Research Report

2017–2018

Ohio Supercomputer Center
An OH·TECH Consortium Member

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"Researchers at universities, businesses, and laboratories across the state leverage the powerful high performance computing systems, services, and expertise of the Ohio Supercomputer Center to help make new discoveries, produce amazing innovations, train a high-tech workforce, and provide a solid foundation for Ohio's future prosperity."

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

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

Tag Index

• Type of computing

Data-intensive computing
High performance computing
High throughput computing

■ Resource type

Dense compute
GPU
Huge Memory

▲ Service type

Education
Facilitation
Research Data Storage
Research Partnership
Scientific Software Development
Visualization & Virtual Environments
Web Software Development

◆ Research field

Engineering & Technology
Natural Sciences
Social Sciences

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

Ohio Technology Consortium: Governed by the Chancellor of the Ohio Department of Higher Education, 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.

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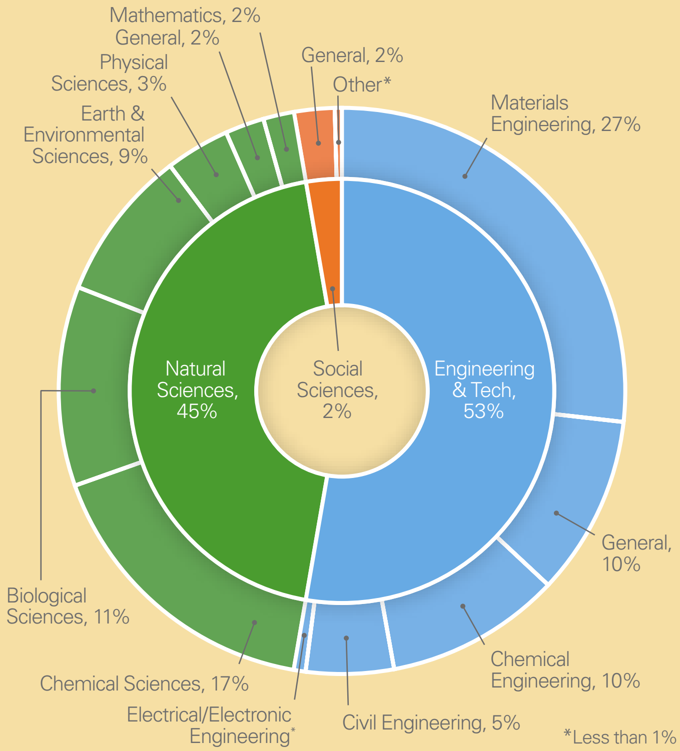
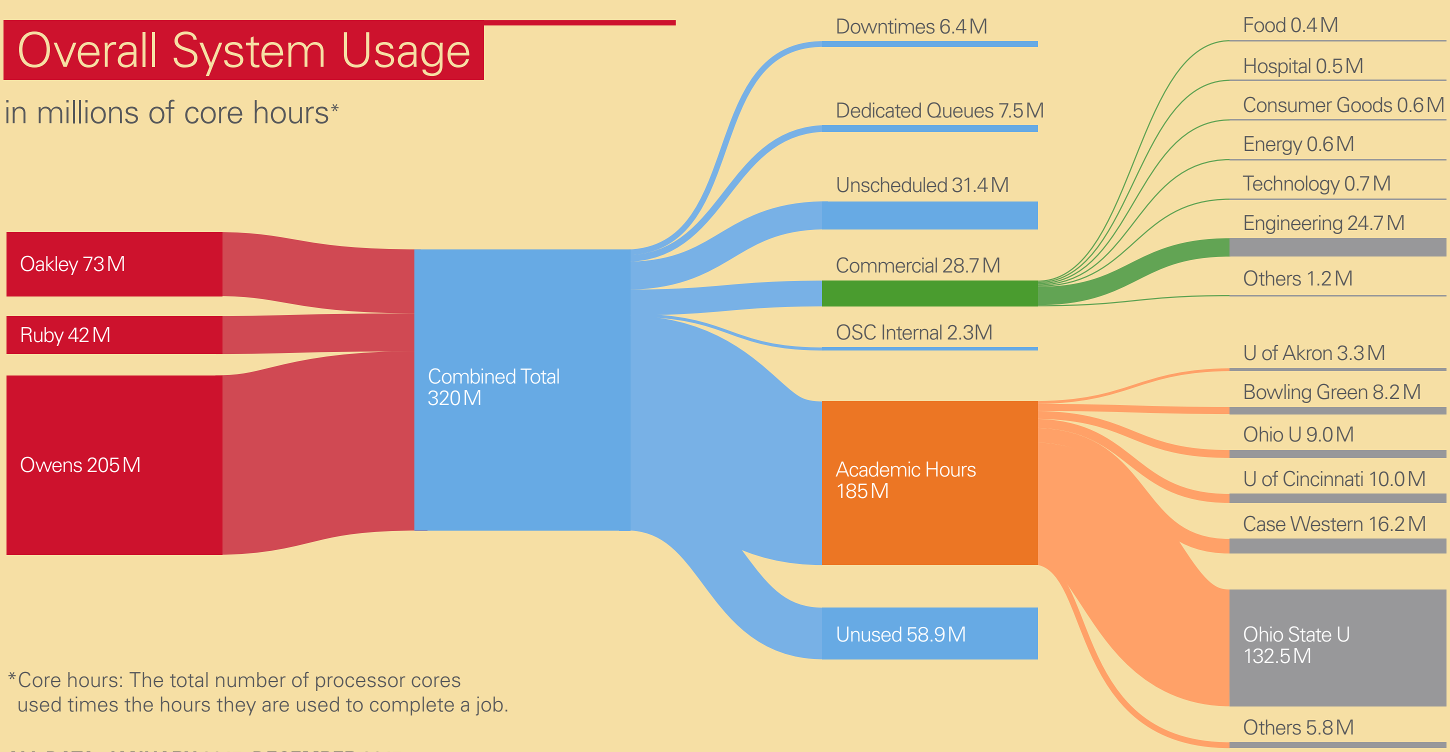
Active Academic Projects

Academic Fields of Science



Overall System Usage

in millions of core hours*



*Core hours: The total number of processor cores used times the hours they are used to complete a job.

ALL DATA: JANUARY 2017–DECEMBER 2017

OSC Overview

The Ohio Supercomputer Center was established in 1987 to "place Ohio's research universities and private industry in the forefront of computational research." Today, more than 30 years later, the Center continues to provide researchers and faculty members across Ohio with the resources, services and expertise that bolster graduate education, provide a foundation for discoveries and help propel innovation.

In 2017–18, OSC increased support the use of high performance computing in the classroom, expanded its statewide training efforts, increased collaboration, extended consulting efforts and promoted its innovative web-based, open-source HPC portal. The Center also refined its streamlined but thorough allocations procedures, upgraded storage systems and began the aquisition process for its newest HPC system—the Dell/Intel Xeon Pitzer Cluster.

Education

Research using OSC services spans a variety of disciplines, such as medicine, business, computer science, economics, engineering, chemistry, mathematics and physics, at various types of institutions—public and private, large and small. Computationally based research programs at many of the state's large universities play an integral role in the graduate education of many students. Poster and flash-talk competitions held at the Center twice each year allow student and faculty members the opportunity to publicly present their work—practice they need to help earn the higher degrees and accolades they seek.

OSC staff also assist faculty and student researchers by making classroom accounts available for professors who want to incorporate HPC resources into courses. In 2017–18, there were more than 30 instances of colleges and universities leveraging OSC services for instructional purposes, either in the classroom or the laboratory.

Ohio high school students and middle school girls receive extraordinary STEM education through first-hand application of high performance computing and networking during OSC's annual Summer Institute (SI) and the Young Women's Summer Institute (YWSI).

Training

For faculty, student and industry researchers who lack institutional knowledge of the Center—especially as people in new fields come to realize the usefulness of HPC resources—OSC staff members address their learning gaps by providing workshops, one-on-one consulting, web-based training materials. In-person office hours are also offered every other Tuesday in Columbus during the academic year.

In 2017–18, OSC staff nearly tripled the amount of training opportunities offered around the state, instructing 461 academic and industry users on HPC systems and OSC-specific programs.

Collaboration

Since its inception, OSC staff members have sought to partner strategically with Ohio researchers in developing competitive, collaborative proposals to regional, national and international funding organizations to solve some of the world's most challenging scientific and engineering problems.

At the most basic level, staff assist researchers by providing customized letters of commitment to show they have access to vital resources, by providing text describing OSC's computing and storage facilities and data retention policies and by providing quotes for specialized services, such as dedicated computing resources, large storage,

(continued on page 4)

PHOTO // David Hudak, Ph.D., Executive Director

(continued from page 3)

HPC consulting, etc. In 2017, staff collaborated on projects with numerous researchers, including:

DK Panda, Ph.D., professor of Computer Science and Engineering at The Ohio State University

- Next Generation Communication Mechanisms exploiting Heterogeneity, Hierarchy and Concurrency for Emerging HPC Systems
- FAMII: High Performance and Scalable Fabric Analysis, Monitoring and Introspection Infrastructure for HPC and Big Data

Ian Howat, Ph.D., director of the Byrd Polar & Climate Research Center at The Ohio State University

- Automated, High Resolution Terrain Generation for XSEDE

Michael Sokoloff, Ph.D., professor of Physics at the University of Cincinnati

- Enabling High Energy Physics at the Information Frontier Using GPUs and Other Many/Multi-Core Architectures

Raghu Machiraju, Ph.D., TDAI Interim Executive Director; professor of Computer Science and Engineering at The Ohio State University

- Translational Data Analytics Institute Data Commons Portal

Maciej Pietrzak, Ph.D., Technical Director - Biomedical Informatics Shared Resource, Comprehensive Cancer Center; and Research Scientist at The Ohio State University

- Biomedical Informatics Shiny Apps in OnDemand

Sandeep Vijayakar, PhD, President, Advanced Numerical Solutions, LLC

- Transmission3D Web Based Service

Allocations

A thorough, yet streamlined, peer-reviewed grant process is employed by the Center to ensure quick turnaround of allocations requests. The process promotes access for all eligible principal investigators and guarantees Ohio an efficient and equitable utilization of resources. It also insures that the research conducted at the Center meets nationally recognized standards.

This process is coordinated through OSC's Statewide User Group (SUG), whose officers meet regularly with OSC staff to evaluate allocations requests, as well as to discuss hardware, software and general information about the Center.

HPC Portal

In fall 2017, OSC launched Open OnDemand 1.0, a National Science Foundation-funded, open-source version of OSC OnDemand, the Center's single-point-of-entry web portal. OnDemand provides clients with seamless, flexible access to computing and storage services at OSC or any of the other HPC centers that have customized and deployed the platform.

Because of its user-friendly interface and ease of access, OnDemand has changed the game for those needing HPC access; no longer do researchers need to know command line instructions to access a supercomputer. Through OnDemand, users can upload and download files and create, edit, submit and monitor jobs.

In spring 2018, OSC released Version 1.3 of Open OnDemand, featuring quicker installation via Red Hat Package Manager, a common standard for distributing Linux software.

Hardware

While the new Pitzer Cluster is scheduled for public deployment in late 2018, preparations for the acquisition stretched through much of 2017 and 2018. The 18-month process included surveying client needs, reviewing vendor technology roadmaps, issuing RFIs and RFPs, and prepping OSC's existing production environment for new technologies.

The Center upgraded its backup capacity and performance with the addition of a new tape library in December 2017. A new IBM storage solution installation was completed mid-2018, and the rest of the year will bring new backup servers and disk storage pools.

Additional information on many of these topics appears throughout the publication.

TAGS: DENSE COMPUTE // RESEARCH DATA STORAGE // NATURAL SCIENCES

Disease Resistance

Karhoff seeks genetic answer to soybean root & stem rot

Stephanie Karhoff grew up on farms with broad fields of soybeans, wheat and corn. Now, as an Ohio State University graduate student in the Translational Plant Sciences Graduate Program under faculty mentor Leah McHale, Ph.D., she leverages Ohio Supercomputer Center resources to search for a genetic answer to Phytophthora sojae, a water mold found in areas with poorly drained soils that causes Phytophthora root and stem rot (PRR).

Soybeans are the largest animal feed protein source and the second largest vegetable oil source in the world, and modified soybean oil is used as fossil fuel replacement in several products. Seed developers have been using selective breeding to generate varieties of soybeans resistant to specific strains of P. sojae. But, the mold has grown more complex and virulent in recent years and can infect plants with multiple resistance genes.

To develop a soybean plant that exhibits stronger resistance to a broad range of P. sojae strains, researchers like Karhoff are working to identify new sections of DNA, areas known as quantitative trait loci or QTL for short, which might contain multiple inheritable genes that together could prove resistant against a combination of strains of P. sojae.

"Major QTL are rare in this pathosystem, and the majority of QTL explain less than 20 percent of the phenotypic variance," Karhoff explained. "Recently, we identified a major QTL on Chromosome 18, which explains up to 45 percent of the phenotypic variance."

Karhoff moved her research from her department's desktop servers to OSC systems to help narrow the potential candidate genes within Chromosome 18 down from an initial 222 locations to a more manageable 24, which she hopes to reduce even further in a future study. She ran several sequencing packages on the Center's Oakley and Owens Clusters.

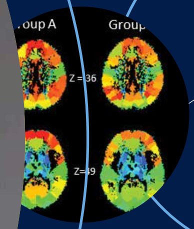
"OSC systems allowed us to study more variables in each run and to use and store much more data throughout the project," she said. "OSC's how-to guides helped make the transition easier, because I don't have an extensive background in coding."

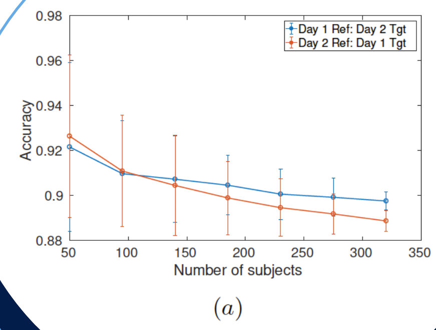
Karhoff believes her work will contribute to researchers' growing knowledge of the trait's genetic architecture. She speculates that once a strong combination of resistance genes is identified, they could be bred into soybean cultivars and made available to farmers to help ensure higher yields in areas where PRR is present. •

PROJECT LEAD // Stephanie Karhoff, Ph.D., The Ohio State University
RESEARCH TITLE // Transcriptomic analysis of soybean near-isogenic lines to identify candidate genes for major Phytophthora root and stem rot resistance QTL FUNDING SOURCE // United Soybean Board
WEBSITE // tpsgp.osu.edu/stephanie-karhoff

PHOTO ABOVE // Soybean field research plots. VIZUALIZATION INSET // Sequencing data for two genes of interest Karhoff analyzed using OSC systems. SMALL INSET // A soybean plant showing symptoms of Phytophthora root and stem rot (PRR) in the field.

TAGS: HIGH PERFORMANCE COMPUTING // DENSE COMPUTE // EDUCATION // RESEARCH DATA STORAGE // ENGINEERING & TECHNOLOGY





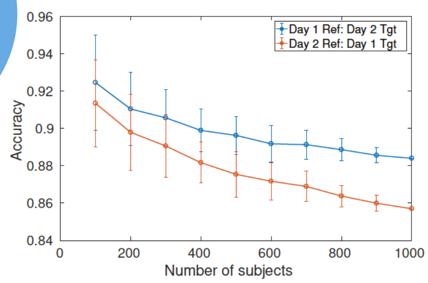
Precision Medicine

Atluri's algorithms deliver higher accuracy FC fingerprinting

The world of personalized medicine is rapidly expanding, with advances in DNA sampling, expanded patient charts and more, creating individualized treatment plans for more diseases and conditions every day. A researcher and his team at the University of Cincinnati are currently making way for precision medicine—in the mind. Gowtham Atluri, Ph.D., develops advanced algorithms for mining data in the neuroscience and public health domains, aided by data-crunching through OSC.

While Atluri's team creates algorithms for many uses in domains as diverse as biomedical informatics to high energy physics, one of these projects analyzes neuroimaging data from the Human Connectome Project (HCP). The HCP is a large-scale project funded by the National Institutes of Health that compounds data from 1,200 individuals to provide a better picture map of human neural connections. More specifically, Atluri's team analyzes over 1,600 hours' worth of functional magnetic

PHOTO LEFT // Gowtham Atluri, Ph.D. University of Cincinnati VIZUALIZATION CENTER // The accuracies of nodes colored in the brain volume.
GRAPH RIGHT // Subject numbers effect on resting state functional connectivity fingerprinting. a) Average accuracy when increased to 320.



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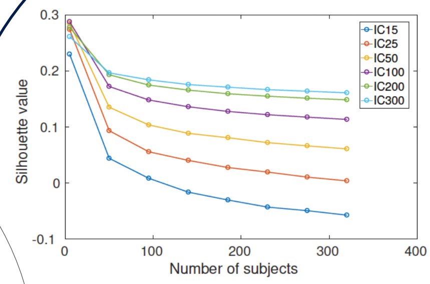
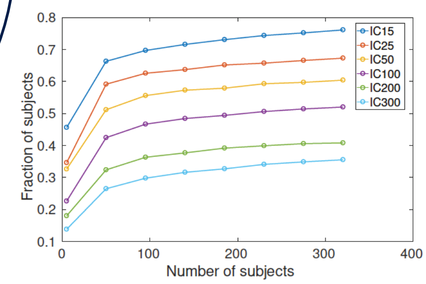


(c)



(d)

resonance imaging (fMRI) scans that capture brain activity at millions of locations.

"Our algorithms that discover interesting patterns and relationships in this wealth of fMRI data require significant computational resources," Atluri said. "These resources are available to us through OSC, and they enable us to effectively test our algorithms and to advance scientific discoveries in neuroscience."

By studying these many data points and discovering the underlying neural connections in a wide variety of subjects, researchers can better characterize an individual's functional connectome (FC). Using such a characterization to uniquely identify individuals is known as FC fingerprinting, an area that is rapidly gaining momentum in the neuroscience community. Atluri's team is trying to determine how accurately an individual's brain connectome can be identified when placed in a group of others' connectomes. The accuracy can depend on how well the underlying patterns and relationships are discovered and characterized. Discovering such patterns and relationships from huge amount of data is a compute-intensive process, and the research would be much more complicated without resources from OSC.

"(Without access to OSC) we will have to either work with a subset of the HCP data to make interesting discoveries or run our algorithms for a much longer period," Atluri said. "While the former limits our ability to detect statistically significant patterns and robustly handle noise, the latter will slow us down in terms of the algorithmic advances we push for."

Higher accuracy FC fingerprinting means these data and algorithms could be used by neuroscientists and mental health experts in the future to provide individualized treatment for mental illnesses such as schizophrenia and Alzheimer's disease.

"The proposed tools and techniques directly enable the investigation of hypotheses relevant to personalized neuroscience—understanding the neurological processes that are shared and unique to individual subjects," Atluri said. "This will help achieve the clinically relevant goals of personalized neuroscience and eventually alleviate the huge societal burden of mental illness."

To ensure the posterity of this work, Atluri also uses OSC resources in the classroom for his course "Advanced Topics in Mining Spatio-Temporal Data." Students become familiar with the OnDemand interface as they learn techniques designed to tackle data mining problems by addressing challenges posed by spatial and temporal characteristics of the data. •

PROJECT LEAD // Gowtham Atluri, Ph.D., University of Cincinnati RESEARCH TITLE // Mining biomedical data FUNDING SOURCE // University of Cincinnati WEBSITE // homepages.uc.edu/~atlurigm

GRAPHS // Subject numbers effect on resting state functional connectivity fingerprinting. b) Accuracy on 1000 subject dataset when increased from 100 to 1000. c) Average subject Silhouette values with varying number. d) Negative Silhouette value subjects for at least one RSFC.

Visual Perception

Golomb lab studies how visual system processes input

If two cups sat in front of you, one blue and one purple, and someone asked you to pick up the purple one, you would know which cup to grab and how to pick it up. Have you ever thought about why? Julie Golomb, Ph.D., spends most of her days answering this question and others related to how the brain perceives, processes and memorizes sensory input. Her lab at The Ohio State University's department of psychology uses supercomputing resources at the Ohio Supercomputer Center to run analyses on behavioral and neural data related to visual perception.

"Vision is for most people our most dominant sense, and we get a lot of information visually," Golomb said. "We know a fair bit about how the visual system works, at least at initial levels, but there's a lot we really don't know. So the sorts of questions that we study in our lab are things like 'how do we perceive different colors and shapes and put them together into different objects?'"

To get a comprehensive picture of what's going on behind the eye, Golomb's group runs a few types of experiments, including a behavioral study that asks subjects to respond to computer tasks based on objects, colors and lights on a screen. Participants' responses are recorded and analyzed in MATLAB. The group also informs its research through neuroimaging with functional MRI scans that show brain activity patterns and with finer temporal data from electroencephalograms, a cap with electrodes that can detect electrical brain activity.

All this data has to be modeled, including large numbers of parameters across hundreds of subjects. By using OSC's clusters to process data, Golomb's group receives results at least three times faster than using desktops in the lab.

"It ends up being a pretty computationally intensive process," said Jiageng Chen, a Ph.D. student in Golomb's lab who runs many of the tests. "We can do that without the supercomputer, but [using the supercomputer is] a lot faster."

While Golomb's group does not directly study vision or visual disorders, their research into discovering more about how the visual system functions could help clue other researchers into solutions for these problems.

"We have distracting stuff happening in our environment all the time… It's a really complex challenge for our brains to solve," Golomb said. "We are constantly bombarded with visual input as we're looking around, and we have to instantaneously put all the pieces together and know which features are part of that object or that person and not get them confused." •

PROJECT LEAD // Julie Golomb, Ph.D., The Ohio State University RESEARCH TITLE // Behavioral and neuroimaging investigations of perception, attention, memory, and cognition FUNDING SOURCE // National Institutes of Health WEBSITE // u.osu.edu/golomblab

GRAPHS BOTTOM // An example of results from one of the eye experiments run by Golomb's group.

TAGS: DENSE COMPUTE // EDUCATION // ENGINEERING & TECHNOLOGY

Neural Networks

Plummer's class trains systems to learn, observe, create

What if you discovered your favorite song, or your favorite work of art, came straight out of a computer? It is possible future generations will experience exactly that.

Andrew Plummer, Ph.D., recently supervised a classroom project at The Ohio State University that explored how artificial neural networks could potentially produce music. As part of the project, students experienced the benefits of high performance computing through the Ohio Supercomputer Center to complete the computationally intensive research.

Neural networks are computing systems inspired by biological neural structures and built to perform similar tasks. Not only have they shown the ability to learn and observe, but also to create.

For instance, by taking images or doodles in a data set, researchers have trained neural networks to create complex pieces of original art. Other projects have used audio files to produce music.

Plummer, senior lecturer/research engineer in Ohio State's Department of Computer Science and Engineering, teaches a course in which students are given the freedom to develop projects of interest to them. In this particular one, students investigated a project by Stanford University researchers called GRUV that uses raw audio waveforms as seed sequences to train long short-term memory (LSTM) neural networks. Theoretically, these networks could create new songs from the seed sequences.

"It's a hot topic right now, being able to do generation not just with music but with stories, narratives or images," Plummer said. "A lot of research teams are looking at this from a high level, my students wanted to figure out the nuts and bolts of what actually goes into building these systems."

The classroom project had three objectives in order to improve on the limitations of GRUV's overall creative output:

- Taking GRUV and observing what can be achieved from various sets of training data
- Attempting to improve the seed generation process
- Using a generative adversarial network model involving a variant of GRUV's LSTM network to see if the quality of musical output could be improved.

Plummer's students built their adversarial network using Python's TensorFlow software on OSC's Owens and Oakley clusters.

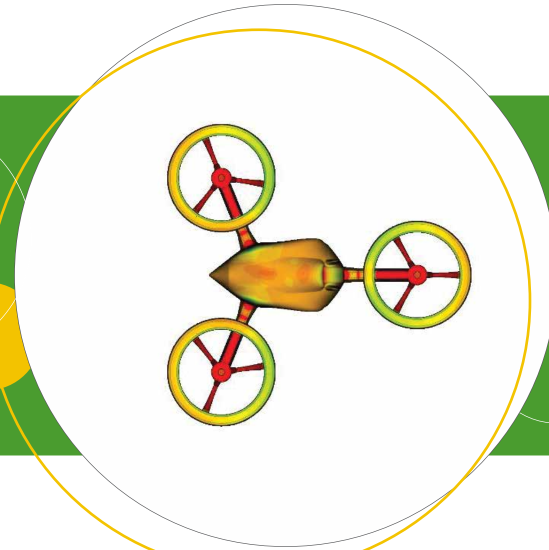
"It's very computationally intensive," Plummer said. "The students were initially building the models on their own computers and they weren't sufficient for quick prototyping and experimentation on the system design. OSC was very valuable for them to have those resources and do quicker experimentation to get them up and running." •

PROJECT LEAD // Andrew Plummer, Ph.D., The Ohio State University. RESEARCH TITLE // NUGRUV: Using and improving the GRUV Project for music generation FUNDING SOURCE// The Ohio State University WEBSITE // arplummer.info

Drone Transportation

TotalSIM, OSC team up to provide inventors with app

VISUALIZATION LEFT PAGE // An aerodynamics test run on TotalSim's TS Aero app. VISUALIZATION RIGHT PAGE TOP // TotalSim's intuitive computational fluid dynamics TS Aero App simuates how GoFly devices will respond to specific conditions.



While widely used for aerial photography and video, the next frontier for drones could be human transportation. The GoFly challenge, sponsored by Boeing, is culling the brainpower of the world's most creative innovators and engineers to create personal flying devices. With $2 million of prize money on the line over the course of two years, teams of inventors, engineers and dreamers are reaching outside their comfort zones to make human flight a reality.

To do this, many must reach for unfamiliar technology and tools to model and design a device capable of carrying a person. That's where TotalSim US and the Ohio Supercomputer Center enter the picture. GoFly approached Ray Leto, president of TotalSim, about providing contestants with computational fluid dynamics (CFD) insights. TotalSim's TS Aero app, built on OSC's AweSim industrial platform, offers an intuitive interface for users to upload their aerospace vehicle designs and test digital prototypes against various forces. In partnership with OSC, TotalSim created a portal based on OnDemand and a specific app for GoFly, based on TS Aero, specialized for devices that use vertical takeoff.

"What we offer that other people don't is an app-based workflow specifically made for these types of vehicles that doesn't require expert knowledge to run," Leto said. "Many of the people using it have never done CFD before, many of them are not aerodynamicists, they're innovators, inventors, and now we're enabling them to do that."

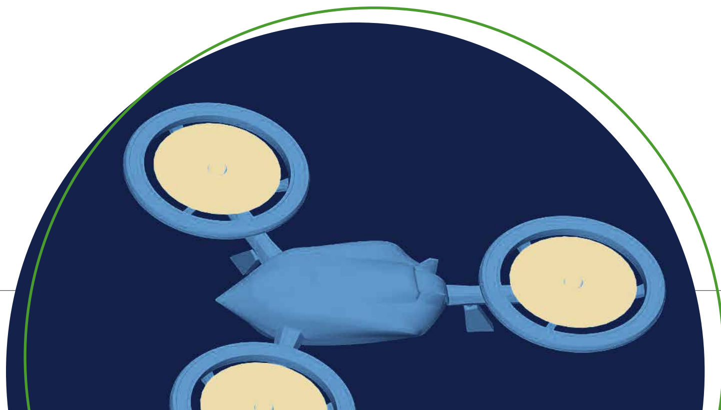
TotalSim allows all GoFly contestants to use its app at no cost, so they can log in and run simulations on their drone designs. Each team can run 10 or more simulations, approximately a $5,000 value.

"OSC was really accommodating in having us do the account setups," Leto said. "We've got a streamlined account creation process with OSC where we create the account and share the application. And we've got a website full of documentation, training information and videos. We launched all that, and we've had pretty good success in getting people up and running."

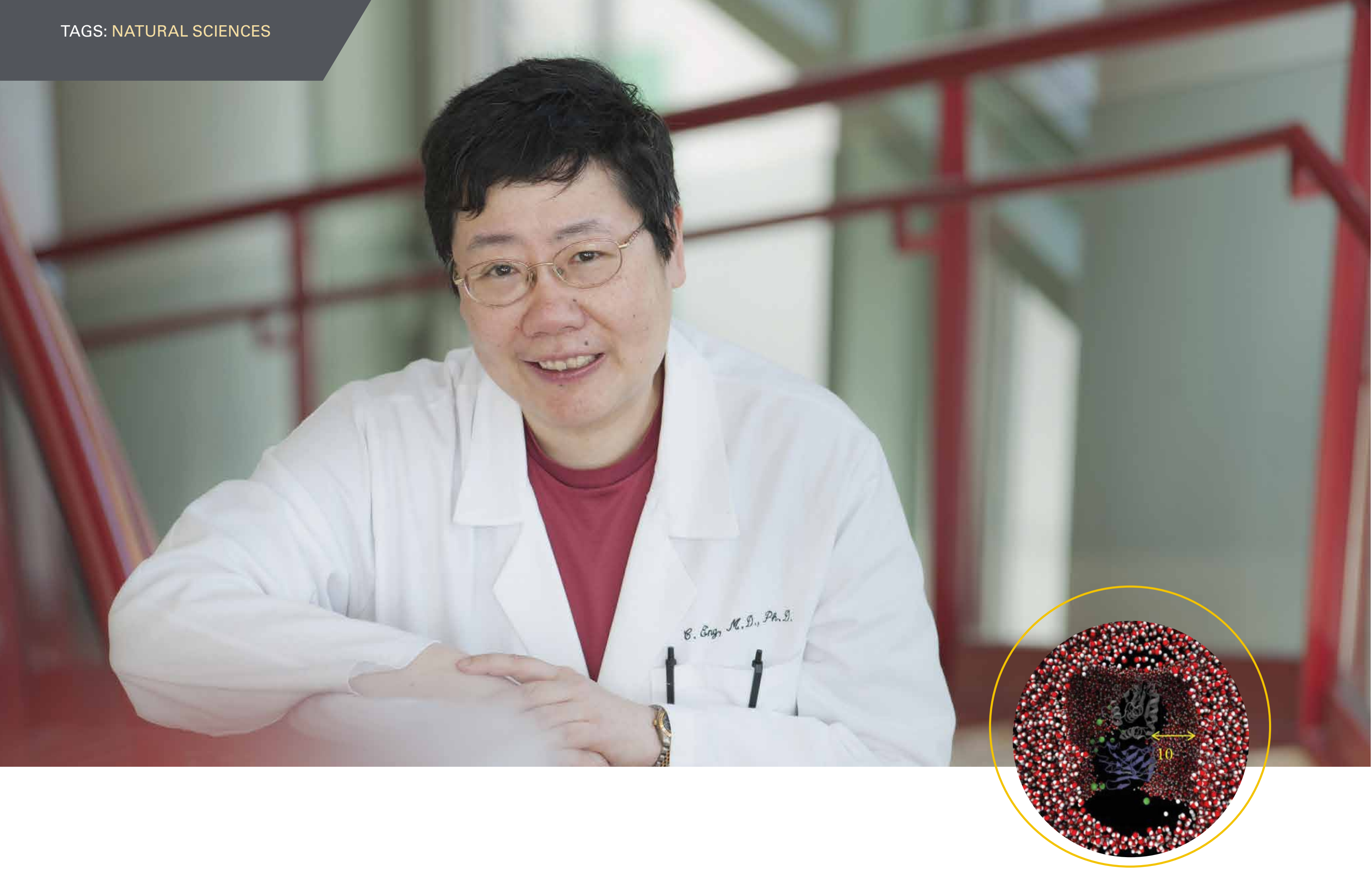
GoFly users have challenged TotalSim since the contest's launch, allowing the company to refine its aerospace application, which it offers to commercial customers as well.

"It's been a good advanced beta testing process for us in some ways, both from the CFD and aerodynamics side of it, and maybe more importantly from the software and the infrastructure side of it with OSC involved," Leto said. •

PROJECT LEAD // Ray Leto, President, TotalSim RESEARCH TITLE // TotalSim's TS Aero App helps GoFly teams outperform the competition FUNDING SOURCE // TotalSim, Boeing WEBSITE // totalsim.us/gofly



VISUALIZATION BOTTOM // A 3D rendering of drone created using TotalSim software for GoFly.



Genetic Mutation

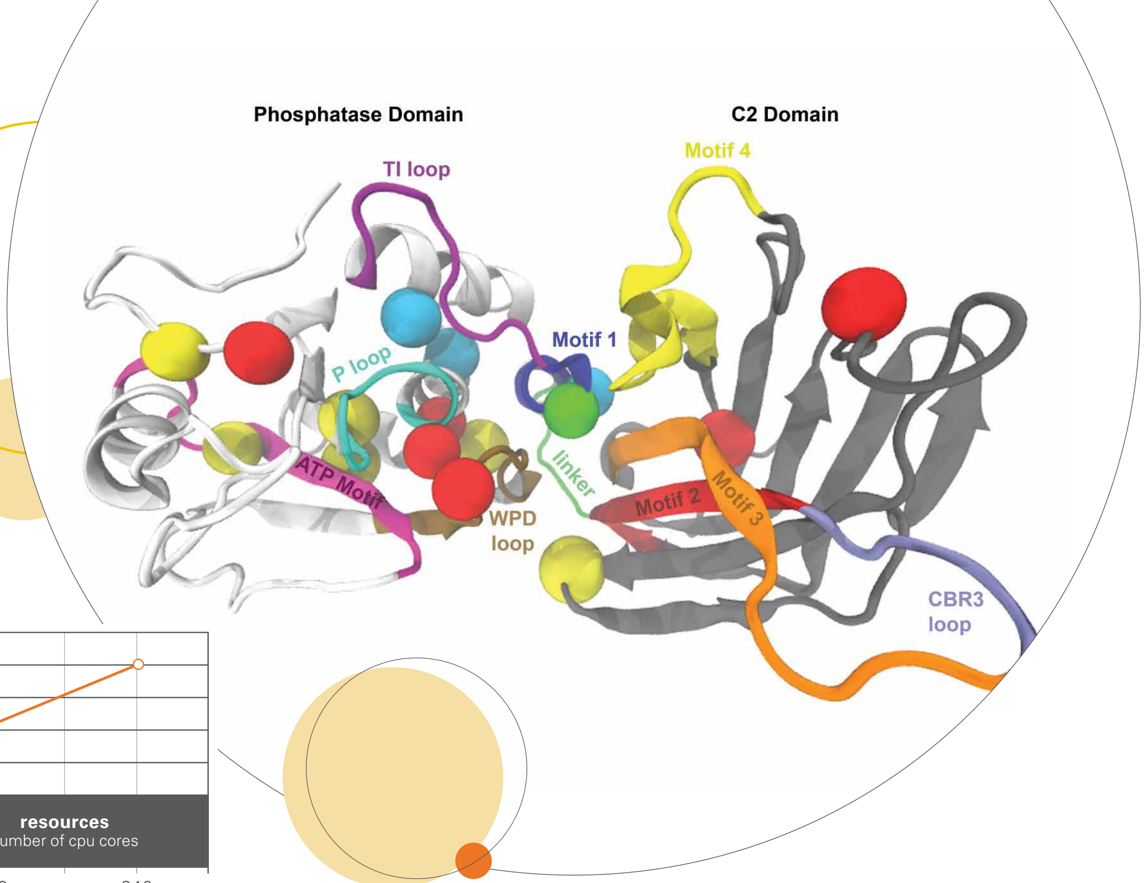
Eng lab lays groundwork for informed diagnosis, prediction

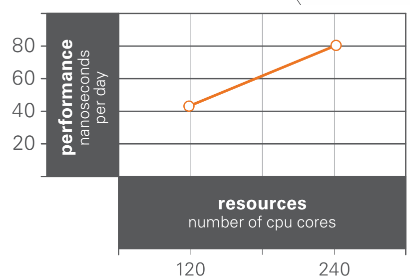
Charis Eng, M.D., Ph.D., takes a gene-informed approach to personalized risk assessment and medical management of her patients and families. Her patient-focused research in genes, when altered, or mutated, associating with specific clinical features, such as cancer and autism spectrum disorder (ASD), provides the scientific evidence on which she practices precision medicine. Eng utilizes these insights as she evaluates the patients she sees at the Center for Personalized Genetic Healthcare (CPGH), the clinical arm of Cleveland Clinic's Genomic Medicine Institute (GMI). Eng is also the chair and founding director of the Cleveland Clinic's Genomic Medicine Institute.

Eng first identified germline mutations in the cancer fighting gene, phosphatase and tensin homolog (PTEN), in Cowden syndrome patients in 1997. Since then, her study of PTEN has resulted in characterizing increased risk of cancers (e.g. breast, thyroid, endometrial, kidney, colorectal, melanoma) and autism (ASD). Yet, it remains unclear why mutations in one gene, PTEN, can result in ASD and/or cancer.

Recently, Eng's lab turned to the Ohio Supercomputer Center (OSC) to use molecular dynamics (MD) simulations on the Oakley Cluster to gain atomic-level insight into the protein encoded by PTEN, which acts as a tumor suppressor. These simulations help further investigate the dynamics of proteins and understand mutation-induced changes in the structure and function of PTEN.

PHOTO TOP // Charis Eng, Ph.D., The Cleveland Clinic VISUALIZATION OVERLAY // A PTEN molecular dynamics simulation containing water molecules and chloride ions arranged around protein in a cubic box.





"Molecular dynamics simulation is an invaluable tool for investigating the behavior of proteins and to decipher the effects of mutation-induced changes in structure and function," according to Eng. "Understanding the functional impact mutations have on the structure of PTEN will aid in the identification of specific mutations that contribute to ASD or cancer."

In 2017, Iris Smith, Ph.D.—a postdoctoral fellow in Eng's lab—used an OSC startup allocation to complete initial benchmarks for PTEN systems, which included about 76,000 atoms. Smith built each system and performed the simulations using GROMACS (GROningen Machine for Chemical Software) on the Oakley cluster, which significantly sped up the simulations previously run on an in-house system.

With the initial benchmarks complete, Smith plans to run larger simulations, analyzing hundreds of thousands of atoms. "These tools allow us to see [inside] how molecules are working and give us a much deeper understanding of the disease mechanism," Smith says.

Images from simulations may someday be used to help physicians understand the structure and function of a particular mutation, enabling a personalized, gene-informed medical management plan, including appropriate screenings and early interventions for either cancer or ASD risk.

"Performing MD simulations at times can be far removed from patient care," Smith said. "But we will utilize this to aid in the prediction of specific mutations, directly informing our patient care."

Gene-based diagnosis and prediction of cancer versus ASD risks will help in tailoring diagnosis and prevention strategies, along with helping patients educate their own doctors as to the nature of their inherited cancers and/or neurodevelopmental risk in their future children.

"Our lab has greatly benefited from our...Ohio Supercomputing Center allocation where we modeled in silico germline missense PTEN mutations associated with autism spectrum disorder and with cancer, and where we performed MD simulations," Eng said. •

PROJECT LEAD // Charis Eng, M.D., Ph.D., Cleveland Clinic RESEARCH TITLE // Insight into structure and dynamics from computational modeling and simulation: The effects of germline PTEN mutations in autism spectrum disorder and cancer FUNDING SOURCES // National Institute of Neurological Disorders and Stroke, National Cancer Institute, The Ambrose Monell Cancer Genomic Medical Clinical Fellowship WEBSITE // my.clevelandclinic.org/staff/6757-charis-eng#education-content

VISUALIZATION TOP // An image of mapping an ASD- vs. cancer-associated mutations on a PTEN three-dimensional structure. GRAPH OVERLAY // OSC helped Eng's lab perform base benchmarks from its initial start-up allocation resources using GROMACS MD simulation software.

Inventive Activity

Corredoira team studies federal funding, tech patent links

The 1960s Soviet/U.S. space race put men on the moon but also developed basic technologies that would result in subsequent breakthrough inventions in related fields: prosthetics, water purifiers, freeze-dried foods, satellite television, memory foam and many more. These advances were wrought from federally funded research and today serve the interests of broad swaths of the general public.

Defining the relationship between federal funding and the rate and direction of inventive activity has been the focus of a research team led by Rafael A. Corredoira, Ph.D., an assistant professor in the Department of Management and Human Resources at The Ohio State University.

"In 2015, we introduced technological influence as a variable to measure an invention's direct and indirect impact on the evolution of technology. This provides a novel means to study the short- and long-run effect of invention antecedents on technological evolution, invention activity and economic growth," Corredoira said.

Corredoira explained that access to Ohio Supercomputer Center services was integral to the 2017 project's success. Running R statistical computing software on OSC's Owens Cluster allowed his team to study a large, complex database of patent-citing articles in top scientific journals. It also helped him tackle the alpha-centrality measure, which calculates the impact of influence, via computationally intensive quantile-regression techniques.

"Quantile regression has advantages over the normal regression because it lets you assess the effect of one variable into another, but across a whole distribution," Corredoira said. "We cared only about the patterns that were in the top five percent of the distribution in influence, because those are the ones that really change the world. If you use median-regression, it assumes that the effect of, for example, federal funding would be the same for a patent in that breakthrough group as it would for the average patent, and that is not the case."

Corredoira and his colleagues found that research funded by the federal government is associated with more active and diverse technological trajectories, more often tied to breakthrough inventions than research funded by private corporations. Industry typically must focus on a shorter development window than many federally funded projects, and single companies often cannot develop the full breadth of potential products coming out of a single breakthrough technology.

They also determined that the most fertile projects for breakthrough inventions were those that tap collaborators outside of the funding agency, such as those found within universities or independent laboratories. •

PROJECT LEAD // Rafael A. Corredoira, Ph.D., The Ohio State University RESEARCH TITLE // Federal funding and the rate and direction of inventive activity FUNDING SOURCE // National Science Foundation WEBSITE // fisher.osu.edu/people/corredoira.2

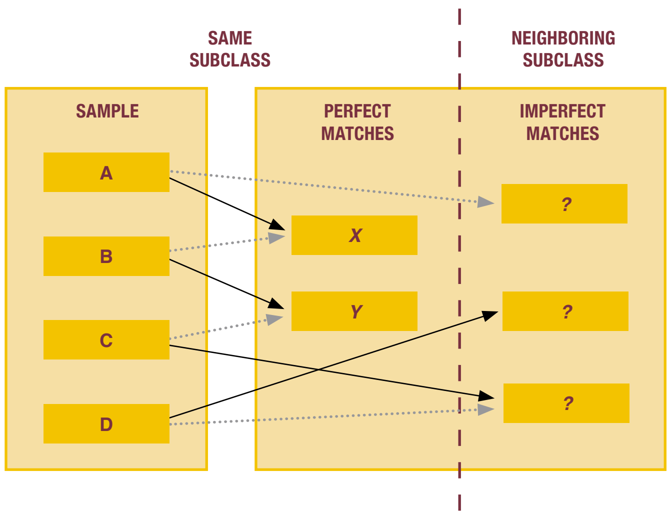


CHART RIGHT // Scenarios of Repeated Matching Scheme: To account for the issue of multiple matches, Corredoira's team accounted for randomness of selecting matches into multiple rounds for each sample patent.

Energy Conversion

Shafaat lab modeling nickel enzymes

The old adage goes, "it's what's inside that counts." While most people aren't talking about proteins when they say it, it certainly applies. Approximately half of all known proteins contain metal ions, which play a crucial role in energy conversion reactions: think photosynthesis or carbon dioxide fixation. Hannah Shafaat, Ph.D., an assistant professor at The Ohio State University's Department of Chemistry and Biochemistry, uses computationally guided spectroscopy to study the role of metal, specifically nickel, centers in proteins.

"It's an underrepresented metal in biology, and certainly underappreciated, because it is capable of performing some very challenging reactions," Shafaat said, "Certainly in the context of trying to understand primordial energy conversion processes, and then applying those fundamental principles to our own anthropogenic energy conversion, understanding the nickel center is key."

Shafaat's group uses high performance processors at the Ohio Supercomputer Center to build model proteins for large nickel enzymes, looking to see what is required for activity. Once these large models are computed, they run experiments on them to validate the models so they can be used for experimental predictions later on. By using these calculations run on the models in an iterative cycle between experiment and theory, they hope to reduce the amount of trial and error necessary in the lab. This helps run more efficient experiments, saving the group time and cost.

"OSC allows us to perform calculations on the proteins in a way that we can never do on a desktop, and would be hard to do even with a local cluster," Shafaat said. "In order to get a good description of our nickel active site you have to include quite a large portion of the protein. This motivates our continued use of OSC because we need such a large model."

While Shafaat's group may be looking at the fundamentals of proteins and their functions, their work has the potential to offer key insights into the building blocks of life. While nature has fine-tuned the processes of producing hydrogen and reducing carbon dioxide, researchers have yet to reproduce these phenomena in the lab with the same efficiency and speed. If these model systems can be built, researchers can get a better understanding of nature's inner workings to manipulate these molecules and proteins in new ways.

"If we can understand how the natural enzymes work, then we can take those fundamental principles into the lab and construct molecules that have those components built in," Shafaat said. "That's the ultimate goal." •

PROJECT LEAD // Hannah S. Shafaat, Ph.D., The Ohio State University RESEARCH TITLE // Mechanistic investigations of small molecule activation reactions in model nickel metalloenzymes through computationally-guided spectroscopy FUNDING SOURCES // National Science Foundation, Department of Energy, American Chemical Society WEBSITE // research.cbc.osu.edu/shafaat.1

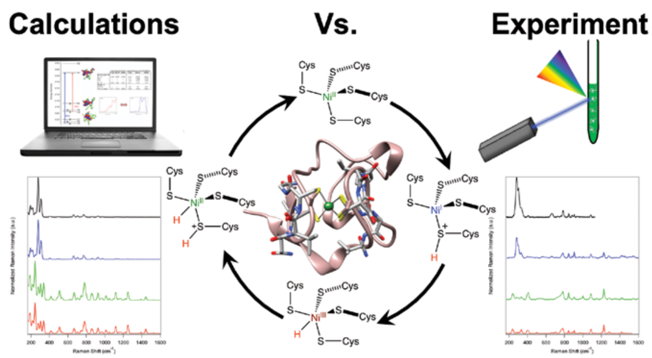


PHOTO TOP // Hannah Shafaat, Ph.D., and Kelly Wrighton, Ph.D. Photo courtesy of the College of Arts and Sciences at Ohio State PHOTO BOTTOM // The direct comparison of experiment to theory for the spectra that Shafaat's group measures.

TAGS: EDUCATION // FACILITATION // ENGINEERING & TECHNOLOGY

Campus Champion

Miami's Mueller supporting HPC needs of university's faculty, students

The demand for high performance computing at Ohio's universities has significantly grown and diversified. Jens Mueller, Ph.D., has witnessed that first hand at Miami University.

Mueller is the director of high performance computing services at Miami University and a Campus Champion for the Ohio Supercomputer Center, supporting faculty and students in all stages of their HPC needs.

"In some way, I'm the person for everything," said Mueller, who has worked with OSC for more than 10 years. "The highlight at Miami is the broad spectrum of fields using computational research. I've only gotten busier because everything is more data driven, increasing demands."

Traditional HPC users at Miami and many Ohio campuses include the engineering departments, computer science, math, physics, chemistry, geography and geology. However, Mueller has witnessed a growing demand from the business school, economics, finance, humanities, political sciences and even the English department.

And the broad spectrum of disciplines also means a broad spectrum of computational skill sets.

"One of the challenges in my role is to identify the proper computational resources based on experience and expressed needs," Mueller said. "This includes software tools and specific hardware resources."

Mueller and his team follow a tiered approach to helping researchers meet HPC needs. They start with Miami's local clusters and, once they are exhausted, Mueller facilitates the transition to OSC.

Mueller also helps facilitate a class partially taught on OSC machines to assist people through the process of using HPC resources, everything from applying for an account to reserving compute nodes to gaining software licenses and even using OSC OnDemand.

"I look at what challenges they'll face and how they can be eliminated," he said. "I just want to make sure the transition is smooth."

Mueller also works one-on-one with research groups and faculty labs. And while he helps Miami's researchers a great deal, he also helps OSC. He was part of the OnDemand committee to give feedback on its usability and regularly

PHOTO TOP // Jens Mueller, Ph.D., (left) is the director of high performance computing services at Miami University and a Campus Champion for the Ohio Supercomputer Center, supporting faculty and students in all stages of their HPC needs. Photo courtesy of Miami University.

communicates to OSC what is working well and what isn't.

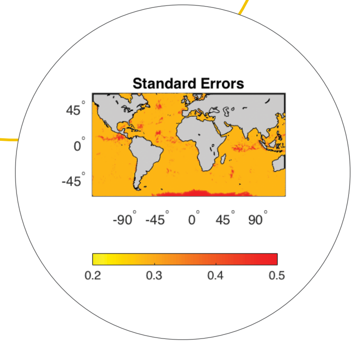
"We contribute to OSC and that's beneficial to them, of course the benefit to us is great as well," he said. "Researchers can get amazing things accomplished using OSC."

Mueller highlighted a few recent Miami projects in which he helped researchers make the most of OSC's resources:

- Graduate student Melvin Ikwubuo, with David Munday, Ph.D., associate professor in mechanical and manufacturing engineering, is studying the effect of geometric features on film cooling efficiency. The project was featured in a poster presentation during the OSC Statewide Users Group in April.
- Amelie Davis, assistant professor of geography, is in a research collaboration on computational analysis of satellite imagery, using the tool R at OSC to predict forage suitability for honey bees and other pollinators.
- Graduate student Erik Brodin, with Professor Jessica Sparks, Ph.D., in chemical, paper and biomedical engineering is in a research collaboration on 3D printer syringe modeling.
- Amy Yousefi, Ph.D., a professor in chemical, paper and biomedical engineering, has a senior design student project attempting to model flow of cell culture fluid in bioreactors with the goal to improve bone growth in artificial scaffolds.
- Rachel Blum, Ph.D., assistant professor of political science, used automated content analysis to study the dynamics of political parties via a topic model. The sources were a vast collection of blog posts and interview data.
- Dr. Andor Kiss, Ph.D., director of the Center for Bioinformatics and Functional Genomics, had a project studying the genome of the wood frog, a species that freezes in the winter and comes back to life in spring when it thaws. •

PROJECT LEAD // Jens Mueller, Ph.D., Miami University RESEARCH TITLE // Campus Champion FUNDING SOURCES // Miami University, Ohio Supercomputer Center WEBSITE // blogs.miamioh.edu/researchcomputing/people

TAGS: HIGH PERFORMANCE COMPUTING // DENSE COMPUTE // RESEARCH DATA STORAGE // NATURAL SCIENCES



Data Analysis

Kang team creating novel modeling methods

Whether it's the ability to predict and respond to natural disasters, analyze brain imaging data, or understanding social network information, scientific researchers and engineers are increasingly turning to high performance computing (HPC) to tackle design obstacles or study real-world phenomena.

The University of Cincinnati's Emily Kang, Ph.D., is carrying out extensive simulation studies through the Ohio Supercomputer Center's resources to create methods and algorithms that will reduce uncertainties in computer modeling and make the process easier and more efficient for researchers.

"The methods and algorithms we have developed can be used to analyze data in many fields, including but not limited to geography, climate science, agriculture, biomedical sciences, and marketing," said Kang, an associate professor in the Department of Mathematical Sciences in the McMicken College of Arts and Sciences. "We are interested in studying how variables are associated with each other or using spatial/spatio-temporal dependence to improve prediction."

Kang has collaborated with researchers in many different research fields to develop robust and efficient statistical models that allow scalable memory and computational complexity, including efficient algorithms to fit high-dimensional social network data and flexible models to analyze massive global remote sensing data, which can be widely used in marketing and environmental engineering.

"Creating a novel method requires both theoretical justification and empirical demonstration," Kang said. "Although our project is viewed as more like fundamental research, we need to carry out extensive simulation studies to validate our new methods and compare their performance with existing ones."

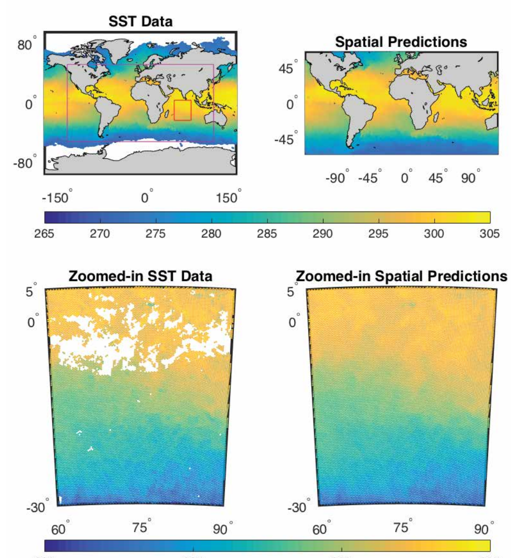
Using software such as Matlab, Julia and R on OSC's Owens Cluster, Kang's analyses requires processing a huge amount of data.

"Using the supercomputer helps my group implement these numerical studies effectively and efficiently," she said. "OSC has enabled us to run simulation replicates in parallel and to easily implement scalable algorithms, which have been essential for the success of our project."

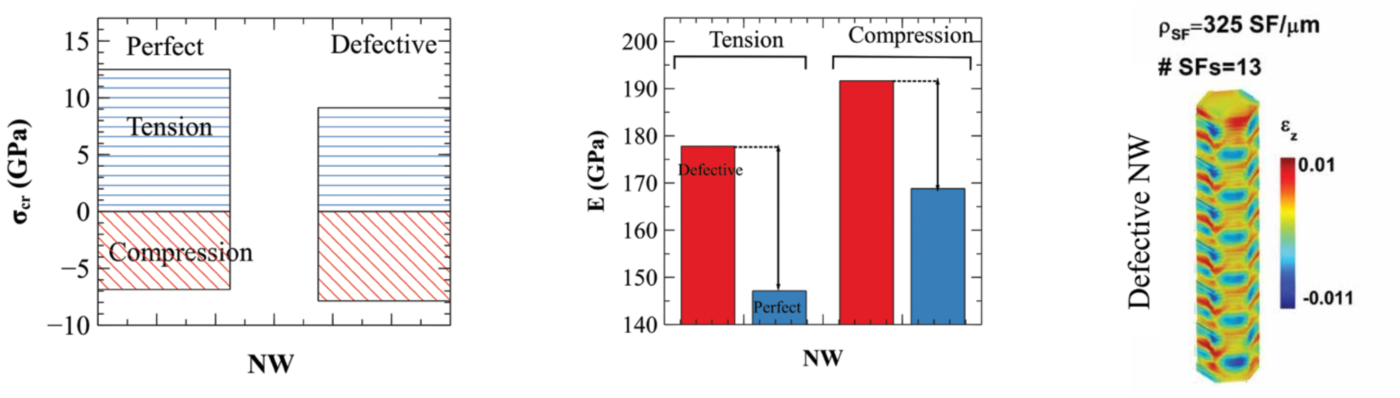
To complete all the studies in many different areas of research, Kang uses multiple students focusing on different topics in the project.

"OSC has enabled them all to investigate different problems and implement their own numerical studies simultaneously," Kang said. "It is essential for my students, the next generation of data scientists, to have the training and experience with high performance computing resources." •

PROJECT LEAD // Emily Kang, Ph.D., University of Cincinnati
RESEARCH TITLE // Statistical models for massive data with complex dependence structure FUNDING SOURCE // University of Cincinnati
WEBSITE // emilystat.wixsite.com/gdads



VISUALIZATIONS // Kang's lab develops multiresolutional models for analyzing massive data with complex dependence structures such as massive remote sensing data and outputs from physical and computer experiments.



Nanostructure Defects

Attariani engineers flaws to improve materials' properties

Hamed Attariani's lab can't look past the flaws in the materials they study—and that's exactly the point. Attariani, assistant professor in Wright State University's department of mechanical and material engineering, is flipping the script in the field of nanostructures by exploring how inherent defects in materials could enhance their mechanical properties rather than deteriorate them. Because the material response to an external stimulus is a function of atomic interactions, Attariani uses LAMMPS Molecular Dynamics Simulator on the Ohio Supercomputer Center to model the mechanical characteristics of these structures.

"We're trying to investigate the mechanical property of materials by changing the defect concentration and type," Attariani said. "By this method we can explore the material design space and accelerate the material discovery."

Although nanomaterials are manmade, they inherit defects during the fabrication process. The common belief is these point/planar defects degrade the material. Rather than trying to eliminate these defects through precise control over the synthesis process, Attariani looks to intentionally engineer defects that can improve the mechanical properties of the nanomaterials. While this method has been studied some on the macroscale, using it at a nano level is novel.

"If you move toward the nanoscale you will find a lot of free surfaces that change the material properties," Attariani said. "Typically, nanostructures are very strong compared to the macrostructures and they show unique characteristics."

To model the behavior of these nanostructures, researchers need to model a huge number of atoms—Attariani's current models contain approximately 300,000 atoms. This is where the power of supercomputing comes in.

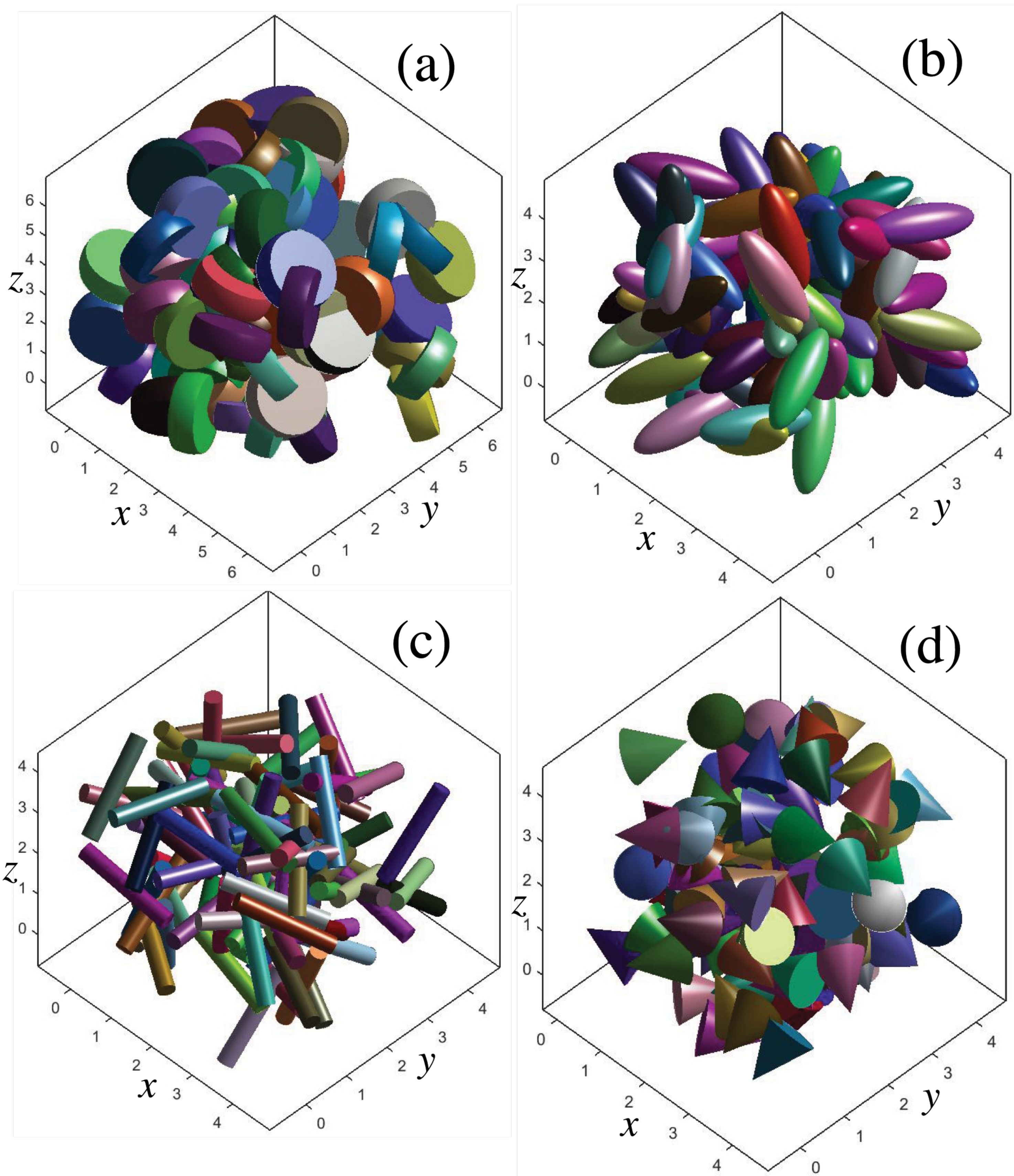
"There's no way that we can do it with a single processor. If I were to do it with a single processor, it might take years to model just one single nanocrystal," Attariani said. "So that's the reason that having access to the supercomputers and parallel processing is a must. Without having access to these types of advance computing infrastucture, there is no way we could do this."

The one-dimensional materials with which Attariani works include zinc oxide that serves as a nano energy-generator; when a mechanical load is applied, it generates electricity. As electronics such as cell phones, lasers and remote sensors shrink, these materials can provide a power source for devices that no longer have space for a battery.

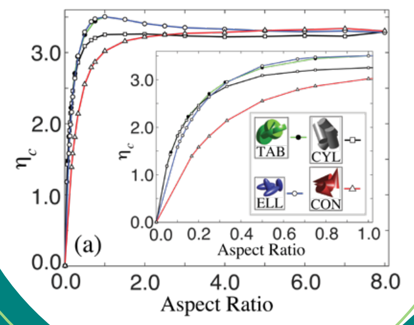
"It's going to be the future generation of nano-energy harvesters," Attariani said. •

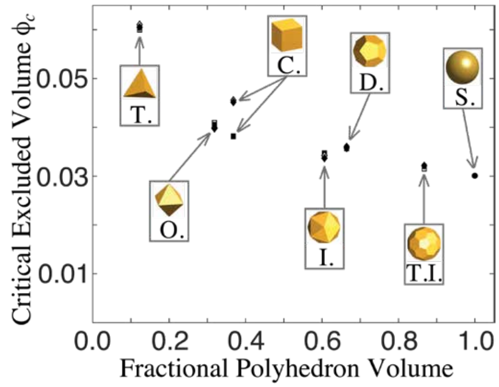
PROJECT LEAD // Hamed Attariani, Ph.D., Wright State University
RESEARCH TITLE // Material by design: A new road map to strengthen low-dimensional nanosources with defect engineering
FUNDING SOURCE // Wright State University WEBSITE // people.wright.edu/hamed.attariani

GRAPHS // A figure and model of the nanostructures Attariani's group is testing.



VISUALIZATIONS // Priour's lab uses the Langevin technique in large-scale molecular dynamics (MD) simulations, which they use to examine systems ranging in size from 20 to 5000 sites.





Void Percolation

Priour leverages Platonic solids to study nature's thresholds

While Youngstown State University physics professor Donald J. Priour, Ph.D., isn't a barista, his field of research—percolation—does have ramifications for brewing a cup of joe, as well as for seepage of hydraulic fracking chemicals, the spread of forest fires and the galactic formation of the universe.

"There's a class of problems called percolation theory, and it's been studied for a long time," Priour said. "Water percolates down through coffee grounds. Because the spaces between the grounds are wide enough, the water can get through. If the spaces weren't, water couldn't get through easily. Something's either permeable or it isn't."

More specifically, Priour's research group is studying void percolation, finding how densely packed the barrier particles need to be before the flow cuts off completely. To determine this limit, Priour simulated a quantity of spherical particles aligned at a certain density, set the surface attribute to reflective and then directed a simulated light beam into the particles from various positions and angles. He calculated each ray of light as it bounced off of each particle. The average point at which the light failed to pass through the voids surrounding the particles established the percolation threshold for a specific particle type and density.

However, Priour understood spheres don't approximate natural granularity very closely. "If you look at sand, its particles are very random and pointy, more polyhedral, so we started looking at faceted particles," he said.

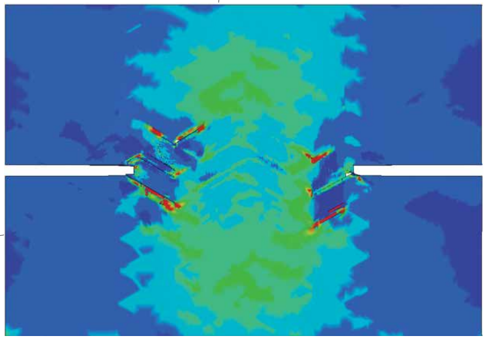
Priour's group began examining the Platonic solids: the tetrahedron, cube, octahedron, dodecahedron and icosahedron. To remain computationally efficient, the researchers initially simulated each barrier particle as a sphere, except when the light ray intersected with the particle boundary, at which point that particular sphere was recalculated as a multi-faceted shape.

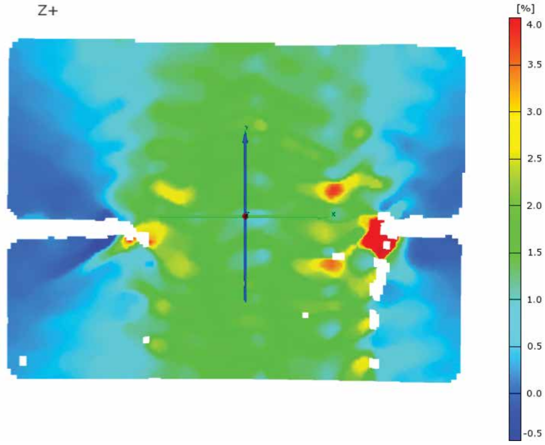
Platonic solids, though, presented an additional complication over spheres; rotated spheres don't change the results. On the other hand, randomly rotated polyhedral might be expected to produce different reflective angles than aligned polyhedra. To find out for certain Priour had to code for 40,000 light rays, each bouncing a million times through 125 million barrier particles for each of five types of particles presenting four, six, eight, 12 or 20 facets. Surprisingly the result was that only for the case of cubes was there a difference between the rotated and non-rotated cases.

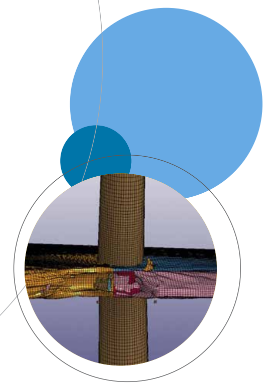
"That was computationally intensive, and in one week we calculated percolation thresholds for all five platonic solids using Fortran and 256 cores of the Owens Cluster," Priour said. "My job would still be running right now if it hadn't been for the Ohio Supercomputer Center." •

PROJECT LEAD // Donald J. Priour, Ph.D., Youngstown State University RESEARCH TITLE // Percolation through voids around randomly oriented Platonic solids FUNDING SOURCE // Youngstown State University WEBSITE // ysustem.com/faculty-faction-dr-donald-priour

TAGS: HIGH PERFORMANCE COMPUTING // DENSE COMPUTE // ENGINEERING & TECHNOLOGY







Aircraft Crashworthiness

Binienda performs simulations to reveal critical details

It's a bit frightening to ponder, but in the past, to understand how safe an airplane was, engineers had to wait for a crash. There wasn't much physical testing that could be done, as with cars.

However, in today's age of high performance computing, understanding aircraft crashworthiness can be analyzed through reverse engineering simulations. Wieslaw Binienda, Ph.D., professor and chair of The University of Akron's Civil Engineering Department, is using the Ohio Supercomputer Center's Owens and Oakley clusters to perform these types of simulations to make airplanes lighter, stronger and safer.

Most current airplanes are made of aluminum, steel and titanium. But the future is in composite material designs, such as carbon fibers locked into place with plastic resin, to make planes lighter, cheaper and more comfortable.

But there's a problem.

"How do you know if a new design is safe?" Binienda said. "Fortunately, there hasn't been a crash of a large composite plane yet. And nobody is going to crash an airplane on purpose and compare it to see how passengers would survive. We don't want accidents, but they happen. The only way to see what happens is to simulate crashes and computer power now is significant enough to simulate crash physics."

Binienda is conducting numerical projects using LsDyna3D and Fluent software to perform simulations that reveal complicated details of airplane crashes. To do that, he and his four graduate students have three phases within the overall scope.

In one, his group is conducting multi-scale modeling for impact analysis and material characterization of advanced composite materials. The goal is to develop an efficient modeling method at the micro, meso and macro scale to predict weaknesses in composite structures.

Another project uses reverse engineering via 3D scans of airplanes to build finite element models of large structures and creating digital terrain topography needed for digital crash scenes to understand how trees, soils and other materials affect crashing planes.

The third phase is conducting aerodynamic wind tunnel simulations of airplane structures and subcomponents using Fluent for forensic engineering of airplane crashes.

"The modeling work has a lot of challenges," Binienda said. "But even large simulations are less expensive and more informative than any experimental crash test.

"We usually submit several jobs using the Owens and Oakley clusters. The memory requirement for these calculations is significant and OSC's resources highly accelerate our research." •

PROJECT LEAD // Wieslaw K. Binienda, Ph.D., The University of Akron RESEARCH TITLE // LsDyna simulation of impact problems FUNDING SOURCE // University of Akron WEBSITE // uakron.edu/engineering/CE/profile.dot?identity=1064521

VISUALIZATIONS // Experimental and numerical results of a deformed shape after impact.

Fluid Performance

Afton Chemical simulates fuel, lubricant characteristics

From wind turbines to motorcycles, Virginia-based Afton Chemical Corporation produces fuel and lubricant additives to increase performance and efficiency such as fuel economy. To stay on the cutting edge of fluid performance, as well as industry standards, Afton's scientists have to create new additives and formulations. Simulation is an integral component to this and is partially powered by the Ohio Supercomputer Center's computing resources.

Lubricant components include solutions such as dispersants and detergents that help prevent sludge and deposits from forming on critical surfaces and friction modifiers that help prevent scoring and reduce wear and micropitting. Afton Senior Research and Development Engineer Joshua Moore models these new molecules and examines their characteristics relating to oil performance—which takes a lot of computing power.

"We're trying to design new molecules to improve performance," Moore said. "As an example, for an engine oil, we want to design new additives, new molecules which improve engine performance in terms of friction/fuel economy, wear, or fatigue."

Moore and Afton engineers teamed up with AweSim at the Ohio Supercomputer Center for molecular modeling, molecular dynamics of additive components as well as system-level modeling using computational fluid dynamics (CFD). AweSim levels the playing field for companies such as Afton, that can benefit from modeling and simulation but may not wish to host it in-house.

"Afton is a great example of how AweSim can provide services to a company outside of Ohio to increase awareness our state's great resources for businesses, in the hope of attracting them to Ohio," said Alan Chalker, director of strategic programs at OSC. "This helps fulfill OSC's role as a technology-based economic development entity for the state."

Simulation-driven design with modeling and simulation on HPC supplements physical product prototyping and allows researchers to take a deeper, mechanistic look at materials such as chemicals, polymers and surfactants.

"We knew our local resources would benefit greatly by working with a supercomputing center. I was looking for an external computer resource with the latest hardware capabilities… and finally found that OSC had the best resources for the best price." •

"I was looking for an external computer resource with the latest hardware capabilities… and finally found that OSC had the best resources for the best price."

— *Joshua Moore, Afton Senior Research and Development Engineer*

PROJECT LEAD // Afton Chemical Corporation RESEARCH TITLE // Molecular CFD modeling for engine lubricants and fuel additives FUNDING SOURCE // Afton Chemical Corporation WEBSITE // aftonchemical.com

PHOTO // Afton Chemical headquarters located in Richmond, Va.

Rubber Dispersibility

Akron's Dong, Ma seek to improve tire operating efficiency

Improving the tires on which we drive can go a long way toward improving the overall efficiency of operating the cars we drive.

Yalin Dong, Ph.D., assistant professor, and Chi Ma, graduate student in The University of Akron's Department of Mechanical Engineering, are using the Ohio Supercomputer Center's resources for a project designed to improve the rubber dispersibility in tires, thus decreasing energy loss and improving the rolling resistance of tires.

The typical filler for rubber—the base material in tires—is silica. The nature of silica's surface often makes it difficult to achieve good dispersion in rubber, which results in energy loss and worse rolling resistance in tires. Dong is working to understand the reaction mechanisms of silane with silica and rubber during the mixing process to achieve excellent silica dispersion in rubber and reduce tire rolling resistance. Silane is the most widely used chemical agent for silica surface modification.

"Traditional silica-silane-rubber mixing is mostly based on experience and optimization," Dong said. "The major novelty of this project is to establish an understanding of silane reactivity with both silica and rubber by combining experiment and simulation studies."

By relating silane reactivity to silica dispersion, the rolling resistance and energy efficiency of tires can be qualitatively predicted by the model being developed through this research, according to Dong.

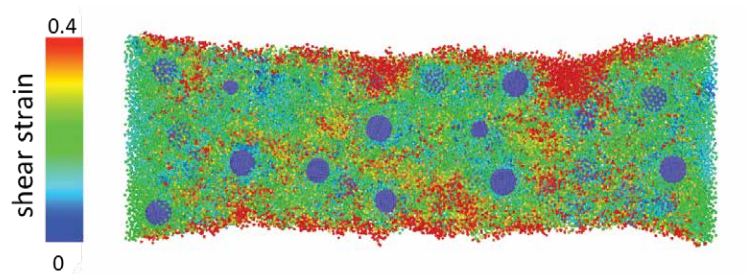
Dong's project is assisting ongoing research by the National Science Foundation Center for Tire Research. He is collaborating with a University of Akron colleague, Jiahua Zhu, Ph.D., to understand mechanical properties of rubber from the molecular level and help with the fundamental understanding through experimentation.

Dong used the LAMMPS (large-scale atomic/molecular massively parallel simulator) software for molecular dynamics simulations on the OSC Owens Cluster to better understand the reactivity of silane with rubber and filler on filler dispersion in the mixing process. He also used high performance computing simulations to develop "a process-microstructure relation to guide the experimental design."

"Our research unleashed the potential of using molecular modeling to advance the understanding of filler dispersion," he said. "Molecular dynamics simulation studies the behavior of material by capturing the dynamics of molecules. Therefore, it demands high performance computation in order to simulate a representative process in terms of size and time.

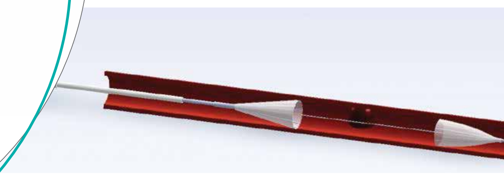
"In my lab, we are equipped with three state-of-the-art workstations, which still do not meet the requirement. OSC provided a solution for this project." •

PROJECT LEAD // Yalin Dong, Ph.D., The University of Akron RESEARCH TITLE // Quantify silane reactivity with silica and rubber for improved silica dispersibility: Towards lowering rolling resistance FUNDING SOURCES // University of Akron, National Science Foundation Center for Tire Research WEBSITE // uakron.edu/engineering/ME/people/profile.dot?u=ydong



VISUALIZATIONS // A molecular view of rubber, a filler-polymer composite, under strain.

TAGS: HIGH PERFORMANCE COMPUTING // DENSE COMPUTE // ENGINEERING & TECHNOLOGY



Mechanical Thrombectomy

Mehrabi team developing device to safely remove clots

Pulmonary embolisms (PE) are a silent killer responsible for hundreds of thousands of deaths each year. Usually caused by a blood clot in the pulmonary artery, PE often originates from blood clots found in the deep veins of the lower legs, a condition known as deep vein thrombosis (DVT). Typical treatment for PE and DVT is less than ideal—anticoagulant medications carry the risk of internal bleeding. Open-heart surgery is extensive and requires a long recovery. A seemingly easy option would be simply removing the clot, but current catheter devices lack the ideal flexibility, and the process can cause smaller blood clots to form. Mohammad Elahinia, Ph.D., professor of mechanical engineering at the University of Toledo, is developing a device that could disrupt the current treatment plan for PE and DVT patients and testing it with computational help from the Ohio Supercomputer Center.

"Current mechanical thrombectomy methods are not effective," said Reza Mehrabi, Ph.D., a partner of Elahinia's on the study. "There is a significant need for a thrombectomy device that is safe, fast, easy to deliver and less expensive."

Elahinia and his team are developing QuickFlow, a revolutionary catheter-directed device for PE and DVT that removes blockages in a variety of anatomical locations. Elahinia is in mechanical engineering—which means the team is working with metals. Nitinol is a superelastic nickel and titanium alloy that can be difficult to work with due to its thermomechanical properties. The team is developing the device using selective laser melting, a technology that uses a laser or electron beam to melt metal powder, creating many micrometer-sized layers. To test the operation of the device and its materials under different types of stress, the team is using ABAQUS and ANSYS software through OSC.

"Numerical simulations will be used to predict behavior of fabricated QuickFlow PE catheters in vivo testing," Elahinia said.

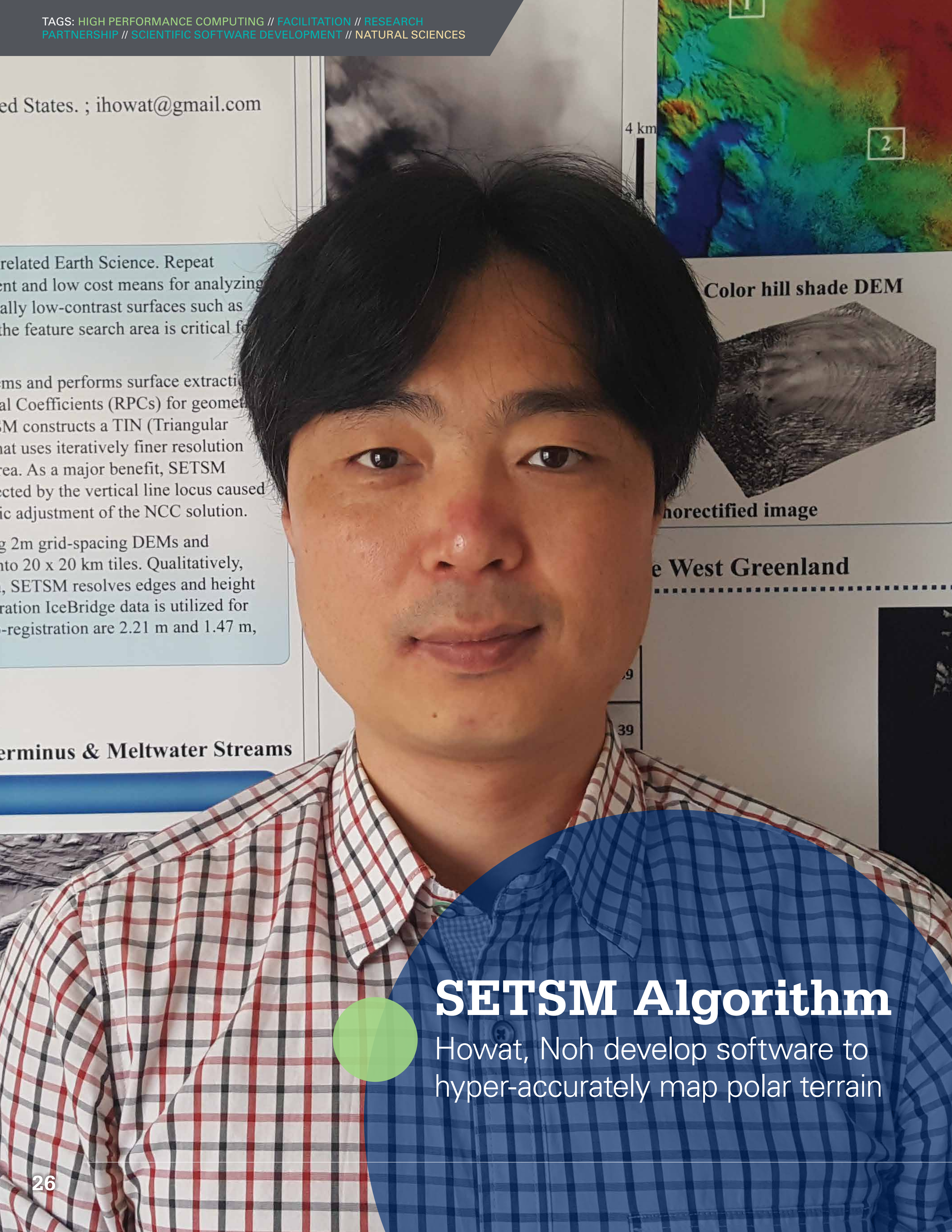
The team will need to solve their current model many times with different boundary conditions.

At the end of the project the team will design and produce the next-generation prototype of QuickFlow and proceed with safety tests and simulated blood clot removal.

"This device shifts the paradigm of care for patients by providing a safe, fast and simple catheter-directed treatment," Mehrabi said. "The current project has an important impact in the human health system and with the support of the Ohio Supercomputer Center will be more effective." •

PROJECT LEAD // Mohammad Elahinia, Ph.D., University of Toledo
RESEARCH TITLE // Addressing pulmonary embolism with Quickflow PE FUNDING SOURCE // University of Toledo WEBSITE // elahinia.net

PHOTO LEFT // A demonstration of the Quickflow PE approximate size. PHOTO RIGHT // The Quickflow PE prototpype consists of two superelastic Nitinol distal and proximal baskets.



SETSM Algorithm

Howat, Noh develop software to hyper-accurately map polar terrain

A detailed understanding of the Earth's land topography is critical to those in geosciences, geographical sciences and even civil engineering. The datasets associated with our land surface topography are the key ingredient to everything from urban planning to plate tectonics.

One of the key tools in this process are Digital Elevation Models (DEMs), which are 3D representations of land surfaces that provide information on a wide range of scientific, navigational and engineering activities. While these models are highly accurate in most areas of the globe, high-latitude, mountainous areas covered in snow and ice have been a challenge to map.

In order to meet this challenge, Ian Howat, Ph.D.—professor at The Ohio State University's School of Earth Sciences Department and director of the Byrd Polar and Climate Research Center—and Byrd Center Senior Research Associate Myoung-Jong Noh, Ph.D., have developed a tool that will accurately produce DEMs of Arctic and Antarctic terrains.

With high performance computing resources from the Ohio Supercomputer Center, Howat and Noh developed the Surface Extraction from Tin-Based Search Minimization (SETSM) algorithm to accurately generate DEMs of these areas.

"The effort was motivated by the fact that no existing commercial or open-source DEM extraction software supports fully automated processing," Howat said. "We've spent years developing SETSM for constructing photogrammetric DEMs from satellite imagery with the objective of creating a fully automated system capable of handling large amounts of data."

DEMs are generated by using satellite images to detect corresponding points between two images taken at different positions, similar to how human eyes have slightly different perspectives. The information is then computed as a 3D coordinate from a sensor model that explains the relationship between a flat image and the Earth's surface.

A step in finding the corresponding points is aligning the pair of images through pattern matching. DEMs are dependent on the accuracy of the image matching algorithm and the sensor model. Traditionally, image matching was done by hand, a procedure far too laborious for a high volume of data. Development of a fully automatic DEM generation software is therefore critical for application to large-scale datasets.

"It's especially important in the Arctic and Antarctic," Noh said. "High-quality stereoscopic DEM extraction over mountainous, snow-covered and glaciated regions is particularly challenging due to the prevalence of low-contrast surfaces such as ice, snow and mountain shadows and repetitively patterned textures."

Noh and Howat used OSC clusters to develop and test SETSM to speed up the procedures with various datasets. The project began in 2012 and in 2015 SETSM became a main DEM-producing software. In 2017, it was released as an open source code. SETSM is the DEM extraction software used for the National Science Foundation's major surface mapping projects; ArcticDEM and the Reference Elevation Model of Antarctica, which are providing the first continental-scale topography datasets at high resolution.

"OSC does a great job of supporting researchers who need rapid processing," Noh said. "The DEMs generated by the SETSM algorithm can be applied to large data sets for a wide range of applications requiring detailed topographic information for mapping, land classification and change detection. In 2015, for instance, the SETSM team that included OSC worked quickly to produce high resolution elevation models for the Nepali earthquake relief effort. These data were critical for a range of uses, including mapping infrastructure, planning rescues and assessing slope stability." •

PROJECT LEADS // Ian Howat, Ph.D., The Ohio State University; Myoung-Jong Noh, Ph.D., The Ohio State University RESEARCH TITLE // Collaboration on SETSM software FUNDING SOURCES // National Aeronautics and Space Administration, National Science Foundation, Polar Geospatial Center WEBSITE // earthsciences.osu.edu

LEFT PAGE PHOTO // Byrd Polar and Climate Research Center Senior Research Associate Myoung-Jong Noh, Ph.D. in front of a poster presentation of the project.

Weld-induced Distortion

EWI, AweSim partner designing 3D weld-prediction app

Weld-induced distortion is an expensive and time-consuming problem for manufacturers of heavy equipment to overcome. However, modeling and simulation can be a major tool to help manufacturers predict and understand possible distortion, avoiding repair costs and waste down the road.

EWI—an engineering and technology organization headquartered in Columbus, Ohio—and the Ohio Supercomputer Center's AweSim program are longtime partners in offering a Weld Predictor app that harnesses the power of high performance computing. The app allows clients to simulate arc welding procedures that predict microstructure, thermal profile, residual stress and distortion in heavy equipment manufacturing.

EWI's current 2.5D Weld Predictor app through AweSim continues to attract clients because cost savings is estimated in the millions of dollars, and the app has been shown to reduce the scrap rate by 60 percent.

Recently, EWI teamed with OSC to create a 3D version of the Weld Predictor.

"The tools used 3D models and are applicable to three common types of welding processes: arc welding, laser welding and hybrid laser arc welding," according to Yu-Ping Yang, who worked with AweSim as EWI's principal engineer on structural integrity and modeling. "Standard weld joints, butt joints, T-joints and lap joints, were included in the software tool. Open source finite element codes were used as a solver and as pre- and post-processing tools. A new web application front end was developed by OSC that allows interactive rotation and zoom controls by a user."

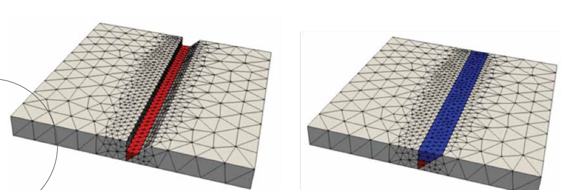
EWI and AweSim developed a whole host of tools for the app, including:

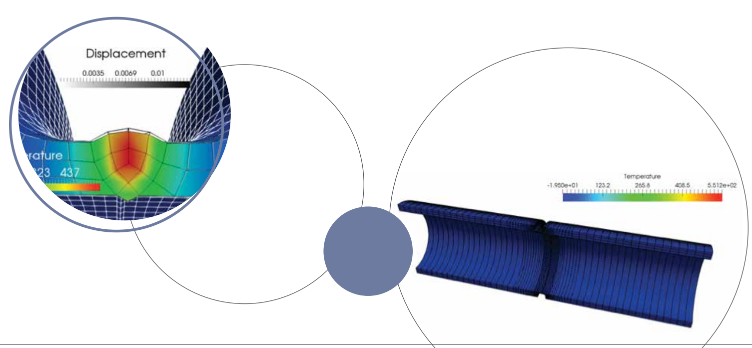
- A python script developed for automatic mesh generation of the three welded joints using an open-source program.
- A material property database containing data for commonly used steels, aluminum alloys, and titanium alloys as well as corresponding filler wires.
- Weld modules for arc welding, laser beam welding, and hybrid laser arc welding to simulate welding processes to predict temperature, stress and distortion.
- An existing open-source software application, ParaView, was integrated for post-processing.
- A simulation flow and script developed for automatic analyses of welding processes.

"This app will be accessed by many users at once," Yang said. "This research will extend to any welded structures. Industrial companies use this app to optimize their product design and manufacturing process, which will create big savings in terms of time and money to develop a new product and improve the existing manufacture processes."

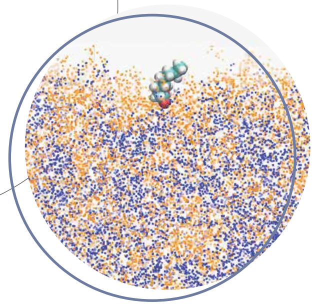
The 2.5D version of the app will remain available to users while engineers continue to refine 3D. •

PROJECT LEAD // Yu-Ping Yang, Ph.D., EWI RESEARCH TITLE // Welding cloud computational applications for digital manufacturing FUNDING SOURCES // EWI, AweSim, Digital Manufacturing and Design Innovation Institute WEBSITE // ewi.org





VISUALIZATIONS BOTTOM LEFT // Modeling the addition of filler metal for a multi-pass weld VISUALIZATIONS BOTTOM RIGHT // Modeling the over-heating of welding filler metal



Molecular Interfaces

Lacks simulates water-alcohol mixtures to gauge products

The way your favorite beverage tastes, how foamy your hand sanitizer is, the way certain products smell or feel or taste or flow is based on whether molecules in a water-alcohol solution go to the surface of the mixture or stay in a group.

Research into the behavior of molecular interfaces from a theoretical chemistry perspective has been fairly common over the years. However, researching these behaviors from an industrial point of view has been sparse. That's where Case Western Reserve University's Daniel Lacks, Ph.D., comes in.

Lacks, the chair of CWRU's Department of Chemical and Biomolecular Engineering and a professor of chemical engineering, performs computational simulations through the Ohio Supercomputer Center to research the behavior of surfactants in water-alcohol mixtures to better understand, and in the future control, the characteristics of products we regularly consume.

A surfactant is a molecule that reduces surface tension at an interface—possibly between two liquids, a liquid and a gas or a liquid and a solid—and their presence alters the overall behavior of a product or system. Not only could Lacks' research apply to personal care products or beverages, but also to biotechnology, with regard to the structure of proteins in the body.

"Originally we were looking at this in regard to personal care products," Lacks said. "But there's really interesting science behind it so we got an NSF (National Science Foundation) grant to study the general idea of solvation (the interaction of a solvent with dissolved molecules) and whether molecules go to a surface."

Products interact with the environment at surfaces, so understanding those behaviors would allow us to manipulate a product's taste, smell, or any number of characteristics a consumer may prefer, Lacks said.

Lacks performed "computationally intensive" simulations on OSC's Owens and Oakley clusters in order to carefully control and validate experiments, artificially changing aspects of a molecule to determine how it will behave.

"With a mixture you need bigger systems," Lacks said. "It takes a lot of averaging to get these small changes to be significantly visible, and to see small differences you need to run long simulations and that's where we use OSC resources.

"The key is understanding what aspects of the molecule would lead to it going to the surface rather than staying in the bulk. That could help design new molecules." •

PROJECT LEAD // Daniel Lacks, Ph.D., Case Western Reserve University RESEARCH TITLE // Molecular dynamics simulation of surfactants at interfaces of aqueous solutions FUNDING SOURCE // National Science Foundation WEBSITE // engineering.case.edu/profiles/djl15

VISUALIZATIONS TOP // Snapshot from a molecular dynamics simulation showing an octanoic acid surfactant molecule at the surface of an ethanol-water solution (ethanol depicted as tan dots, water depicted as blue dots). PHOTO TOP // Daniel Lacks, Ph.D., Case Western Reserve University.

"If I need to move a huge quantity of data over to that storage, I know it's not going to bring the system to its knees. It's designed precisely for that purpose."

— *David Kinnamon, Ph.D., Director of Human Genetics Research Informatics*

Data Management

Kinnamon creates platform to handle troves of genetic info

The more genetics researchers learn about the building blocks of life, the more data they produce. This is a great problem to have—the more they know, and the more detail in which they know it, the better we can treat diseases at the individual level, streamline screening processes and create targeted pharmaceuticals. However, for researchers and genetic counselors, wading through the myriad of genotypes and phenotypic information to get to a specific set of relevant genes or variants is an unnecessary hindrance to the life-changing work they could be doing. Daniel Kinnamon, Ph.D., director of Human Genetics Research Informatics in the Division of Human Genetics at The Ohio State University's Wexner Medical Center, is head of a project that will make their lives easier.

Kinnamon worked directly with staff at the Ohio Supercomputer Center to create a human genetics data management platform that takes advantage of the Center's high performance storage and compute capacity. Most end users of the medical center data only need to view information for a few genes or variants at a time. Searching through a number of large files, many more than 10 gigabytes in size, for the needed information is both infeasible and inefficient.

PHOTO TOP // David Kinnamon, Ph.D., Director of Human Genetics Research Informatics in the Division of Human Genetics at The Ohio State University's Wexner Medical Center

"Alignments are stored in huge files that are not humanly readable," Kinnamon said. "There's an open-source browser for these types of files. We were able to take that software and integrate it into our platform's web interface. Because OSC has high performance storage that we use for our platform's genomic data, we could actually have the web interface submit a request to get just the relevant section of the file off of storage and respond quickly. That allows our end users to interact with these data that otherwise would have been totally inaccessible to them."

The platform comprises two OSC-hosted virtual servers residing on a single physical server. An application server provides a front-end data management and analysis option for users while another server stores and manages data. Small analysis jobs can be performed locally on the application server while larger jobs, e.g., sequence alignment or genome-wide association studies, will be executed on the OSC Oakley or Owens clusters. OSC has also recently provisioned a third virtual server to enable secure access to protected data via the web interface by end users external to the Wexner Medical Center.

Currently, Kinnamon's platform supports 28 different research protocols, including a $12.4 million NHLBI- and NHGRI-funded study on the genetics of dilated cardiomyopathy (DCM), a heart condition in which the left ventricle becomes enlarged and weakened, decreasing the heart's ability to pump blood. Researchers on the project want to identify and characterize genes that cause or predispose an individual to dilated cardiomyopathy, which is a leading cause of heart failure. The project currently has phenotypic data on hundreds of families and exome sequences on hundreds of individuals with DCM within these families. The team is narrowing copious amounts of data down to 35 genes related to DCM. Genetic counselors and molecular geneticists involved in the study need to use information on potentially relevant variants that may exist in several public databases to figure out if they might contribute to disease. Through the use of Kinnamon's platform, they can view this information and curate variants quickly through a user-friendly web interface without having to know cryptic command line instructions.

"We have exome sequences back on 387 people, and we're expecting to get about 1,500 by early 2020 for just this study, so you can get an idea of how rapidly our storage needs are going to scale," Kinnamon said. "If I need to move a huge quantity of data over to that storage, I know it's not going to bring the system to its knees. It's designed precisely for that purpose. Scalability is the reason we decided to build this entire system at OSC from the get-go." Kinnamon adds that the scalability provided by OSC will be crucial for the next DCM genetics study currently in the planning phase, which will be collecting data on 10,000 patients and their families. •

PROJECT LEAD // Daniel Kinnamon, Ph.D., The Ohio State University Wexner Medical Center RESEARCH TITLE // Division of Human Genetics Data Management Platform FUNDING SOURCES // The Ohio State University Wexner Medical Center and Comprehensive Cancer Center, NHLBI, NHGRI, NCI, Pelotonia WEBSITE // wexnermedical.osu.edu/departments/internal-medicine/genetics/team/daniel-kinnamon-phd; dcmproject.com

PHOTO TOP // Kinnamon's research team views programming and graphics related to their data management platform.

Search Engines

Sun's team seeking integration of machine, human sources

How many times a day do you turn to a search engine to answer a question? For most of us, it's often. Of course, when a question has more depth or could confuse your go-to artificial intelligence source, we turn to other people, maybe through direct contact or community platforms. And while both machine and human question-answering avenues have developed rapidly, they each have their limitations.

Huan Sun, Ph.D., assistant professor of computer science and engineering at The Ohio State University, wants to address those limitations by combining the best of both worlds, and she's using the Ohio Supercomputer Center to do it.

"Our grand vision is that humans and machines should team up as an integrated complex system for effective and efficient question answering," Sun said. "But the techniques we're proposing can potentially be generalized to many other scenarios where human and machine intelligence need to be combined in an algorithmic manner."

Sun and her lab began using OSC to collect open source data sets to do analysis and build models for benchmarking. One of those models is based on reinforcement learning, a branch of machine learning that involves human-machine collaborations, allowing the machine to learn from human interaction.

"If we can leverage human-machine collaborations in the task of question answering, there are a lot of opportunities to advance other AI (artificial intelligence) tasks further," Sun said. While one goal of Sun's research is simply helping us all get better answers to our questions faster, a bigger goal is improving AI's ability to discover knowledge from various data sources and using that knowledge to answer questions and help people make decisions in various domains including healthcare, online shopping, education, etc. Sun used Tensorflow, an open source software library in Python, on OSC's Owens and Oakley clusters to model the large-scale data sets that included an encyclopedic knowledge base with hundreds of millions of entities in the world as well as their relations. The research also includes modeling deep neural networks that take a massive number of model parameters to be optimized .

The GPU capabilities on Owens and the storage OSC offers are critical to Sun's research.

"We heavily use methods like deep learning models, which can easily have millions of parameters to build, and the models may take two days to train even when using one or two GPUs," Sun said. "It could take weeks or months to fully develop and refine these models and so HPC (high performance computing) is really important." •

PROJECT LEAD // Huan Sun, Ph.D., The Ohio State University RESEARCH TITLE // Advancing human and machine question answering via human-machine collaboration FUNDING SOURCES // The Ohio State University, Army Research Office. WEBSITE // web.cse.ohio-state.edu/~sun.397

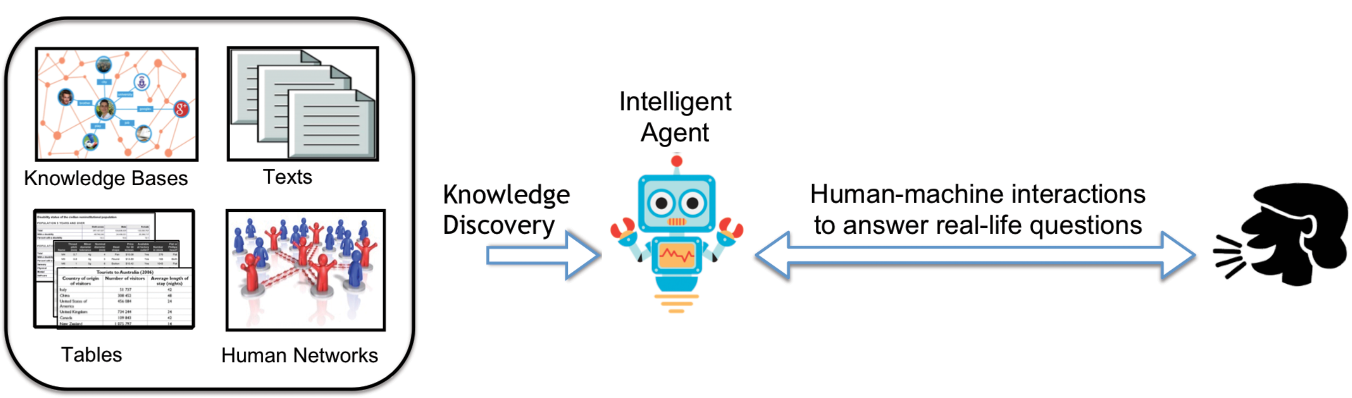
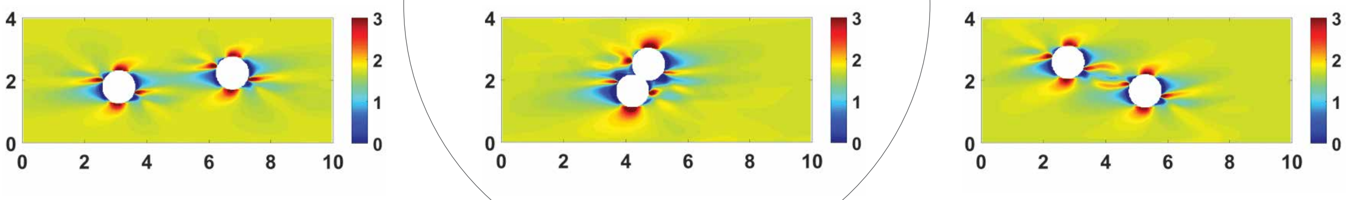


DIAGRAM // Huan Sun, Ph.D., is building advanced intelligent agents that can discover knowledge from various data sources to answer user questions in an interactive and collaborative manner, helping people make decisions in various domains including healthcare, online shopping and education.



Complex Suspensions

Hormozi lab simulates landslides, mudslides, avalanches

Researchers in Sarah Hormozi, Ph.D.'s lab refuse to go with the flow: instead, they study it. More specifically, Hormozi, assistant professor of mechanical engineering at Ohio University, investigates complex suspensions in fluids. These occur in natural settings such as landslides, mudslides, underwater avalanches as well as industrial settings such as mining operations and in the petroleum industry. Rather than waiting for one of these natural disasters to happen or traveling to mines and oil fields, the group simulates these flows using resources at the Ohio Supercomputer Center.

"There is a compelling need to study the rheological behaviors of these complex suspensions in order to be able to predict their flow dynamics in various situations," Hormozi said. "However, this prediction is a challenging problem due to the complex rheology of the suspending fluids, the interaction of fluid and particle phases, and multiple-body and short-range interactions of particles."

The suspensions Hormozi's group studies are materials consisting of viscous fluids and solid particles, with a broad range of sizes. The suspending fluid itself may exhibit a wide range of behaviors such as shear thinning, shear thickening, shear banding, yield stress and viscoelasticity. The group intends to create a computational framework based on the Immersed Boundary Method, used to study various types of flow. The large, impactful project is directed by Ohio University and KTH Royal Institute of Technology in Sweden. The group has used OSC for a few projects in this area.

One such project involves the mixing of municipal sludge, or semi-solid sewage material. Understanding the mixing process is important as it influences how to thermally treat the waste, for example, through anaerobic digestion. This can have a profound influence on what gases are released into the atmosphere in this process. Throughout this project, the group identified ways to enhance mixing by redesigning the flows as well as the mixing digester geometry.

"The project is composed of highly expensive simulations which require intensive computational time on multiple CPU," Hormozi said. "Conducting this project is essentially impossible without being able to use a multi-core high performance supercomputer like OSC."

Hormozi intends to integrate this research with educational activities to promote interdisciplinary research, teaching and international collaboration. •

PROJECT LEAD // Sarah Hormozi, Ph.D., Ohio University PROJECT TITLE // Interface-resolved simulations of particle suspensions in complex fluids FUNDING SOURCES // National Science Foundation, European Research Council WEBSITE // hormozilab.com/

VISUALIZATIONS TOP // Colormaps of the first normal stress difference at different times. PHOTO BOTTOM // Photo of Dr. Hormozi, courtesy of Ohio University.

Diagnostic Tests

Chen, Ning evaluating methods for checking test accuracy

When it comes to making medical decisions, sometimes even our tests need to be tested. Ying-Ju Tessa Chen, Ph.D., assistant professor in the Department of Mathematics at the University of Dayton, in collaboration with former advisor Wei Ning, Ph.D., at the Bowling Green State University, is studying the effectiveness of the receiver operating characteristics (ROC) curve analysis using their proposed method: the Adjusted Jackknife Empirical Likelihood (AJEL) method. Chen's research is accelerated through the use of the Ohio Supercomputer Center services to process huge datasets.

In the medical world, the ROC curve analysis is the gold standard for measuring the effectiveness of various diagnostic tests. It provides a graphical display showing the relationship between the true positive rate and false positive rate of test results as the criterion changes. The ROC curve has been widely applied in epidemiology, biometrics, medical research, diagnostic medicine and material testing and model performance assessments.

While the ROC curve effectiveness has been explored previously by other researchers in the field, Chen hopes the AJEL method will be easier to implement and have fewer complications than previous methods.

"There are some computational difficulties in practice while using (previous methods)," Chen said. "To obtain the statistic based on the empirical likelihood, the procedure involves the maximization of the nonparametric likelihood through the calculation of Lagrange multiplier subject to given constraints. When the constraints are either linear or can be switched to be linear, the maximization process of EL method is easy to be accomplished. However, when the constraints are nonlinear, there are some computational challenges. In addition, the convex hull of the estimating equation might not contain the zero vector and then the estimate of interest parameter does not exist. In short, the maximum likelihood estimator of the ROC curve may not exist due to such difficulty."

To test her proposed method, Chen needed to perform an extensive simulation study with a high number of repetitions and large sample sizes to compare the performance of the proposed method against several existing methods. Using the R programming language, Chen wrote parallel algorithms to run the simulations.

"The computing resources in the Ohio Supercomputer Center helped us to speed up the progress of completing this project tremendously," Chen said.

The AJEL method and the corresponding properties were developed based on U-statistics, a class of "unbiased" statistics that is especially important in estimation theory. In future work, Chen and colleagues are interested in extending a similar idea to more general class of statistics than U-statistics and investigating the properties of the AJEL method beyond the ROC curve.

"If we didn't have access to OSC, it would be very difficult to complete this project," Chen said. "The project would only include the simulation study with some simple comparison." •

PROJECT LEAD // Wei Ning, Ph.D., Bowling Green State University
RESEARCH TITLE // ROC curve analysis based on adjust empirical likelihood method FUNDING SOURCE // Bowling Green State University WEBSITE // personal.bgsu.edu/~wning

PHOTO // Ying-Ju Tessa Chen, Ph.D, processes huge datasets at OSC to test her lab's AJEL method.

Statewide Users Group

The demand for high performance computing in Ohio is relentless, and it does not discriminate by field. At the Ohio Supercomputer Center's Statewide Users Group (SUG) conferences, clients in fields spanning everything from astrophysics to linguistics gathered to share research highlights and hear updates about the Center's direction and role in supporting science across Ohio.

Statewide Users Group conferences in September of 2017 and April of 2018 brought OSC clients face-to-face with OSC representative and experts and brought the research being done on their supercomputer clusters to the forefront of both groups.

SUG is a volunteer group composed of the scientists and engineers who provide OSC leadership with program and policy advice and direction to ensure a productive environment for research.

The September conference featured a keynote address from Bryan C. Carstens, Ph.D., associate professor and vice chair of the Department of Evolution, Ecology and Organismal Biology at Ohio State. A longtime client of OSC, Carstens presented his research into the protection of biodiversity. His presentation discussed his thesis that publicly accessible databases contain millions of data points that are relevant to the discovery and protection of biodiversity, but are currently underutilized.

Attendees at the April 2018 conference heard a keynote address from Andrew Siegel, director of application development at Argonne National Laboratory. Breakout sessions provided attendees with deep dives on hardware, software, Big Data, OSC's OnDemand, and app development, as well as a tour of the State of Ohio Computing Center.

Both conferences also featured a variety of topics and poster and flash talk competitions. Nearly 40 participants competed in each conference, with winners receiving 5,000 resource units of time on OSC systems and runners-up receiving 2,500 resource units.

(continued on page 36)

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SUG Conference Winners

Fall 2017 Flash Talks

Alex Trazkovich, an Ohio State student, won the flash talk competition for his presentation "Effects of Copolymer Sequence on Adsorption and Dynamics Near Nanoparticle Surfaces in Simulated Polymer Nanocomposites."

R. Keith Slotkin, also a student at Ohio State, was the runner-up for his flash talk titled "Bioinformatics: From Reference Genomes to Individuals Using Existing Datasets."

Fall 2017 Posters

Mohammad Shahriar Hooshmand, another Ohio State student, won the poster competition for his project, titled "Oxygen Diffusion around (10-12) Twin Boundary in Ti."

There were two runners-up in the poster competition: Dan Gil, a student at Case Western Reserve University, whose project was titled, "The Solvophobic Effect," and Lianshi Zhao, an Ohio State student, whose project was titled, "Large-scale Computation for Plasma Opacities."

Spring 2018 Flash Talks

The Ohio State University's Lifeng Jin won the flash talk competition for his presentation titled "Unsupervised Depth-bounded Grammar Induction Model for PCFG with Inside-Sampling."

Taking the runner-up position, also from Ohio State, was Jorge Torres with "The Role of HPC in the Radio-detection of Astrophysical Neutrinos."

Spring 2018 Posters

Adriaan Riet, from Case Western Reserve University, won first place for his presentation titled "Enhanced Diffusion in an MgO Grain Boundary through Molecular Dynamics Simulations."

There was a tie for the runner-up poster winner. The Ohio State University's Masood Delfarah's poster was titled "Recurrent Neural Networks for Cochannel Speech Separation in Reverberant Environments," and Rosario Distefano, also from Ohio State, shared the distinction with her poster titled "miREpiC: miRNA Editing Profiling in Cancer."

PHOTO LEFT // Andrew Siegel from Argonne National Laboratory presents in April 2018. PHOTO RIGHT // Attendees at SUG poster session.

Training Services

OSC reached out to more clients and potential users than ever this year, expanding its workshop offerings and traveling across the state to bring training and education to users at several universities and the surrounding areas. The Statewide Users Group brought more cutting-edge knowledge to the forefront of OSC clients at its two annual conferences, featuring keynote speakers and peer-led flash talks. And, supporting the next generation of researchers and engineers, OSC invests in its annual summer programs, hosting dozens of bright middle and high-school students from around the state for hands-on learning about high performance computing at an early age.

Workshops

The Ohio Supercomputer Center is an incredible resource for academic researchers across the state—which is why it is imperative they know how to use it.

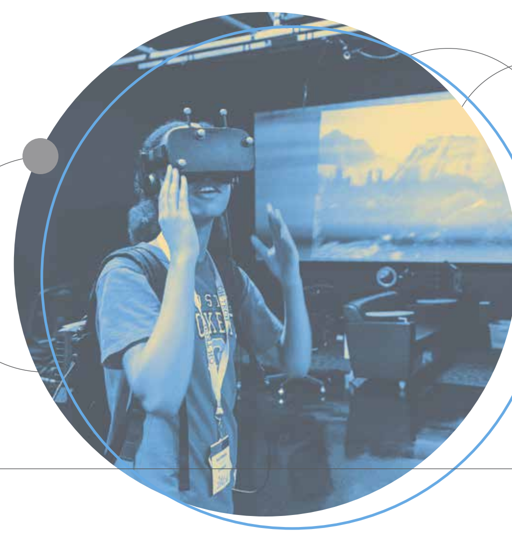
New groups, new departments and new disciplines—such as linguistics, computational biology, or economics—are beginning to use high performance computing more every day. However, in these areas, users don't have many seasoned colleagues to turn to within their own department, or their own college, so it takes them longer to get started and become productive.

This year, OSC took steps to address this learning gap through workshops in a different section of Ohio each month to help introduce academic clients to HPC and to address roadblocks they may have. In the last year, the number of workshops and trainees nearly tripled, with 23 training opportunities attended by 461 people.

Summer Programs

Each summer, OSC has a role in shaping Ohio's future STEM leaders through its summer programs. Summer Institute (SI) is OSC's unique and intense two-week residential summer program for high school students entering their sophomore, junior or senior year. Participants experience the dynamic world of high performance computing as they work alongside peers and experts in the field to research complex, real-world science and engineering challenges using computational science.

Young Women's Summer Institute (YWSI) is a weeklong program for Ohio's middle school girls to gain valuable computer, math, science and engineering skills through hands-on, collaborative projects. YWSI girls develop a deeper interest in science, technology, engineering and math (STEM) as they use the latest computer technology to solve complex, real-world science and engineering challenges with a team of peers.



Software Services

Scientific Software Development

As professionals in high performance computing 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.

OSC also provides more than 130 different software packages to researchers, with about 20 of them licensed packages. Researchers also can bring their own software or applications.

OSC staff members are available for consulting or collaboration with research computing teams that require expertise to tackle problems or reduce the runtime for their analyses. OSC experts have experience with several computing languages, programming models, numerical libraries and development tools for parallel/threaded computing and data analysis.

Overall Client Impact

23 academic institutions

48 companies

2,202 clients

256 awards made

23 training opportunities

461 trainees

604 projects served

33 courses used OSC

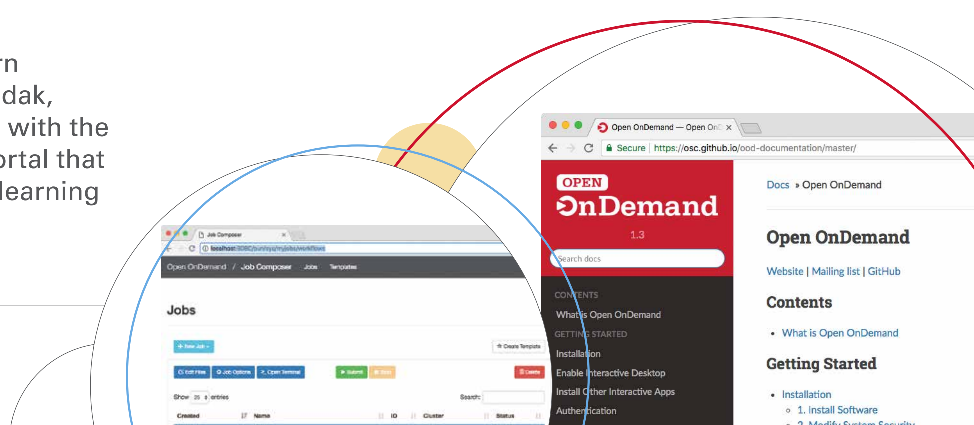
Web Software Development

OSC's expert web development team helps clients create custom web interfaces to simplify the use of powerful HPC resources, allowing data to be the focus. Simplifying workflows allows researchers to dive into finding solutions and making breakthroughs.

OSC's one-stop shop for access to its high performance computing services, OSC OnDemand is a custom-built web portal that provides users with seamless, flexible access to all of OSC's computing and storage services.

"Up until this point, clients had to install software, use a cryptic file editor and learn batch system commands," said David Hudak, executive director of OSC. "Our objective with the OnDemand project has been to build a portal that will allow them to use HPC without a big learning curve. It's about lowering the barrier of entry to the world of supercomputing."

Users can upload and download files, and create, edit, submit and monitor jobs. Because of its user-friendly interface and ease of access, OSC OnDemand has changed the game for those needing HPC access. No longer do researchers need to know command line instructions to access a supercomputer. OSC OnDemand breaks down barriers so researchers with a wide variety of backgrounds can easily access OSC's resources.



Service Highlight

Open OnDemand

In 2017, OSC launched Open OnDemand 1.0, an open-source version of OSC OnDemand, the Center's online, single-point-of-entry application for HPC services.

Open OnDemand is an NSF-funded project to develop a widely shareable web portal that provides HPC centers with advanced web and graphical interface capabilities. Through OnDemand, HPC clients can upload and download files, create, edit, submit and monitor jobs, run GUI applications and connect via SSH, all via a web browser, with no client software to install and configure.

To date, about a half-dozen HPC centers have installed and deployed the package, and another half-dozen have installed the portal for testing and evaluation.

"In my mind, the biggest benefit of Open OnDemand for us is the ability for our users to run graphical applications like Matlab, Ansys, etc., on HPC resources without having to log into these resources directly," said Martin Cuma, a scientific consultant at the Center for High Performance Computing at the University of Utah, where staff already have deployed Open OnDemand. "Learning the basics of the HPC resource use (basic Linux terminal operation, queue manager, etc.) can be a hurdle which Open OnDemand should at least partially reduce."

"We're excited to be offering Open OnDemand for the NSF-funded PSC Bridges system," said Jason Sommerfield, coordinator of systems and operations at the Pittsburgh Supercomputing Center, which also has deployed Open OnDemand. "Beyond providing an approachable onramp for new users, Open OnDemand's recent addition of support for applications, such as the Jupyter Notebooks collaboration tool, further simplifies important, common HPC workflows."

Open, interactive HPC via the web

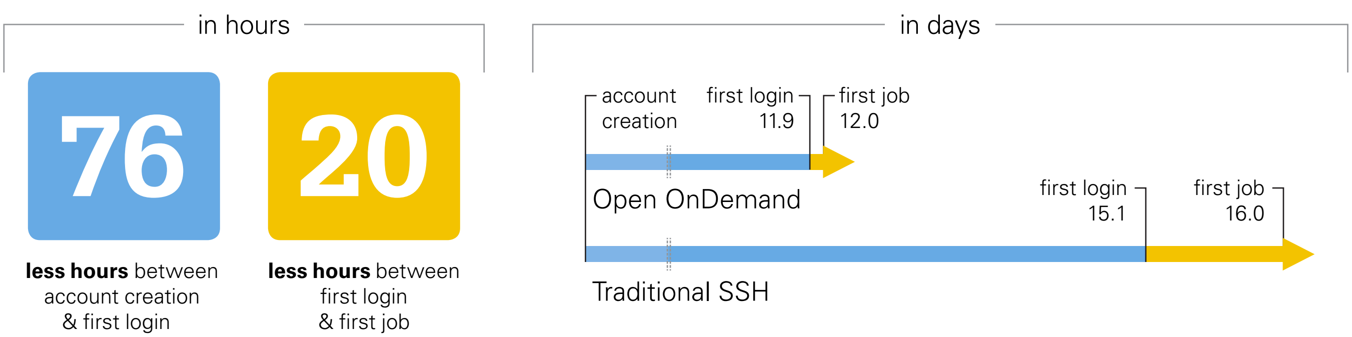
The 1.0 version of Open OnDemand includes the ability to launch interactive HPC desktop sessions with the new dashboard "batch connect" plugin, support for Portable Batch System Professional's (PBS Pro) workload manager and job scheduler software and partial support for IBM's Load Sharing Facility (LSF) 9.1 workload management platform.

OnDemand can be installed on a variety of HPC operating systems, such as RHEL and CentOS; and on a variety of resource managers such as Torque, PBS Pro, LSF, Slurm and SGE.

For more information, visit openondemand.org.

Faster Time to Science

Using OnDemand vs. traditional SSH access*



*Data set: Median times from 1712 OSC accounts created in 2017

Hardware Services

Cluster Computing

OSC offers a fully scalable center with mid-range machines to match those found at National Science Foundation centers and other national labs. Collectively, OSC supercomputers provide a peak computing performance of 1.9 petaflops. As a whole in 2017, OSC clients accomplished 4.4 million computational jobs, used 221.4 million core hours and conducted 604 projects as well as 33 academic courses.

Preparations to install and deploy the new Pitzer Cluster stretched throughout late 2017 and most of 2018. In December 2017, the Center upgraded its backup capacity and performance with the addition of a new tape library. A new IBM storage solution installation was completed mid-2018, and the rest of the year will bring new backup servers and disk storage pools.

Research Data Storage

Ohio researchers have access to many file storage options at OSC. OSC's research data storage includes high performance, large capacity spaces along with others that are perfect for a wide variety of research data. OSC offers clients more than five petabytes (PB) of disk storage capacity distributed over several file systems, plus more than seven PB of backup tape storage.

OSC's scratch service is a high performance file system that can handle high loads and is optimized for a wide variety of job types. OSC also provides a parallel file system for use as high-performance, high-capacity, shared temporary space. The current capacity of the parallel file system is about 1.1 PB.

Services Delivered

221 M+ core hours consumed

78% average HPC system utilization

4.4 M+ computational jobs

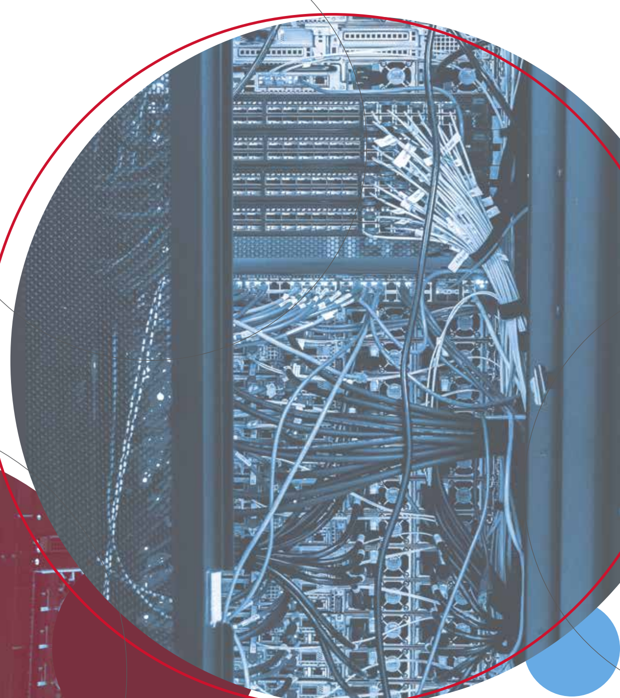
98% up-time

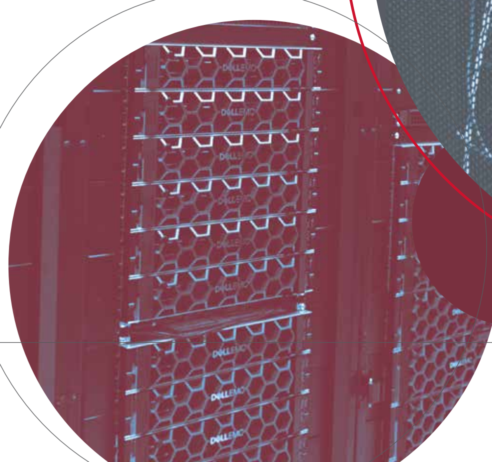
44% average storage system utilization

1.5 PB data stored

2 PB data transferred

79% jobs started within one hour





Supercomputers

Students, scientists, engineers and clinicians depand on these key OSC systems:

Owens Cluster

A 23,392-core Dell/Intel Xeon machine:

- 28 cores & 128 GB of memory per node
- 16 nodes have 1.5 TB of memory & 48 cores
- 160 nodes have Nvidia Tesla P100 GPUs

Ruby Cluster

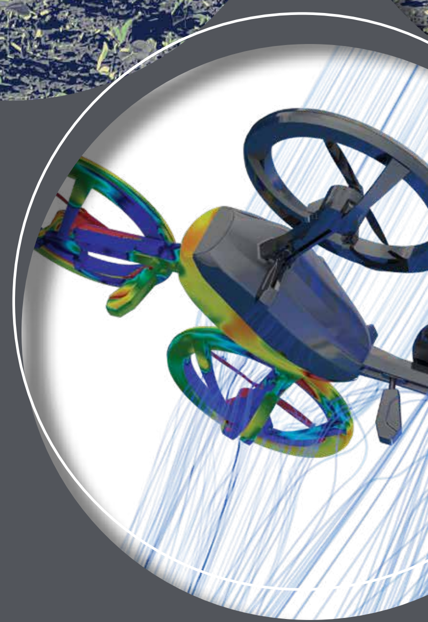
A 4,800-core HP/Intel Xeon machine:

- 20 cores & 64GB of memory per node
- One node has 1 TB of memory & 32 cores
- 20 nodes have Nvidia Tesla K40 GPUs

Oakley Cluster

An 8,304 core HP/Intel Xeon machine:

- 12 cores & 48 GB of memory per node
- One node has 1 TB of memory & 32 cores
- 64 nodes have 2 Nvidia Tesla M2070 GPUs



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