Ohio Supercomputer
An OH·TECH Consortium Member

Annual Report 2014–15

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

"OSC delivers the computational muscle and expertise that boosts scientific discovery and industrial innovation across Ohio."
— John Carey, Chancellor, Ohio Department of Higher Education

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

The Ohio Technology Consortium (OH-TECH) represents the technology arm of the Ohio Department of Higher Education. OSC, OARnet, OhioLINK, eStudent Services and the still-in-development Research and Innovation Center comprise a suite of technology and information member organizations unsurpassed in any other state. Their consolidation under the OH-TECH banner allows each organization to harness boundless synergies and efficiencies.

Ohio Supercomputer Center

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

OSC leadership: (left to right) Basil Gohar, Steven Gordon, Karen Tomko, Alan Chalker, Pankaj Shah, David Hudak, Douglas Johnson and Brian Guilfoos

2014–15

Highlights

Management and Business Changes

Last year was a momentous turning point for OSC's operational business strategy for the coming years. A new OSC management team, built from internal talent and a new business model, is motivated and full of ideas for the future. The new business model takes into account various "condo"-related activities at other high performance computing centers in the country and blends those successful ideas into OSC's statewide service model (see page 4). This includes industrial use of supercomputers along with traditional academic research.

Renewed Outreach Efforts

OSC worked directly with vice presidents of research, deans and high performance computing users to create value-added services. With good traction at The Ohio State University, the center is now beginning to explore condo-related activities with other universities as well. OSC also recycled several retired units of the Glenn Cluster as promotional displays (left) at JobsOhio, the University of Cincinnati and OSC offices, with potential for more placements in the coming months.

New Hardware and Services

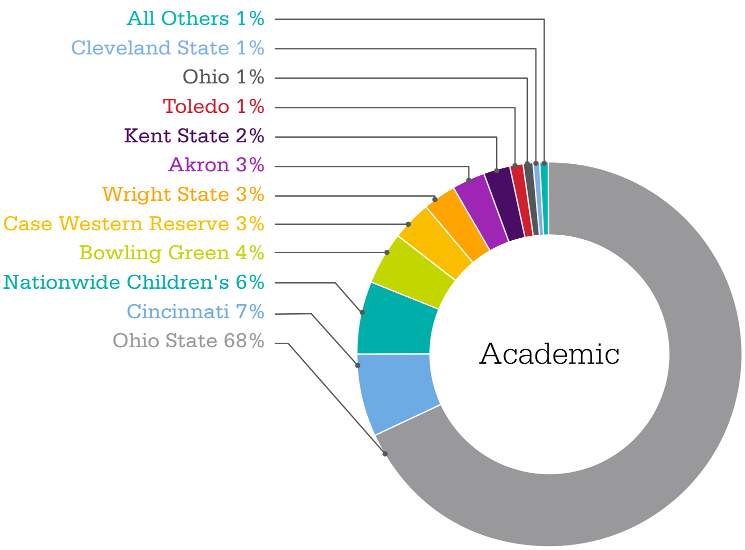
The latest supercomputer, named Ruby in honor of Cleveland-born entertainer and activist Ruby Dee, was dedicated April 9, 2015. The small-but-mighty HP-Intel Xeon Phi-based supercomputer has 240 nodes and 15.3 terabytes of memory, yielding a total peak performance of 144 teraflops. The OSC team also successfully merged first-level support services into the existing OARnet Network Operations Center, providing 24/7 support to high performance computing researchers.

Academic Clients

Recognizing HPC resources as an indispensable springboard for innovative breakthroughs, OSC empowers academic, healthcare and industrial researchers to achieve pioneering scientific discoveries in the biosciences, advanced materials, energy and the environment and a host of emerging disciplines.

The numbers speak for themselves. Last year, 1,173 distinct users engaged OSC's powerful supercomputing and storage resources. As a group, they accomplished:

- 2.4 million computer jobs
- 90 million computing hours
- Tens of millions of dollars in related research funding received by leveraging access to OSC



Top 25 Academic Projects

Principal Investigator	NSF Field of Study	Institution
W. Windl	Metallurgy	OSU
A. Asthagiri	Physical Chemistry	OSU
C. Hadad	Organic & Macromolecular Chemistry	OSU
C. Bartlett	Genetics	RINCH
T. Beck	Physical Chemistry	UC
J. Herbert	Physical Chemistry	OSU
M. Olivucci	Photobiology	BGSU
D. Bromwich	Polar Meteorology	OSU
M. Buck	Biophysics	CWRU
D. Schumacher	Atomic, Molecular, Plasma Physics	OSU
S. Wang	Information Robotics & Intelligent Systems	WSU
R. Yoder	Organic & Macromolecular Chemistry	OSU
M. Davidson	Algebra and Number Theory	KSU
I. Howat	Surficial Processes	OSU
N. Sahai	Biophysics	UA
R. Bruschweiler	Chemistry	OSU
M. Sokoloff	Elementary Particle Physics	UC
J. Steffensmeier	Measurement Methods & Data Improvement	OSU
A. Martinez	Computer & Computational Research	OSU
H. Heinz	Materials Research	UA
J. Chen	Fluid Dynamics and Hydraulic	OSU
R. Furnstahl	Knowledge and Database Systems	OSU
L. Cao	Materials Science	OSU
D. Lacks	Chemical, Biological, and Thermal Engineering	CWRU
P. Schniter	Algorithm Development	OSU

Industry Clients

When OSC was established in 1987, state policymakers "intended that the center be made accessible to private industry as appropriate."[1] Later that year, the Ohio Department of Higher Education formed the center "as a statewide resource designed to place Ohio's research universities and private industry in the forefront of computational research."[2] Since its creation, OSC has been a leader in the field of HPC industrial engagement. From product prototyping to process design, high performance computing can save businesses both time and money, while improving products and streamlining operations.

AweSim

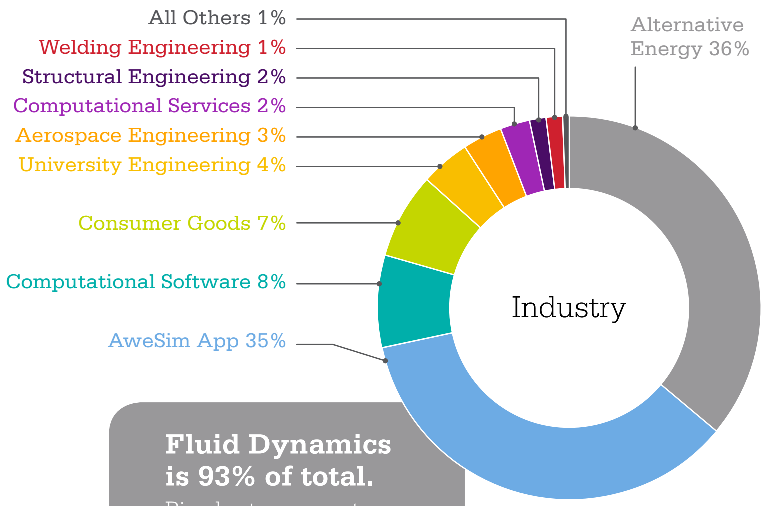
OSC's latest industrial engagement effort, AweSim, creates cloud-based manufacturing apps that extend the competitive benefits of simulation-driven design to small and mid-sized businesses that previously could not afford to leverage such solutions.

The $6-million public/private partnership builds on the success of Blue Collar Computing, OSC's first industry program, and leadership with the National Digital Engineering and Manufacturing Consortium (NDMEC).

Under the AweSim program, OSC and its industry partners are pioneering the field of modeling and simulation as a service—providing research and development scientists with access to computation and storage resources. This service can include various features, such as licensed computational software, mass data storage, web-portal access and more. AweSim can automate the manual prototyping process and create reusable apps to support affordable and accessible HPC modeling, simulation and analysis for manufacturing. This enables companies to more quickly address emerging customer requirements.

Direct Access

OSC industry clients simply seeking access to supercomputing resources can purchase packages that include a wide array of features, including the use of up to 1,024 cores, ample home directory storage space and a combination of basic and advanced technical support. OSC operates according to externally audited policies and procedures based upon industry standards.



Fluid Dynamics is 93% of total.
Pie chart represents the remaining 7%.

[1] Ohio House Bill 171, passed June 30, 1987
[2] Ohio Board of Regents resolution, December 18, 1987

HPC Services

Beyond providing shared statewide resources, OSC works to create a user-focused, user-friendly environment for HPC clients. OSC developers further refined OnDemand, a web browser-based application for “one-stop shop” access to HPC resources. With OnDemand, users can upload and download files; create, edit, submit and monitor jobs; run graphical user interface (GUI) applications; and connect remotely with SSH and other encrypted login protocols—all through a web browser, with no client software to install and configure.

In an effort to create a more sustainable business model, OSC continues to seek partnerships with industry, such as Honda and P&G, as well as “condo” opportunities with individual academic departments. Condo model refers to participants purchasing one or more compute nodes for the shared cluster while OSC provides the infrastructure, as well as maintenance and services. An academic department can share funds with OSC to purchase a system, which OSC staff then manage and maintain. Users on the condo nodes have access to all software packages installed on the supercomputers.

Additionally, OSC has created a pricing sheet for the purchase of computing time or to lease a node. For example, a large commercial client recently reserved about 30 percent of two systems for 12 weeks in the summer of 2015. This model provides needed operational funds that allow OSC to further leverage the state’s capital investment.

For any issues that arise, OSC’s 24/7 support desk is available to provide clients with Level 1 support any hour of any day.

Innovative HPC services often put OSC in the spotlight on the national HPC stage. OSC staff members at left are seen exhibiting at SC14, the national supercomputing conference, in New Orleans, Louisiana.

Training & Education

Since its inception, OSC has earned a national reputation for exceptional training and education programs by creating a pipeline that contributes to a skilled computational science workforce.

Summer Institute & Young Women's Summer Institute

OSC promotes student interest in the STEM fields through its Summer Institute (SI) for Ohio's brightest freshmen, sophomores and juniors, as well as Young Women's Summer Institute (YWSI) for middle-school girls. Students use supercomputers for practical applications, such as solving complex science and engineering problems. OSC also focuses on updating the skills of K–12 teachers so they can apply technology, modeling and simulation and project-based learning in their classrooms.

Ralph Regula School of Computational Science

The center's virtual Ralph Regula School of Computational Science coordinates a statewide initiative in computational science education, which is the use of computer modeling and simulation to solve complex business, technical and academic research problems. Students may take part in the baccalaureate minor or associate concentration program offered at numerous Ohio colleges and universities. The program takes an interdisciplinary approach to allow undergraduates to apply computational tools directly to their area of study.

XSEDE

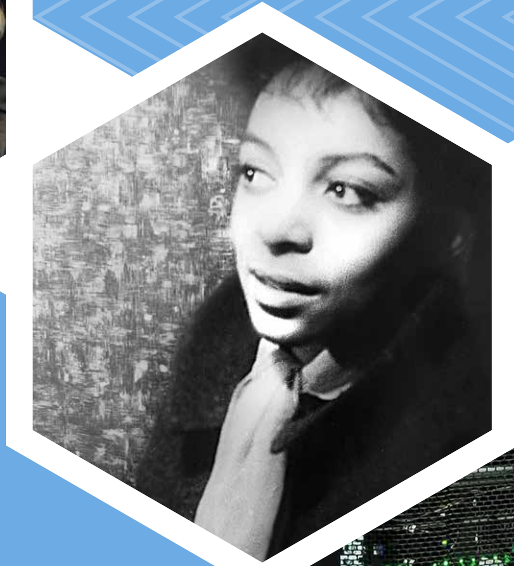
OSC faculty and student researchers can take advantage of ongoing training for various aspects of scientific computing taught by the center's instructors or in collaboration with the National Science Foundation's Extreme Science and Engineering Discovery Environment (XSEDE) program. XSEDE is a single virtual system of resources and services — things like supercomputers, collections of data and new tools — offered to researchers from 18 different sites around the world.

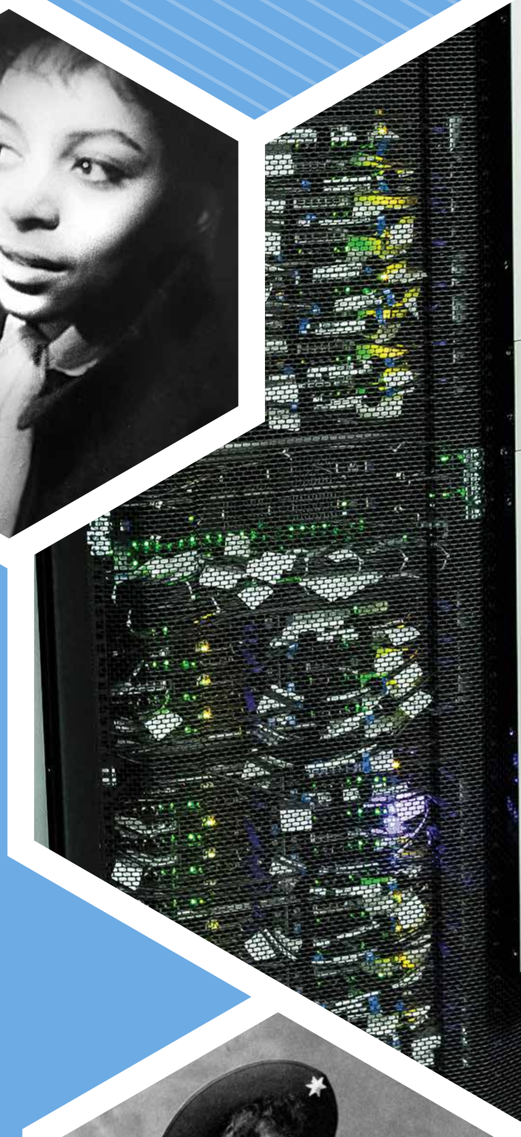
- Steve Gordon serves as XSEDE's national lead for education programs;
- David Hudak serves as XSEDE's manager of industry relations; and
- Karen Tomko is an XSEDE campus champion.

OSC staff plays an active role in providing hands-on learning experiences for programs, such as SI (top) and YWSI (above).

Training and education programs at OSC provide a pipeline from middle school to college to career training.

(Above) In April 2015, Chancellor John Carey, right, and Statewide Users Group Chair Thomas Beck unveiled the center's newest supercomputing system — the 4,800-core HP/Intel Phi Ruby Cluster.





Hardware/Software

Collectively, current OSC supercomputers provide a peak computing performance of 338 teraflops — the equivalent of everyone on earth performing more than 48,000 calculations every second. The center also offers more than two petabytes of disk storage capacity distributed over several file systems, plus almost two petabytes of backup tape storage.

Additionally, the center provides licenses for more than 30 software applications and access to more than 70 different software packages. Researchers can run their own license software, as well. Among the most-used software codes this past year were OpenFOAM for computational fluid dynamics, LS-DYNA for structural mechanics and Parallel MATLAB for numeric computation and visualization.

With the approval of a $12 million capital allocation last year and insights gleaned from the deployment and operation of the Ruby Cluster, OSC engineers have begun preparations for the purchase of a new system that will feature nearly four times the number of processors than found in the current flagship system. Expected to be operational in the 2015–16 academic year, the request for proposal specifications — 1,000 nodes, 1,000 teraflops and total memory of 100+ terabytes — will most likely put the yet-to-be-named supercomputer among the top academic systems in the United States.

Recent OSC systems have been named after Ohioans known as pioneers in their respective careers: The Glenn Cluster for astronaut and statesman John Glenn (above); the Oakley Cluster for legendary sharpshooter and social advocate Annie Oakley (bottom left); and the newest addition, the Ruby Cluster, for Ruby Dee, actress, activist and civil rights proponent (top left).

High Performance Computing & Storage

In 2014–15, researchers statewide depended upon several key OSC systems:

HP Intel Xeon Phi Ruby Cluster
4,800 cores provide a total peak performance of 144 teraflops of computing power

HP Intel Xeon Oakley Cluster
8,304 cores provide a total peak performance of 154 teraflops

IBM 1350 AMD Opteron Glenn Cluster
3,408 cores provide a total peak performance of 60 teraflops

Csuri Advanced GPU Environment
leverages graphics processing units for a robust visualization environment

IBM Mass Storage Environment
contains more than two petabytes of disk storage

Client Profile

Cincinnati researchers aim for early identification of patients with antibiotic resistance

WHO:
Cincinnati Children's Hospital Medical Center

WHAT:
The Ohio Supercomputer Center provides resources that help train a predictive model used to identify patients at risk of developing invasive infections.

IMPACT:
Early identification methods will allow clinicians to more efficiently choose medicines for antibiotic-resistant patients and take preventive measures to limit the spread of infections.

Researchers at Cincinnati Children's Hospital Medical Center are using Ohio Supercomputer Center (OSC) resources to zoom down to the genomic level to identify patients at risk of developing invasive infections that are often difficult to treat due to antibiotic resistance. Early identification methods would allow clinicians to more efficiently choose medicines for these patients and take preventive measures to limit the spread of infections.

Keith Marsolo and his team are developing novel techniques that could be used to more quickly identify patients whose bodies no longer respond to standard-use antibiotics, a serious emerging health threat. Sick children at CCHMC can develop this resistance after the many rounds of different antibiotics they receive to ward off infections from their weakened immune systems.

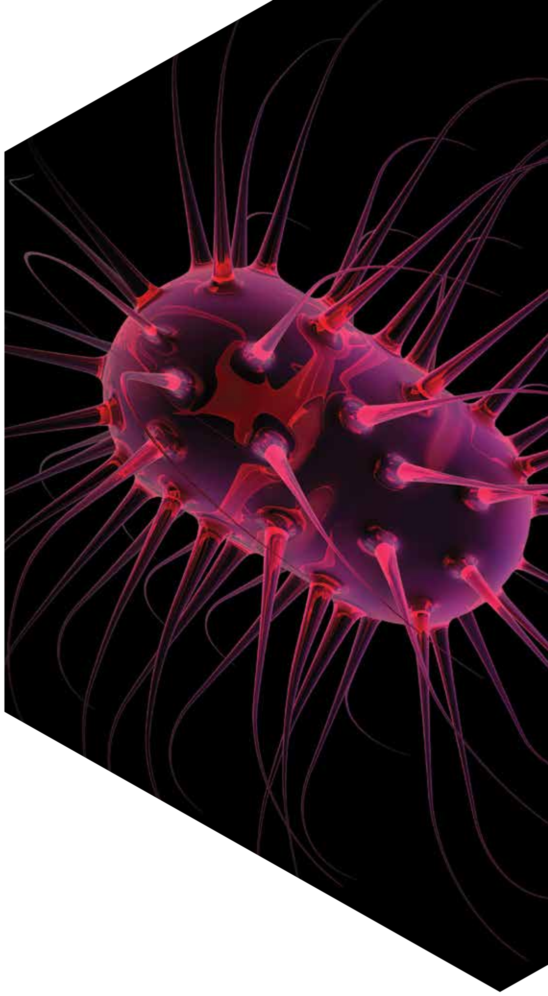
"Once the patients who become sick develop infections, it becomes harder and harder to treat them because they've developed a resistance to so many types of antibiotics that clinicians just run out of options," said Natalia Connolly, a research associate for the study at CCHMC.

The problem is part of a bigger picture: The overuse of antibiotics in the medical field, as well as in the food industry, is a rising threat to public health.

"Because [antibiotics] are overused, the bugs react to them. So the more times you expose them to the antibiotics, the less likely [the antibiotics] are to work," Marsolo said. "The problem occurs when you get multi-drug resistant bacteria. The superbugs, they're often called, as they grow and spread, there's essentially nothing you can do to stop them."

When we ingest antibiotics, most of the targeted bacteria in our bodies are killed. Any bacteria that remain reproduce and evolve their genetic makeup to be resistant to the antibiotics. The antibiotic-resistant genes in bacteria become part of the human body's gut metagenome, which includes the microbiome, (all the bacteria, viruses and fungi that live within the digestive system) and the resistome (all the antibiotic-resistant genes found in the

Antibiotic resistance is a serious emerging health threat, especially to children with chronic medical conditions.



digestive system). It is in the metagenome where Marsolo and his team are uncovering the answers to antibiotic resistance.

The study began when Drs. David Haslam and Heidi Andersen, clinicians at CCHMC Division of Infectious Diseases, obtained and sequenced fecal samples from three cohorts: sick pediatric inpatients, healthy outpatient children and healthy adults. Their bold vision was that gut metagenomics offered a much more precise way than traditional fecal cultures to identify patients at risk for developing infections. The clinicians turned to bioinformaticians to help analyze the data in innovative ways. After removing the human DNA from the samples, approximately 1,700 genes remained to be analyzed. With data-processing help from OSC, Marsolo's team used a machine-learning approach known as support vector machines. The SVM was first trained on data from patients with a known classification label, such as inpatient or control, to build predictive models to make a decision when presented with new samples. OSC's resources were crucial in training the SVM, as multiple parameters had to be tested in order to discover the optimal model.

"Because you have so many parameters and each one of them has a multitude of options, you really can't do it without some serious computing power," Connolly said.

Their initial results showed that the antibiotic-resistant genes varied greatly among the three categories of cohorts. As healthy subjects should be expected to have a metagenome that showed less antibiotic resistance, this was good news. With promising results from the initial study, the team is continuing its successful partnership with Drs. Haslam and Andersen as part of a larger prospective study. With a limited number of antibiotic drugs on the market, the researchers' hope is that the study will provide early measures for identifying sick patients most prone to developing infections, as the current process is quite slow.

"This is still very new and very novel, but that's where I hope that this work will go," Connolly said.

"Because you have so many parameters and each one of them has a multitude of options, you really can't do it without some serious computing power."

— Natalia Connolly, research associate for the study at CCHMC

Client Profile

Astrophysicists leverage OSC resources to unlock mysteries of dark matter

WHO:
Center for Cosmology and AstroParticle Physics at The Ohio State University

WHAT:
The Ohio Supercomputer Center provides computational resources needed to simulate "the biggest bound structures in the universe."

IMPACT:
Astrophysicists do not know what particles make up dark matter (which makes up a quarter of our universe) but hope that this first study of its kind will shed some light on the mysterious substance.

To begin to understand dark matter in astrophysics, one must first step into a world where galaxies are considered small. Annika Peter, Ph.D., and graduate student Stacy Kim are leveraging the powerful systems of the Ohio Supercomputer Center (OSC) to better grapple with this novel perspective and advance their research at The Ohio State University's Center for Cosmology and AstroParticle Physics. Their study could help define the substance that makes up over a quarter of the universe.

Very little is known about dark matter. Astrophysicists know that it exists, the amount of it that exists and its large-scale distribution in the universe. They also know that it is gravitationally attractive, causing nearby gas and stars to move faster and cluster more than they would without the close proximity of dark matter. While the particles that make up gases and stars, such as atoms and molecules, are well known, scientists do not know what particles make up dark matter —only that they are new, undefined particles.

The dominant hypothesis is that dark matter is made up of weakly interacting massive particles, or WIMPs, which would mean that dark matter is a very stable particle that interacts with itself only weakly. While the idea of WIMPs fits nicely into many astrophysical observations, there is some observational evidence that the hypothesis is not valid.

"The problem with [WIMPs] is that on scales that we consider small, which, to us, is the size of clusters of galaxies and smaller, it looks like things aren't what they should be," Kim said.

To better define the properties of this mysterious matter, astrophysicists look at how dark matter might interact with itself. According to the

> *"This is sort of the missing link that allows us to translate between theories of dark matter and what astronomers see in the sky."*
>
> *— Annika Peter, Ph.D., The Ohio State University's Center for Cosmology & AstroParticle Physics*

NASA, ESA, and the Hubble SM4 ERO Team

(Above) Three of the galaxies in this famous grouping, Stephan's Quintet, are distorted from their gravitational interactions with one another. One member of the group, NGC 7320 (upper right), is actually seven times closer to Earth than the rest.

WIMP theory, gravitationally attractive dark matter should settle into dense clumps. After observing the movement of stars within galaxies, some researchers noticed that stars were not orbiting as quickly as they would expect them to be if dark matter were as stable and weakly interacting as the WIMP theory suggests.

Peter and Kim are exploring a model of dark matter that is less stable, called self-interacting dark matter. To do this, they are researching the "stickiness" of dark matter—in other words, if particles of dark matter can collide with each other.

While some physicists are able to physically test theories of collisionality by using particle colliders, Peter and Kim are working on a much larger scale. To test their theory of dark matter collisionality, Kim is smashing together immense, virtual galaxy clusters within large simulations created on OSC systems.

"The clusters that Stacy has been simulating are the biggest bound structures in the universe, and when they hit each other, it's like the largest particle collider in the universe," Peter said.

A galaxy cluster can grow larger when a galaxy or smaller galaxy cluster collides with it, in an event called a merger. When Kim runs merger simulations, she watches to see how dark matter and the galaxies move when two galaxy clusters with equal mass collide. Galaxies on their own do not interact with each other in a collisional sense. By looking at the distribution of galaxies versus the location of dark matter halos after a merger, Kim may be able to determine the "stickiness" of dark matter, based on what is already known about the collisionality of galaxies.

"We don't expect the distributions of dark matter particles and galaxies to resemble each other," Peter said.

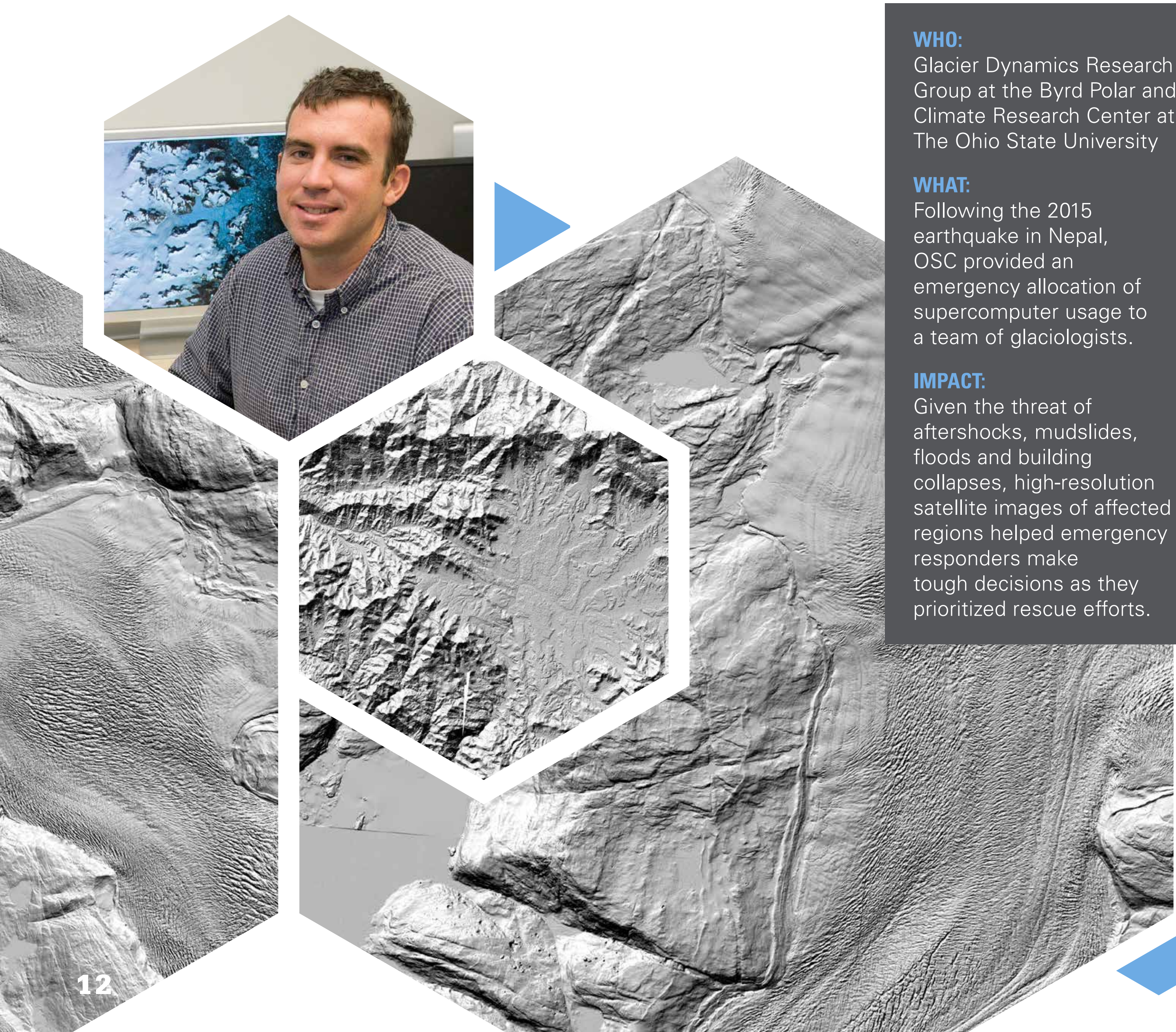
As the first study of its kind, Peter and Kim hope to provide astronomical observers with a better understanding of what they are seeing as they stargaze.

"This is sort of the missing link that allows us to translate between theories of dark matter and what astronomers see in the sky," Peter said.

A detection of dark matter collisionality would upend the presiding WIMP paradigm and could finally begin to define the illusive properties of this mysterious particle. •

Client Profile

Glaciologists refocus on Nepal to aid in disaster relief efforts



WHO:
Glacier Dynamics Research Group at the Byrd Polar and Climate Research Center at The Ohio State University

WHAT:
Following the 2015 earthquake in Nepal, OSC provided an emergency allocation of supercomputer usage to a team of glaciologists.

IMPACT:
Given the threat of aftershocks, mudslides, floods and building collapses, high-resolution satellite images of affected regions helped emergency responders make tough decisions as they prioritized rescue efforts.

> *"To support this effort, we have granted the SETSM team priority queuing . . . for use of our flagship supercomputer system, the Oakley Cluster."*
> *— Brian Guilfoos, HPC Client Services Manager*

Researchers who normally use high-resolution satellite imagery to study glaciers used their technology and a computational boost from the Ohio Supercomputer Center (OSC) to help with disaster relief and longer-term stabilization planning efforts in Nepal.

In April 2015, a violent earthquake struck central Nepal, killing more than 7,000 people and destroying hundreds of thousands of homes. The deadliest earthquake in Nepal since 1934, the tremor killed at least 19 climbers and crew on Mount Everest and reportedly produced casualties in the adjoining countries of Bangladesh, China and India.

Two research teams—one at The Ohio State University and another at the University of Minnesota—worked quickly to produce high-resolution, 3-D digital surface maps for use in the Nepali relief effort. OSC provided the computing power for data-intensive calculations that employ Surface Extraction for TIN-based Searchspace Minimization (SETSM) software.

"These data are critical for a range of uses, including mapping infrastructure, planning rescues and assessing slope stability," explained Ian Howat, Ph.D., an associate professor of earth sciences at Ohio State and a principal investigator in the Glacier Dynamics Research Group at the university's Byrd Polar and Climate Research Center. "Thus far, we have produced a mosaic that models the Kathmandu area with measurements at eight-meter intervals."

"To support this effort, we granted the SETSM team priority queuing and an emergency allocation of up to 60,000 core hours for use of our flagship supercomputer system, the Oakley Cluster," said Brian Guilfoos, HPC client services manager at the Ohio Supercomputer Center.

The SETSM software is a fully automatic algorithm for deriving the surface maps, called Digital Terrain Models, or DTMs. The maps are created from applying the algorithm to sets of overlapping pairs of high-resolution satellite images acquired by colleagues at the Polar Geospatial Center at the University of Minnesota. The satellite images are acquired from the Worldview-1 and Worldview-2 satellites, owned by DigitalGlobe Inc., and are licensed through the National Geospatial-Intelligence Agency's NextView program. The Polar Geospatial Center is distributing the final products on the organization's website.

"Besides improving on this DTM, we will be processing the entirely useable archive of Worldview stereo imagery over Nepal in order to expand coverage," said Myoung-Jong Noh, a member of the Glacier Dynamics Research Group at the Byrd Center and the lead author of a scientific paper on SETSM in the journal GIScience & Remote Sensing. •

Ohio State glaciologists turned their focus from Greenland ice sheets (large images, left) to the mountains of Nepal (center, left) following the April 2015 earthquake.

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