



# Annual Report

2017–2018



# Ohio Supercomputer Center

An **OH·TECH** Consortium Member

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“The Ohio Supercomputer Center delivers an assortment of powerful, cutting-edge services that propel academic research and business innovation across Ohio.”

— John Carey, Chancellor, Ohio Department of Higher Education

**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.

osc.edu

# Beyond first impressions

After visiting the Ohio Supercomputer Center (OSC) for the first time, many people leave with a singular impression of racks of powerful hardware sitting inside a comfortably air-conditioned room. While that observation is perfectly valid—without compute and storage systems, you don't have a supercomputer center—there are many equally essential aspects.

A center thrives on clients who leverage advanced computing to make discoveries, unlock innovations and identify trends. Ohio's rich legacy of invention and discovery continued in 2017 through the efforts of over 2,200 students, scientists, engineers and clinicians from 23 universities and multiple commercial companies.

Also, a center needs the support of consistent and supportive stakeholders. The State of Ohio, through the Ohio Department of Higher Education, has been investing in OSC since its 1987 creation, tasking the Center with placing "Ohio's research universities and private industry in the forefront of computational research." Industry clients help support OSC's mission, and universities contribute to OSC's ongoing sustainability.

Dynamic networking technologies must be identified to connect a center's systems to its clients. OARnet, our sister organization and a leading statewide research and education network, delivers data to and from our clients throughout Ohio, across the country and around the world.

An efficient, expert staff offering systems services, software development, support and training is crucial to helping clients get the most out of each computing session, whether through system configuration, coding, training, troubleshooting or other services.

In short, OSC is fortunate to be so much more than just amazing machines in the middle of a floor; it is an immeasurable blend of brilliant researchers, dedicated stakeholders, robust connecting technologies and expert support. That's the reality behind the first impressions.



**David Hudak, Ph.D.**  
Executive Director



## Highlights

### **Prioritizing education and training**

In 2017–18, OSC staff nearly tripled the number of education opportunities around the state, training 461 users on high performance computing (HPC) systems and OSC-specific programs. For those who lack institutional knowledge of OSC—especially as more new fields realize the usefulness of HPC resources—OSC addresses this learning gap through its workshops, across Ohio. In-person office hours are also available every other Tuesday in Columbus during the academic year.

### **Open OnDemand**

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

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

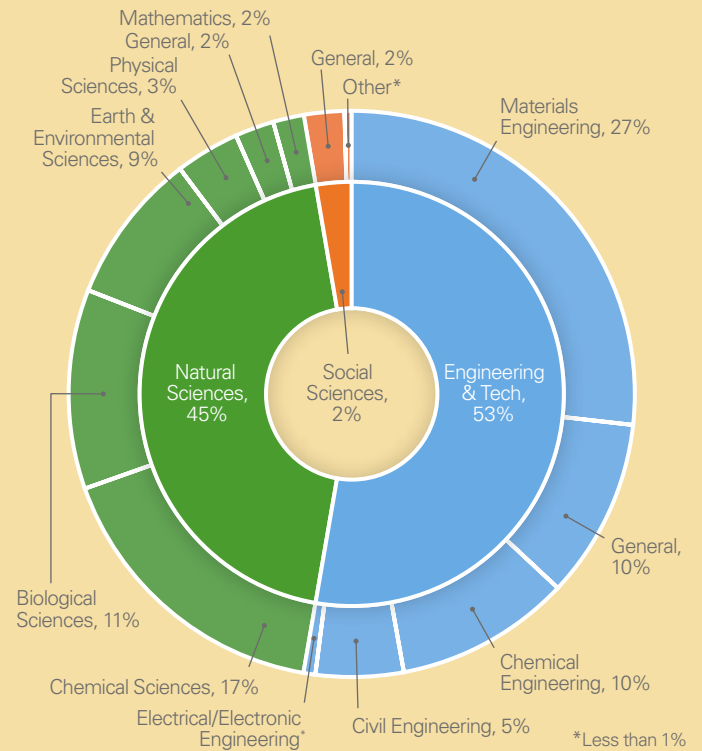
### **Storage and facility upgrades**

The Center upgraded its backup capacity and performance with the addition of a new tape library in December. 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.

## Active Academic Projects



## Academic Fields of Science



## Overall Client Impact



**23**  
academic institutions



**48**  
companies



**2,202**  
clients



**256**  
awards made



**23**  
training opportunities



**461**  
trainees



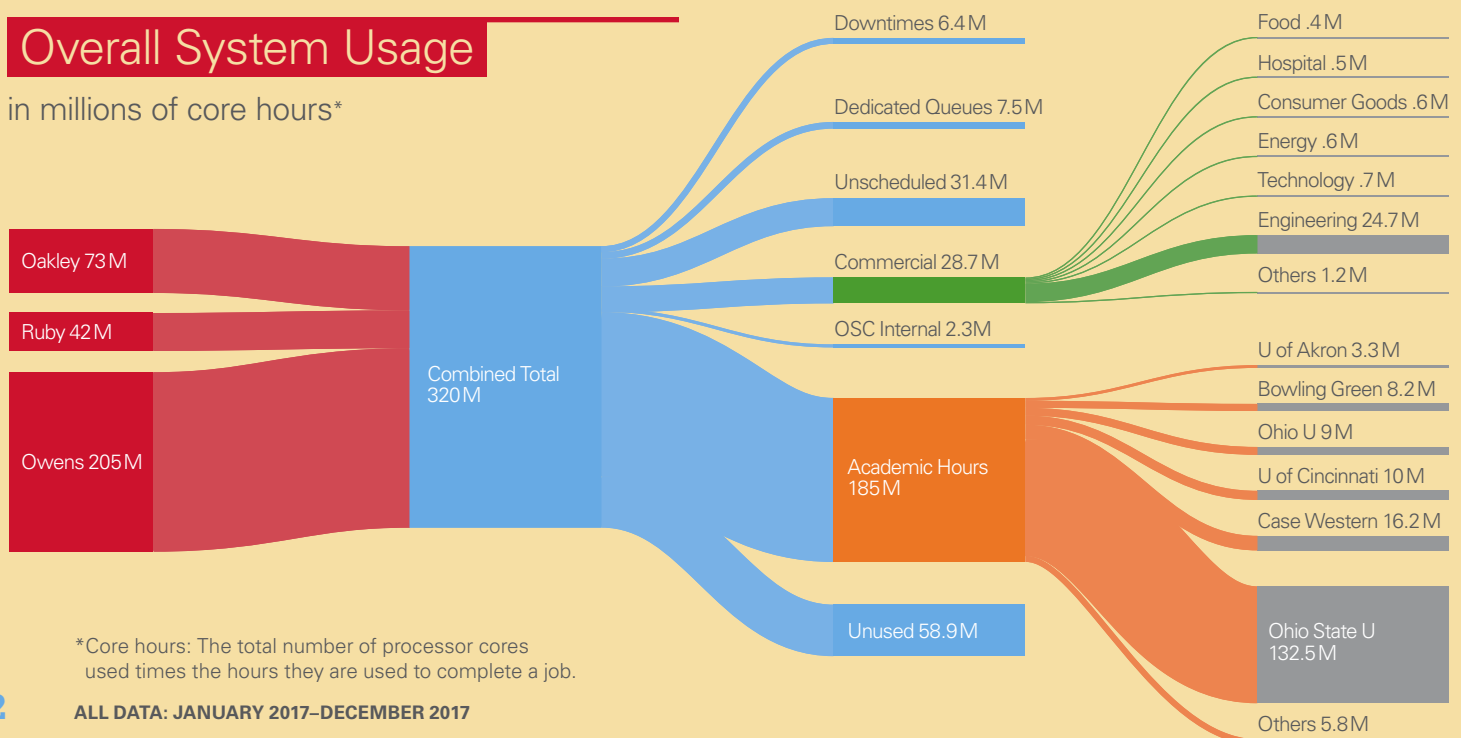
**604**  
projects served



**33**  
courses used OSC

## 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.

# Clients

OSC provides statewide resources to empower Ohio researchers on their way to new innovations and discoveries that will lead to new products, services and breakthroughs in a vast array of scientific disciplines. Through partnerships with Ohio industries, supercomputing provides businesses with a competitive force. And, by educating Ohio's workforce in the key skills required for future jobs, OSC helps move the needle in economic development.

Beyond providing shared statewide resources, OSC works to create a user-focused, user-friendly environment for our clients. In 2017, 2,202 distinct students, faculty and staff members across 23 Ohio universities and 48 companies accessed OSC's resources. As part of our expanding training programs, we had 461 people attend 23 individual training opportunities throughout the year—nearly triple the numbers from the prior year.

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## Academic

OSC supports educational activities at various types of institutions—two-year and four-year, public and private, large and small—across a broad range of disciplines and degree programs. Academic clients include students, faculty, staff and special interest groups, such as the Formula Society of Automotive Engineers (FSAE) teams who used an app at OSC for their racing design competition.

More than 30 colleges and universities leveraged OSC services for instructional purposes, either in the classroom or the laboratory. The largest areas of academic study are the natural sciences, engineering and technology.

A thorough, yet streamlined, peer review process is used to ensure quick turnaround of allocations requests, as well as to prioritize high-quality science and promote efficient utilization of resources.

“My simulation would still be running right now if it hadn't been for the Ohio Supercomputer Center.”

— Donald J. Priour, Ph.D., Professor of  
Physics, Youngstown State University

## Industrial

The AweSim program is OSC's industrial outreach initiative, designed to provide OSC's HPC resources to businesses throughout Ohio.

Company owners and management, engineers, industrial designers and IT professionals from a variety of businesses are learning more about the “HPC in the cloud” advantages available to them through AweSim.

AweSim works with a team of engineering service providers who are experts in a variety of computer-aided engineering disciplines. With assistance from OSC, businesses of all sizes and across a variety of industries can use HPC for virtual product design, testing simulations and data-intensive projects.

This allows small- to mid-sized manufacturers to push the boundaries of innovation and be more competitive economically. AweSim provides affordable, accessible and scalable modeling and simulation on high performance computers via:

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

# Education & Training

## Workshop and training expansion

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.

## Statewide Users Group (SUG)

SUG is a volunteer group composed of the scientists and engineers who provide OSC's executive director with program and policy advice

and direction to ensure a productive environment for research. Participants gather at the SUG conference twice a year for deep-dive breakout sessions on vital topics, such as hardware, software, Big Data, OSC's OnDemand and app development, as well as a tour of the OSC suite at the State of Ohio Computing Center.

The ever-popular poster and flash talk competitions allow student and faculty participants an opportunity to publicly present their work—practice they need to help earn the higher degrees and accolades they seek. OSC staff and directors provide updates on the center's direction as well as a forum for OSC's client base to give constructive feedback.

## Summer programs

Each summer, OSC has a role in shaping Ohio's future STEM leaders through its Summer Institute for high school freshmen, sophomores and juniors and Young Women's Summer Institute for middle school girls. Students use hands-on, collaborative projects to experience the dynamic world of high performance computing as they work with peers and a variety of experts.



# Systems & Software

Collectively, OSC supercomputers provide a peak computing performance of 1.9 petaflops. The center also offers more than five petabytes of disk storage capacity distributed over several file systems, plus over seven petabytes of backup tape storage.

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

## 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

## OSC OnDemand

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

Users can upload and download files, and create, edit, submit and monitor jobs. 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. OnDemand breaks down barriers so researchers with a wide variety of backgrounds can easily access OSC's resources.

## 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



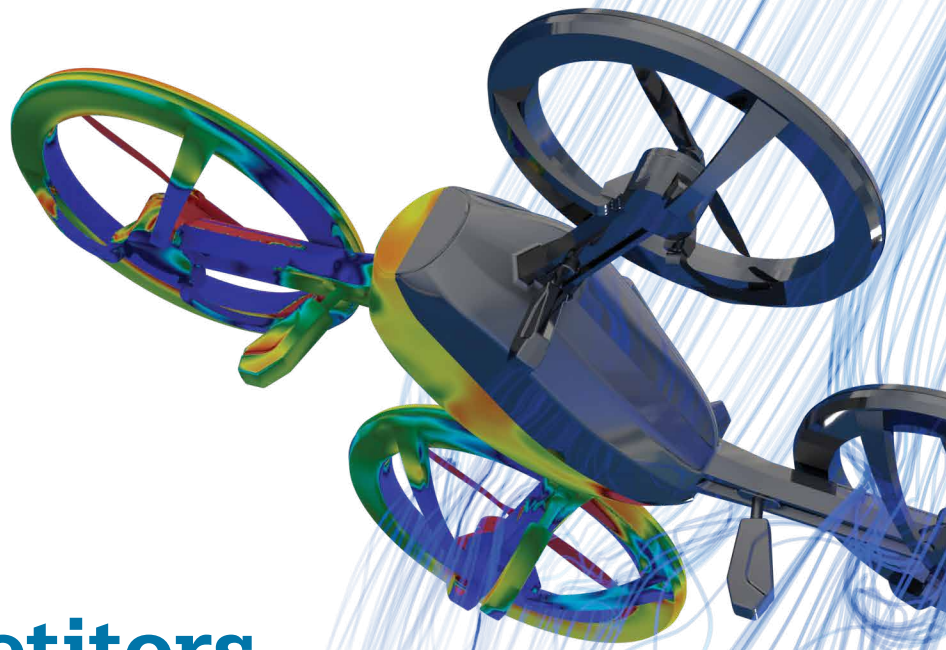
**1.5 PB**  
data stored



**2 PB**  
data  
transferred



**79%**  
jobs started  
within one  
hour



# GoFly competitors take flight with TotalSim CFD

## WHO:

TotalSim US, an engineering consultant firm in Ohio that works in partnership with AweSim, OSC's industrial engagement platform

## WHAT:

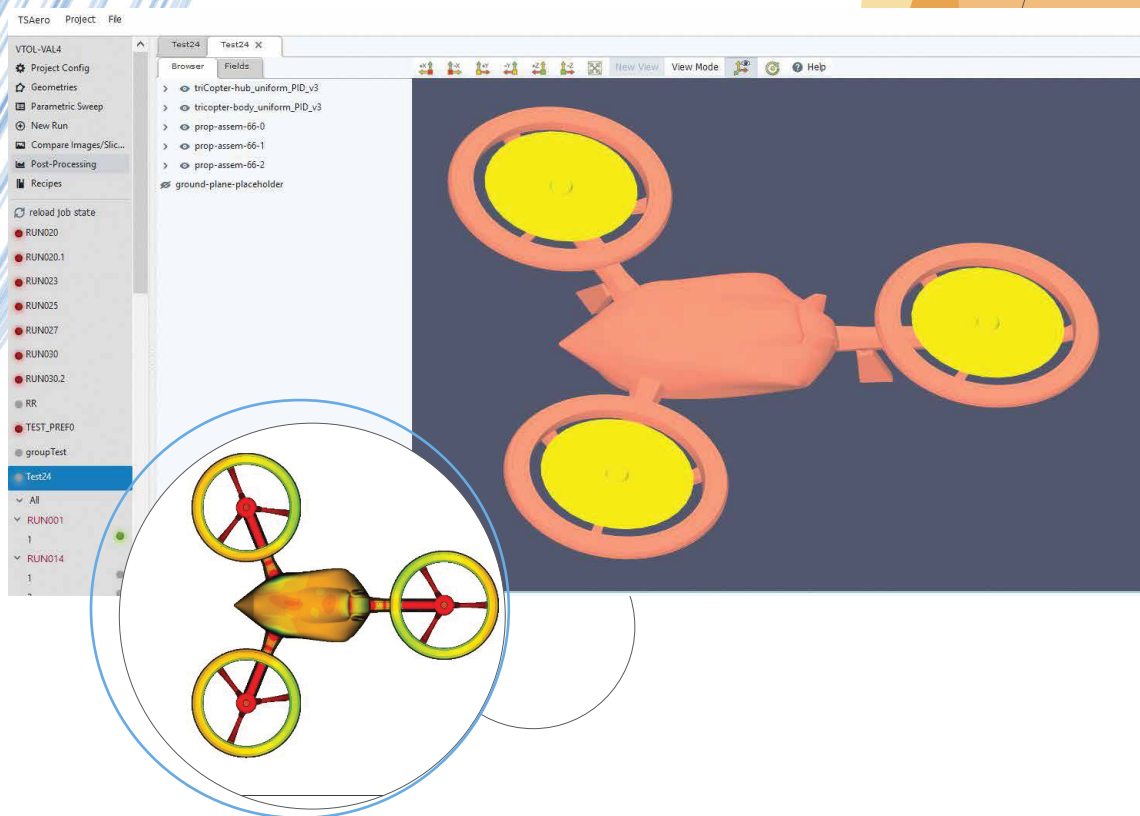
TotalSim, with help from OSC, customized a version of its TS Aero computational fluid dynamics app for competitors in Boeing's GoFly challenge.

## IMPACT:

By testing the aerodynamics of personal flying devices, GoFly competitors using TotalSim's app have allowed the company to refine the software and infrastructure, improving a potential commercial version.

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.

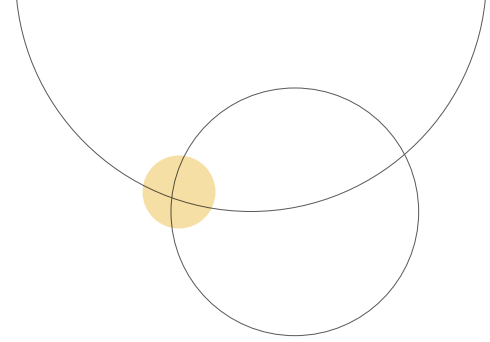
“OSC was really accommodating in having us do the account setups,” Leto said. “We’ve got a streamlined account creation process with OSC where we create the account and share the application. And we’ve got a website full of documentation, training information and videos. We launched all that, and we’ve 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. •

“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 ...”

— Ray Leto, President of TotalSim



# Simulations help Cleveland Clinic researcher practice precision medicine

## WHO:

Charis Eng, M.D., Ph.D., chair and founding director of the Cleveland Clinic's Genomic Medicine Institute and director of its clinical arm, the Center for Personalized Genetic Healthcare

## WHAT:

Eng's lab studies the PTEN gene, which acts as a tumor suppressor. PTEN mutations can result in a number of cancers and have been linked to autism spectrum disorder. Molecular dynamics simulations on OSC's Oakley Cluster help Eng's lab further investigate the dynamics of proteins and understand mutation-induced changes in the structure and function of PTEN.

## IMPACT:

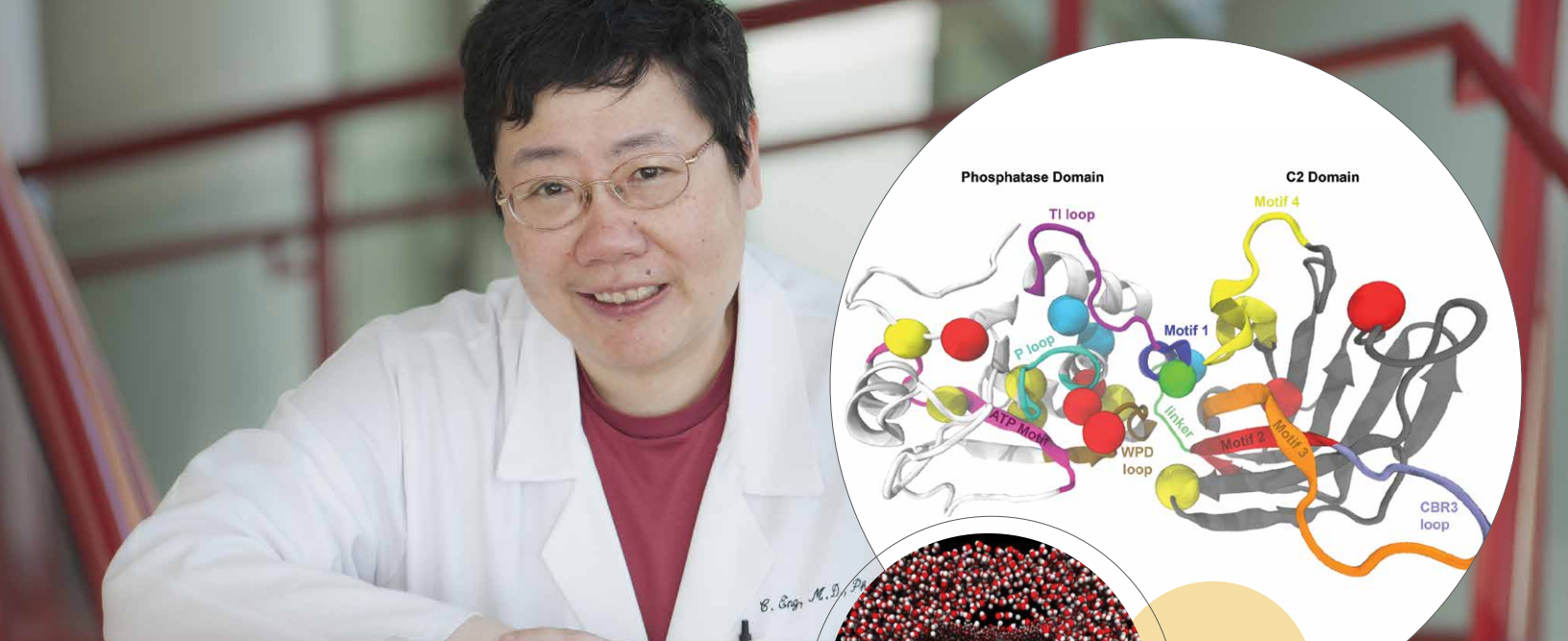
Gene-based diagnosis and prediction of cancer vs. autism spectrum disorder risks will help in tailoring diagnosis and prevention strategies, along with helping patients educate their own doctors as to the nature of their inherited cancers and/or neurodevelopmental risk in their future children.

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 for her precision medicine. Eng utilizes these insights as she evaluates the patients she sees at the Center for Personalized Genetic Healthcare, the clinical arm of 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 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 simulations to gain atomic-level insight into the protein encoded by PTEN.

"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."

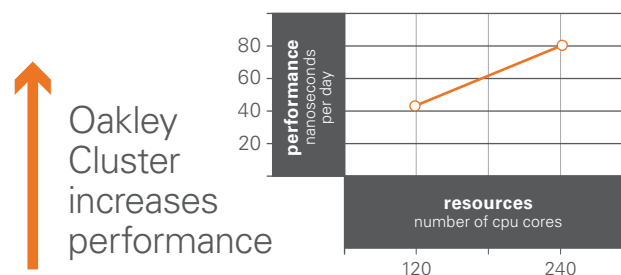


“Understanding the functional impact mutations have on the structure of PTEN will aid in the identification of specific mutations that contribute to ASD or cancer.”

— Charis Eng, Ph.D., *The Cleveland Clinic*

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 involved 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 how molecules are working [inside] and give us a much deeper understanding of the disease mechanism,” Smith says.



OSC’s Oakley Cluster helped Eng’s lab perform base benchmarks from its initial start-up allocation resources utilizing GROMACS MD simulation software platform.

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 molecular dynamics 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.” •



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