced support, Monday through Friday, 9 a.m. to 5 p.m., oschelp@osc.edu or 614-292-1800.
- Real-time System Status Updates: Follow @HPCNotices on Twitter

Consulting

Consult with OSC staff experts on HPC and software engineering issues, including optimizing code and debugging.

Research Collaboration

Find collaborators on the OSC staff for various research and education projects, including major new grant-funded interdisciplinary initiatives.

SOFTWARE AND WEB PORTALS

Software

Utilize a broad selection of applications, including more than 200 software packages that OSC staff update and test regularly, as well as getting started guides.

OnDemand

Access OSC's HPC and storage services through OnDemand, a central, web-based portal. Users can upload and download files and create, edit and submit jobs without the need for software installation. A simplified classroom version is available at class.osc.edu.

Open OnDemand

Remotely use the open-source version of OnDemand, supported by the National Science Foundation, from any device. Features include file management, command-line shell access, job management and monitoring across multiple

99.7%
Availability*

5.7 PB
Stored on Disk

65%
Average Storage Utilization

3.4 PB
Data Transferred

200+
Software Packages

*includes planned outages

batch servers and resource managers, and graphical desktop environments and applications.

MyOSC

Manage your account through OSC's client portal. Clients can adjust passwords and contact information, manage project access, report funding and publications and run custom usage reports. The OSC team continually updates MyOSC to enhance the user experience.

HARDWARE SERVICES

Cluster Computing

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 7.5 Petaflops. OSC routinely upgrades its clusters to ensure that researchers can access top-of-the-line supercomputing resources.

Research Data Storage

Researchers can access upgraded storage services and a tape backup infrastructure capable of redundantly storing up to 23.5 PB of data. Protected Data Service (PDS) addresses the most common security control requirements encountered by researchers. Protected data types include 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.

Globus Server

This free cloud-based service allows clients to move, share and discover research data through a single interface, regardless of its location or number of files or size. Globus is used extensively at supercomputer centers and major research facilities.

Ascend is OSC's new Dell Technologies-based high performance computing cluster with advanced NVIDIA graphics processing units (GPUs).

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. The name of OSC's new cluster, Ascend, evokes the state of Ohio's long history of advancements in the aviation and aeronautics fields.

Compute	**Owens** 2016	**Pitzer** 2018	**Pitzer Expansion** 2020	**Ascend** 2022	**TOTALS**
Cost	$7 million	$3.4 million	$4.3 million	$1.8 million	$16.5 million
Theoretical Performance	~1.6 PF	~1.3 PF	~2.6 PF	~2 PF	~7.5 PF
Nodes	824	260	398	24	1,506
CPU Cores	23,392 Intel Broadwell	10,560 Intel Skylake	19,104 Intel Cascade Lake	2,304 AMD Milan	55,360
RAM	~120 TB	~70.6 TB	~93.7 TB	~24 TB	~308.3 TB
GPUs	160 NVIDIA Pascal P100	64 NVIDIA Volta V100	102 NVIDIA Volta V100	96 NVIDIA Ampere A100	422

ENGAGEMENT

Statewide Users Group
Join the software or hardware and operations committee on our Statewide Users Group to contribute to OSC's planning efforts and help shape services and resources.

Researcher Recognition
Nominate yourself or a colleague for recognition in OSC communications by submitting your research accomplishments and news.

Campus Champions
Advocate for OSC's HPC resources at your academic institution and receive project accounts with no-cost access to a range of OSC services.

Client Continuity
Inquire about opportunities to continue to use OSC resources at your next institution or private sector employer.

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