Greetings

A Message from the Executive Director

For more than a quarter century, the talented and diligent staff of the Ohio Supercomputer Center (OSC) has provided our clients with powerful resources for accelerating discovery and promoting prosperity. The highlights featured on these pages provide snapshots of the facilities, expertise and initiatives that served our users in 2013-14.

As a member of the Ohio Technology Consortium, a division of the Ohio Board of Regents, OSC works closely with stakeholders, policymakers, colleagues and our consortium partners to provide a seamless foundation for Ohio's discovery and innovation efforts.

As we embark on the next fiscal year, we are beginning the process through which we expect to procure and launch even more powerful computational tools, benefiting both academic and industry researchers.

In compiling this report, we believe that technology should be transparent. The value should be – and, as highlighted on these pages, definitely is – the people: our staff members and our researchers.

Pankaj Shah
Executive Director
Ohio Supercomputer Center & OARnet

OSC Leadership: (front, l-r) Karen Tomko, Ph.D., interim Director of Research and Scientific Applications Group Manager; David Hudak, Ph.D., Director of Supercomputer Services; Basil Gohar, Web and Interface Applications Manager, (rear) Alan Chalker, Ph.D., Director of Technology Solutions and Director of AweSim; Pankaj Shah, Executive Director of the Ohio Supercomputer Center and OARnet; Doug Johnson, Chief Systems Architect and HPC Systems Manager; and Brian Guilfoos, HPC Client Services Manager.

Ohio Supercomputer Center

The mission of the Ohio Supercomputer Center is to empower our clients, partner strategically to develop new research and business opportunities and lead Ohio's knowledge economy. Since 2011, the Center has operated as a member of the Ohio Technology Consortium, a division of the Ohio Board of Regents.

OH·TECH | Ohio Technology Consortium
A Division of the **Ohio Board of Regents**

OSC, OARnet, OhioLINK, eStudent Services, and the still-in-development Research and Innovation Center comprise the consortium's suite of technology and information member-organizations, providing Ohioans the foundation of a comprehensive technology infrastructure unlike that found in any other state.
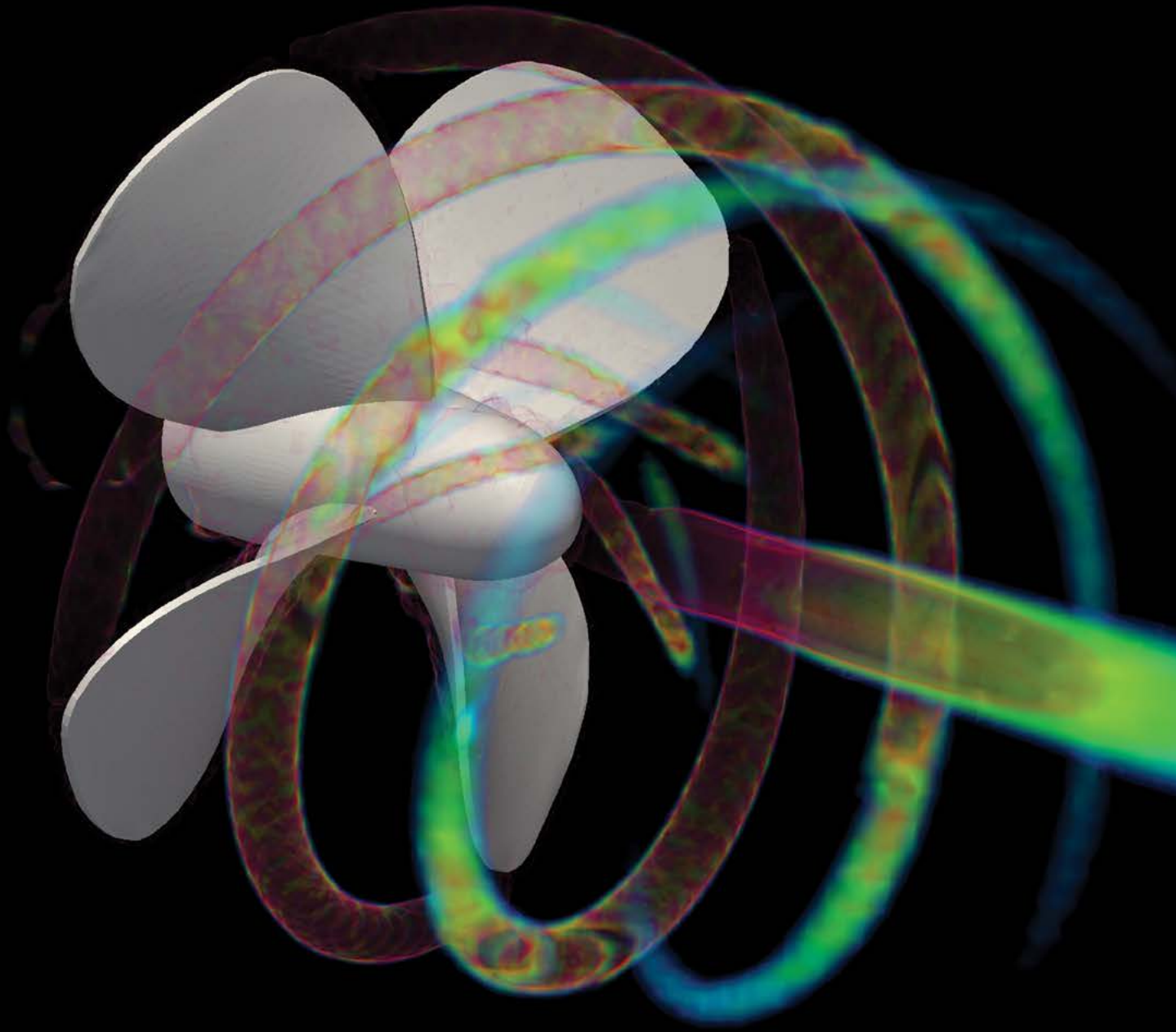
Fans play instrumental roles in countless ways: from climate control to vehicle propulsion and from power generation to cleaning. Funded through the Small Business Innovation Research (SBIR) program at the Department of Energy, engineers created FanSim to help enhance fan design. The application accepts user input on parameters, such as fan geometry, blade number, shroud diameter, fan immersion, flow rate / speed and rotational direction and then provides the customer with visual and numerical results, such as pressure, torque, power and efficiency.

2013/14 Highlights

The past year at the Ohio Supercomputer Center involved a great deal of looking ahead to new opportunities and challenges, as well as looking back at a record of accomplishment.

One of the most significant achievements of the year was the launch of the Center's multi-million dollar industrial engagement initiative, AweSim, in Denver at SC13, the international conference for high performance computing, networking, storage and analysis. We believe that an access approach featuring "manufacturing apps" will finally place simulation-driven design squarely on the doorsteps of small- and mid-sized businesses across Ohio and the Midwest.

Another important milestone was celebrated when we marked the 25th anniversary of summer K-12 programs during the closing ceremonies of this year's Summer Institute for high school boys and girls. In the quarter-century since the first 20 students spent two weeks at the Center exploring technology and other STEM-related projects, OSC has developed an international reputation for innovative and effective HPC training and education programs. These programs have created a pipeline of STEM graduates and future scientists.

Addressing Research Needs

Over the last year, OSC has closely collaborated with officials from The Ohio State University, who have been planning a strong foray into data analytics as part of the university's 10-year, multi-million dollar Discovery Themes Initiative. The initiative aims "to leverage Ohio State's special strengths to address the technological, social, and environmental stresses that define today's global world." OSC leadership has recommended that Ohio State pursue a shared-infrastructure strategy to meet its data analytics needs, lower costs, increase quality and improve interoperability.

The Center has proposed offering a 'condo' model for High Performance Computing (HPC) hardware, where researchers can purchase compute or storage hardware to augment OSC systems as an alternative to department- or lab-level HPC clusters. OSC will work with researchers to determine the best hardware for their needs, and will procure, deploy and manage the hardware as an extension of systems already available at OSC.

Additionally, OSC staff members have been pursuing research interests of their own through a variety of projects funded through agencies, such as the National Science Foundation, Air Force Research Laboratory, Department of Health and Human Services, and the Sao Paulo Research Foundation-Brazil and Ohio State University Partnership. The broad array of projects ranged from analyzing radio frequency (RF) signal processing to simulation of home healthcare hazards and to supporting international research collaboration.

Boosting Systems, Efficiencies

In April 2014, Ohio Gov. John Kasich signed a two-year capital appropriations bill, which included a $12 million allocation for a powerful, new supercomputing system for OSC. This investment in Ohio-based research and innovation represents the most capital funding allocated to OSC in the Center's 26-year history.

OSC staff worked closely with officials from the Ohio Board of Regents, Ohio State's Office of Research and the Statewide Users Group to refine a business model that will streamline clients' access to services while enhancing OSC's sustainability.

And, in recent months, renovations have been made to our offices, located on Ohio State's West Campus. Facility improvements included upgrading of the networking and communication infrastructure, modernization of service desk facilities and reorganizations of some departments to improve efficiencies.
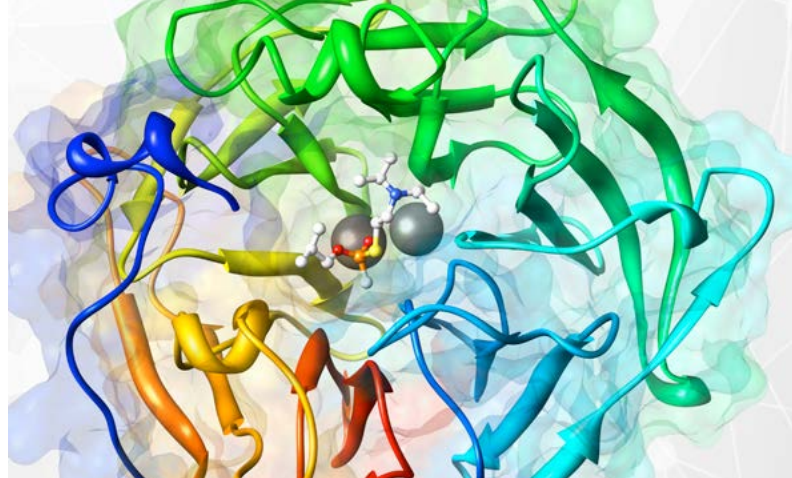
The Ohio Supercomputer Center provides computational and storage resources for research into countless areas, such as harnessing the body's own defenses to counteract nerve agents (the enzyme acetylcholinesterase, above) and designing an electric landspeed vehicle that can travel more than 400 mph (the Buckeye Bullet 3, above, left).
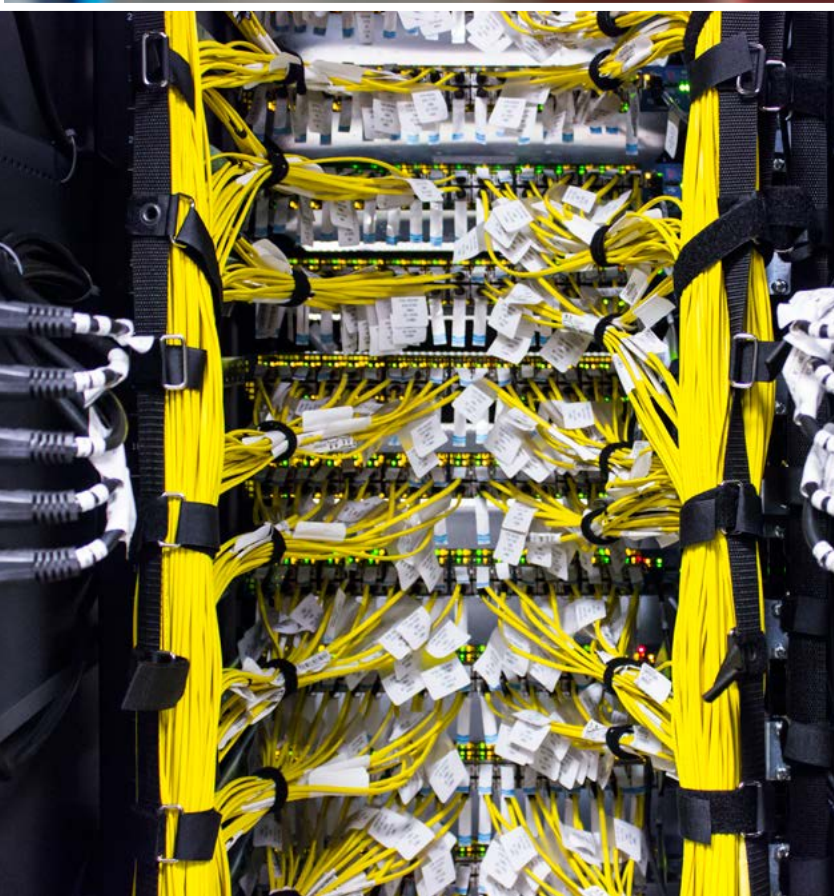
Our clients

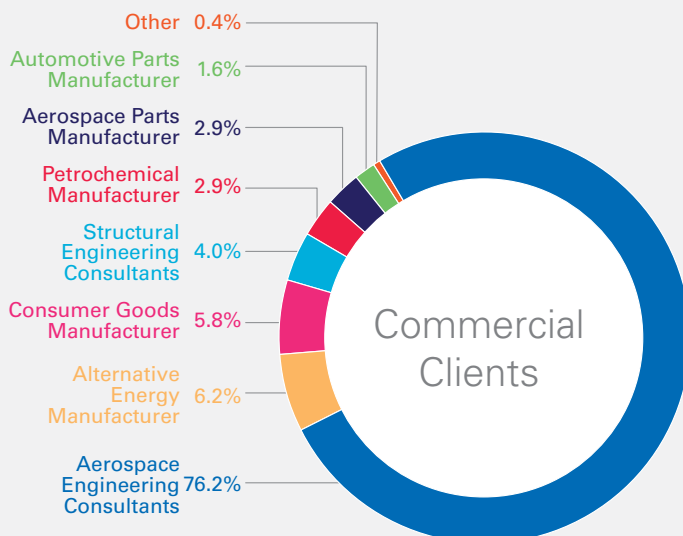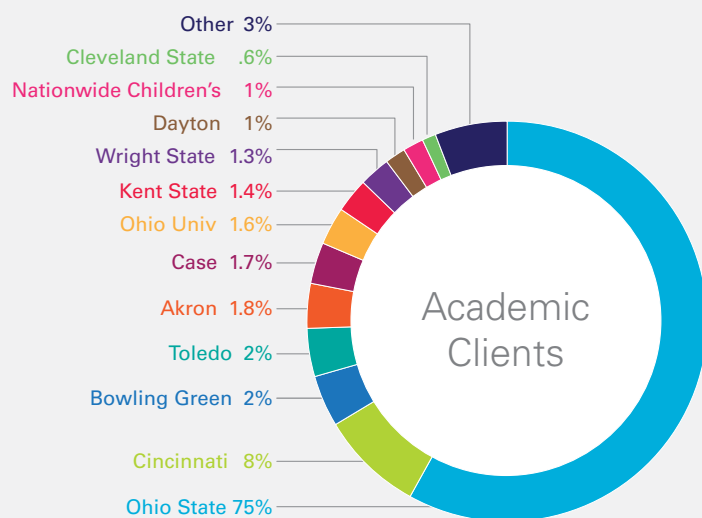## Empowering Academic Research and Industrial Innovation

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

The numbers tell our story best. Last year, 1,180 distinct users – representing academic, healthcare and industrial researchers from across Ohio – engaged OSC's powerful supercomputing and storage resources. In the process, they:

- Ran more than three million computer jobs
- Used more than 80 million computing hours
- Leveraged access to OSC for tens of millions in related research funding

The graphs below provide a snapshot view of the center's system usage by academic institution and by commercial research organization.

On the following page, you also will find a list of research projects that were conducted by many of the top users of OSC systems in FY 2013-14.

Academic Clients

Institution	%
Other	3%
Cleveland State	.6%
Nationwide Children's	1%
Dayton	1%
Wright State	1.3%
Kent State	1.4%
Ohio Univ	1.6%
Case	1.7%
Akron	1.8%
Toledo	2%
Bowling Green	2%
Cincinnati	8%
Ohio State	75%

Commercial Clients

Organization	%
Other	0.4%
Automotive Parts Manufacturer	1.6%
Aerospace Parts Manufacturer	2.9%
Petrochemical Manufacturer	2.9%
Structural Engineering Consultants	4.0%
Consumer Goods Manufacturer	5.8%
Alternative Energy Manufacturer	6.2%
Aerospace Engineering Consultants	76.2%

Top Academic Clients by Usage of OSC Resources: 2013-14

Principal Investigator	Research Title	Institution
Wolfgang Windl	Computational Design of Metallic Glasses	OSU
Aravind Asthagiri	Multi-scale Modeling of the Electrochemical Reduction of CO^2 to Alcohols	OSU
John Herbert	Development of Novel Electronic Structure Methods for Large Systems	OSU
Christopher Hadad	Development of Functionalized Molecular Baskets for the Encapsulation of Organophosphorus Compounds	OSU
David Bromwich	Atmosphere-Ocean Coupling Causing Ice Shelf Melt in Antarctica (ACCIMA)	OSU
Thomas Beck	Computational Studies of Specific Ion Effects in Water and Ion Channels	UC
Douglass Schumacher	Modeling Intense Laser Plasma Interactions Driven by Next Generation Short Pulse Lasers	OSU
Massimo Olivucci	Investigating Anabaena Sensory Rhodopsin Mutants for the Design of Novel Optogenetic Tools	BGSU
Christopher Bartlett	Childhood Language Impairment and Gene Expression in the Brain	NWCH
John Wilkins	Development of Classical Potentials for Modeling TI and TI-NB Alloys	OSU
Shaojun Wang	Developing Large-scale Distributed Syntactic Semantic and Lexical Language Models for Machine Translation and Speech Recognition	WSU
Aleix Martinez	Compound Facial Expressions of Emotion	OSU
Chenglong Li	Protein Arginine Methyltransferase 5 (PRMT5): Structural Dynamics and Drug Discovery	OSU
Hendrik Heinz	Design and Testing of Nanoalloy Catalysts in 3D Atomic Resolution	UA
Philip Schniter	Active Sensing via Compressive Illumination	OSU
Ian Howat	Demonstration of SETSM Phase 2: A 2-Meter Digital Surface Model of the Greenland Ice Sheet	OSU
Daniel Lacks	Molecular Dynamics Simulation of Surfactants at Interfaces of Aqueous Solutions	CWRU
Thomas Humanic	Continuing Use of OSC Computing Resource by OSU Heavy Ion Group in Support of ALICE Computing Program Year 2013	OSU
Richard Furnstahl	In-Medium Similarity Renormalization Group With Chiral N N + 3N Hamiltonians, Part III: Toward Heavy Nuclei	OSU

Dr. David Bromwich is one of more than a thousand academic research scientists who leverage OSC high performance computing and storage systems each year to better understand our world.

"Computational support from our OSC allocations has been key in the completion of 12 substantial publications over the past four years. These works combined were based on more than 10 million CPU hours, with a large fraction at OSC, and equally extensive analysis. Together, these papers utilize methods that span the scales of materials physics... ."

– John Wilkins, Ohio Eminent Scholar, Professor of Physics, The Ohio State University

Industrial Engagement

## AweSim: Virtual Design. Real Benefits.

OSC's newly launched industrial outreach program – AweSim – is designed to provide the benefits of modeling and simulation to small and mid-sized manufacturers. Many large manufacturers already have embraced simulation-driven design to achieve a higher degree of competitive advantage. Smaller manufacturers are largely missing out on this advantage because they cannot afford access to such solutions.

Simulation-driven design supplements physical-product prototyping with less expensive computer simulations, reducing the time to market, while improving quality and cutting costs. Modern manufacturing simulation applications (or "apps") integrate essential manufacturing domain knowledge, sophisticated simulation software and powerful computational resources inside a web-based work flow.
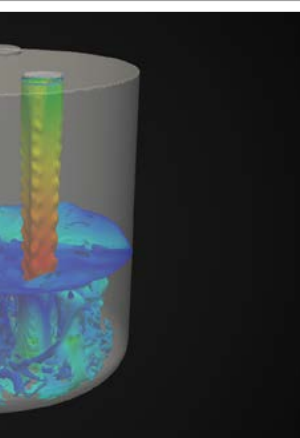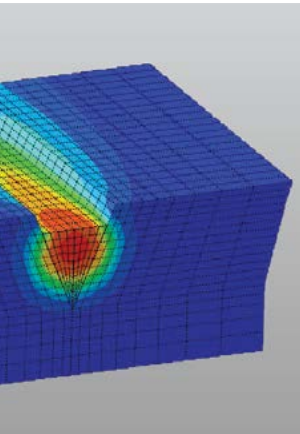
Based upon these concepts, the Ohio Supercomputer Center has developed unique technology capabilities and, together with its client partners, a product strategy to help reduce the barriers for entry into this largely untapped market. The $6.4 million public/private initiative is funded by Ohio's Third Frontier Commission and program partners P&G, Intel, AltaSim Technologies, TotalSim USA, Kinetic Vision and Nimbis Services.

In addition to the AweSim initiative, OSC continues to provide commercial clients with conventional access to HPC computation and storage, meeting a charge that was spelled out in the state funding allocation that created the Center in 1987.
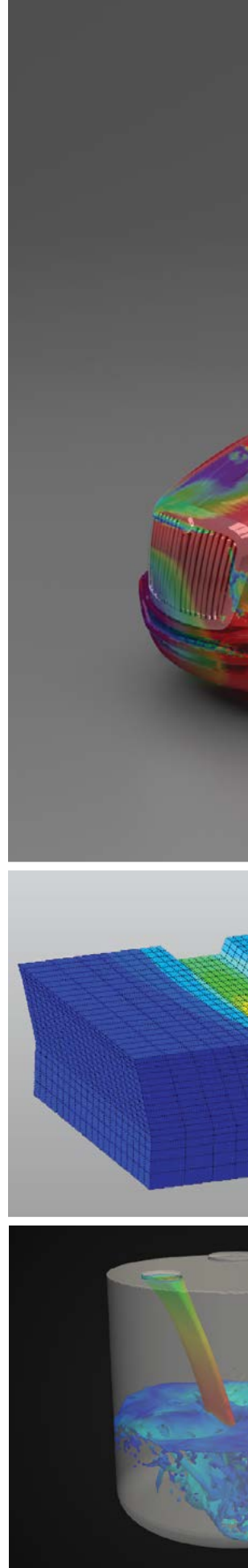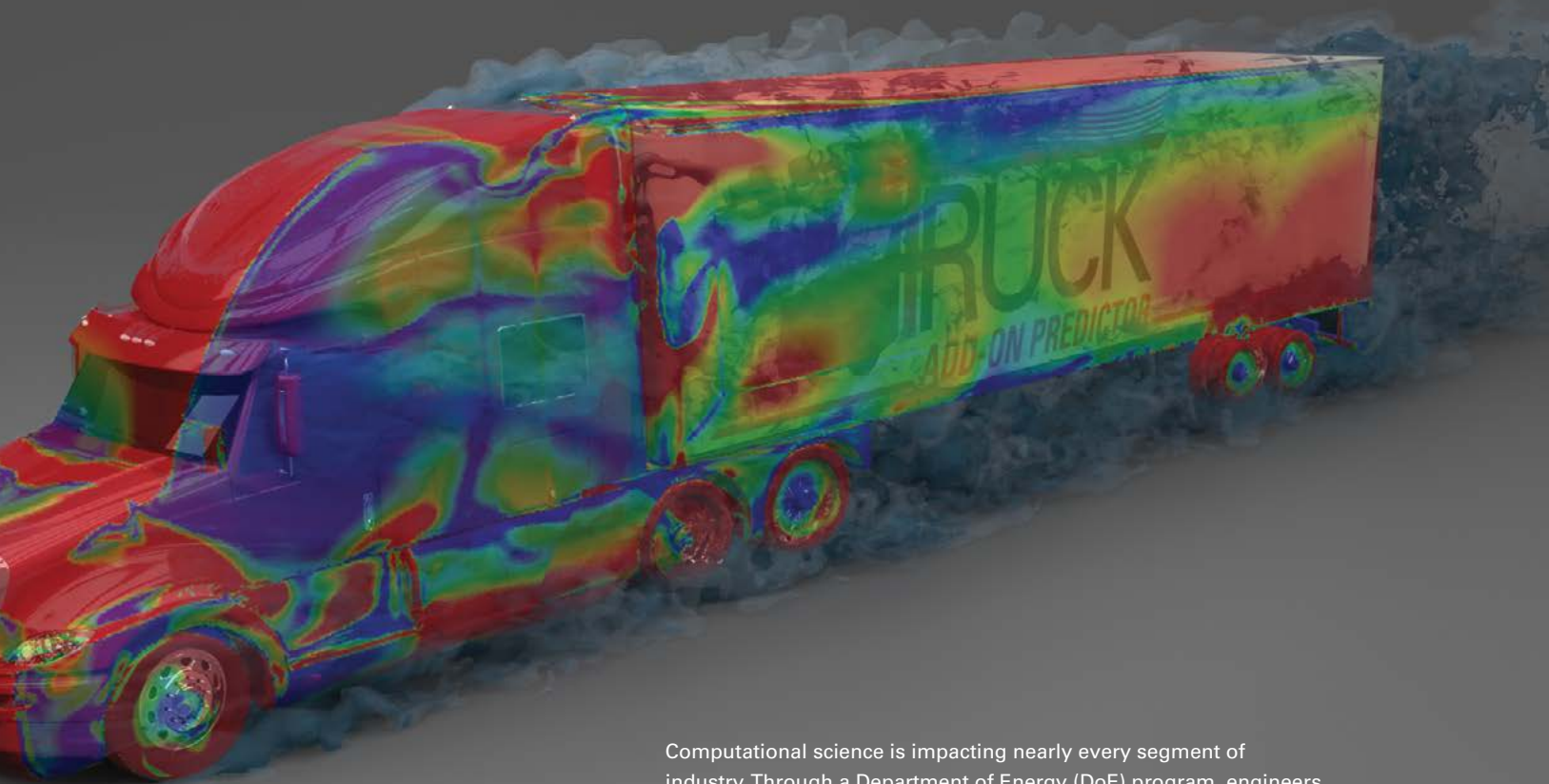
Computational science is impacting nearly every segment of industry. Through a Department of Energy (DoE) program, engineers developed a Truck Add-on Predictor that models aerodynamic forces over a joint vehicle/trailer body.

AWE**SIM** PARTNERS

ALTA**SIM** TECHNOLOGIES
REALIZING TOMORROW'S TECHNOLOGY

(intel)

TOTAL SIM USA

P&G

kinetic**vision**

Ⓝ **Nimbis Services**

Ohio Supercomputer Center
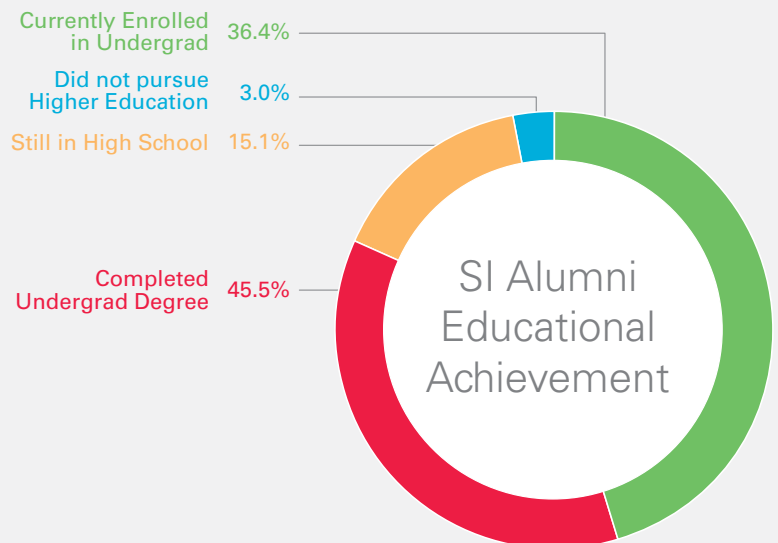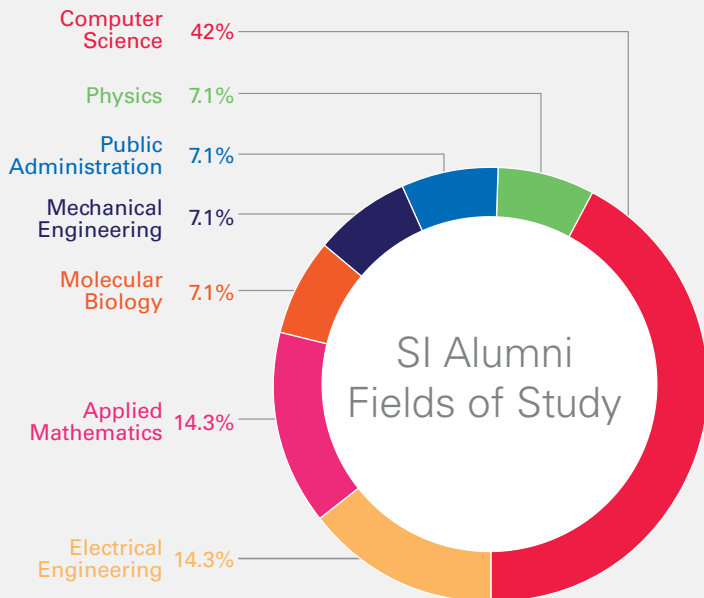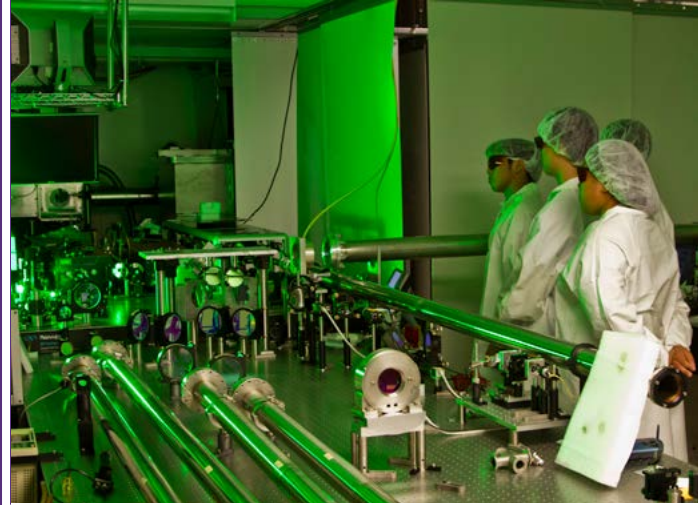An OH·TECH Consortium Member

Several AweSim pilot applications have been developed to demonstrate the value of modeling and simulation to industry. Weld Predictor (middle left) helps to predict weld strength using variables, such as material, angle, depth and temperature. Container FillSim (bottom left) helps to increase manufacturing-line speeds by forecasting how fluids can be poured into and mixed within a container.

Twenty-five Years of Summer Institute

To encourage interest in the Science, Technology, Engineering and Mathematics (STEM) fields, OSC has offered summer programs for 25 years. Each year, Ohio's brightest freshmen, sophomores and juniors participate in OSC's Summer Institute, a two-week camp where participants experience firsthand high performance computing and network.

Likewise, the Young Women's Summer Institute encourages middle-school girls to develop an interest in STEM subjects and careers. Next year, YWSI alumni will celebrate its 15th anniversary.

In FY2014, OSC initiated a Summer Program alumni organization, drawing upon the skills and experience of nearly 400 SI alumni and 225 YWSI alumni. These former participants today work for major technology corporations and innovative start-ups, such as Apple, CozyBit, Google, Hewlett Packard, Kaprica Security, Lockheed Martin Space Systems and Uber.

SI Alumni Fields of Study

- Computer Science 42%
- Physics 7.1%
- Public Administration 7.1%
- Mechanical Engineering 7.1%
- Molecular Biology 7.1%
- Applied Mathematics 14.3%
- Electrical Engineering 14.3%

SI Alumni Educational Achievement

- Currently Enrolled in Undergrad 36.4%
- Did not pursue Higher Education 3.0%
- Still in High School 15.1%
- Completed Undergrad Degree 45.5%

2014 SI Alumni Survey Results

Training & Education

Educating the Next Generation of Computational Science Leaders

Since 1987, OSC has earned a national reputation for exceptional training and education programs by creating a pipeline that contributes to a skilled computational science workforce.

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 computational science minor or associate degree program offered at numerous Ohio colleges and universities. A stackable workforce certification program allows workers to learn computer modeling and the underlying mathematics and computer programming skills.

Within the Center, more than 30 undergraduate and graduate students annually gain real-world experience through a variety of internships at OSC and its partner organizations in the Ohio Technology Consortium.

OSC's faculty and student researchers can take advantage of ongoing training for 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

Extreme Science and Engineering Discovery Environment

Three OSC staff members play significant national or regional leadership roles within XSEDE:

- Steve Gordon, Ph.D., OSC Senior Education Specialist, serves as XSEDE's national lead for education programs;
- David Hudak, Ph.D., OSC Director of Supercomputer Services, serves as XSEDE's manager of industry relations; and
- Karen Tomko, Ph.D., Interim Director of Research and Scientific Applications Manager, is an XSEDE campus champion.

Hardware, Software & Services

214 Teraflops of Peak Computing Power

2013-14 was a year of diligent preparation for OSC engineers. With existing capital allocation funding, the staff planned to boost a small pilot cluster into a system that in fall 2014 will nearly rival existing production systems.

And, with the approval of a new $12 million capital allocation in the spring and insights gleaned from the test cluster, the engineers began preparing for the purchase of a new system that will feature nearly four times the number of processors in the current flagship system. Expected to be operational in 2015, engineers requested information from vendors about HPC hardware offerings and timelines, cloud services, alternative purchase options and partnership opportunities.

Collectively, current OSC supercomputers provide a peak computing performance of 214 Teraflops – the equivalent of everyone on earth performing more than 30,000 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.

The Center also provides licenses for more than 30 software applications and access to more than 70 different software packages. Researchers can run software for which they provide the license, 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.

Beyond providing these shared statewide resources, OSC works to create a user-focused, user-friendly environment. For example, OnDemand, a web-based application that enables "point-and-click" access to the supercomputers, was further refined by a team of OSC developers. In 2013-14, more than 550 users launched apps over 39,000 times through OnDemand.
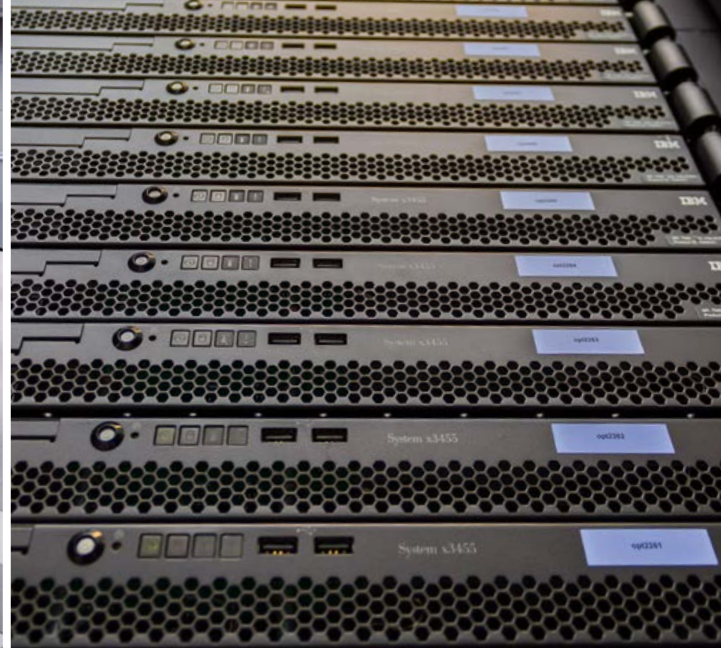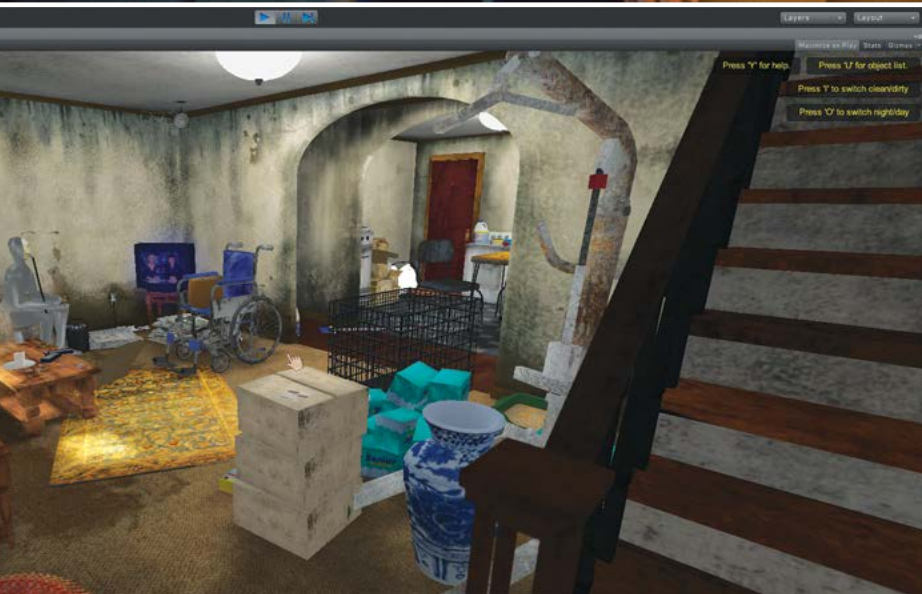
High Performance Computing & Storage

In 2013-14, researchers statewide depended upon several key OSC systems:

- HP Intel Xeon **Oakley Cluster** (top left), which provides a total peak performance of 154 Teraflops of computing power.

- IBM AMD Opteron **Glenn Cluster** (top right), which provides a total peak performance of 60 Teraflops.

- HP Intel Xeon Phi **Ruby Pilot Cluster** (left), which was developed in partnership with Intel and Ohio State to test pre-production Intel Xeon Phi processors.

- **Csuri Advanced GPU Environment**, which leverages Graphics Processing Units for a robust visualization environment.

- IBM **Mass Storage Environment**, which contains more than two Petabytes of disk storage.

Virtual Environments

Virtually Exploring Big Data

An interdisciplinary team of scientists and clinicians within OSC's Virtual Environments and Simulation Group applies high performance computing and advanced interface technology to explore complex computational data virtually. As advanced simulations integrate progressively larger computational data sets from multiple sources, OSC staff members create intuitive methodologies to integrate these vast caches of multisensory data into a single coherent simulation that can facilitate a researcher's explorations and interactions.

The following examples illustrate the wide array of funded modeling and simulation projects OSC supported in 2013-14:

- Geoscience students with mobility impairments can explore the geological structures of Mammoth Cave through an interactive virtual interface (previous page, bottom right) developed through National Science Foundation funding.

- Home health care providers are able to identify household threats to the health of patients, their family, or themselves within a virtual training environment (previous page, bottom left) funded by the National Institute for Occupational Safety and Health.

- Future surgeons can practice delicate drilling techniques on a computer-based teaching system, known as the Virtual Temporal Bone Project. The simulator was developed in partnership with Nationwide Children's Hospital – Columbus and Ohio State's Department of Otolaryngology through funding from the National Institute on Deafness and Other Communication Disorders at the National Institutes of Health.

- Automotive engineers can improve the design and implementation of vehicle instrument panels and in-vehicle information systems at The Ohio State University Driving Simulation Laboratory (previous page, top), developed through collaborations with Honda R&D Americas, oversight from Ohio State's Office of Research and technical expertise from OSC.

Promoting OSC

News and Social Media

The great work at OSC made for great news throughout 2013 and 2014. OSC press releases, in most cases, focused on the computational aspects of work done by researchers leveraging OSC resources. A release on the polar climate studies of Ohio State's David Bromwich resulted in a podcast with HPCwire; likewise, Columbus-based NBC4 reported on the 25th anniversary of Summer Institute.

Extensive news media outlets, including the Associated Press, HPCWire and Computerworld, reported on the launch of our AweSim industrial outreach initiative. This coverage yielded an invitation for OSC to present at the National Governor's Conference in November 2013.

On the social media front, a new blog provided a platform for OSC staff members and guest bloggers to share their expertise. We generated further buzz by cross-posting to Facebook, Twitter and LinkedIn. The blog articles garnered media interest as well, including Scientific Computation magazine and Lawrence Livermore National Labs.

To showcase the Center, AweSim and our OH-TECH partners, we designed and produced a new booth. The booth, which premiered at SC13, the international conference for high performance computing, commands a presence at these large-scale events.

The annual OSC Research Report featured 20 academic investigations and five industrial projects. The 44-page report was distributed at SC13 and other conferences and to policymakers and stakeholders.

Contact Us

Pankaj Shah
Executive Director
Ohio Supercomputer Center
and OARnet
(614) 292-1486 • pshah@oh-tech.org

Alan Chalker, Ph.D.
Director of Technology Solutions
and Director of AweSim
(614) 247-8672 • alanc@osc.edu

Basil Gohar
Web and Interface
Applications Manager
(614) 688-0979 • bgohar@osc.edu

Steven Gordon, Ph.D.
Senior Education Specialist
(614) 292-4132 • sgordon@osc.edu

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

Dave Hudak, Ph.D.
Director of Supercomputer Services
(614) 247-8670 • dhudak@osc.edu

Doug Johnson
Chief Systems Architect
and HPC Systems Manager
(614) 292-6286 • djohnson@osc.edu

Karen Tomko, Ph.D.
Interim Director of Research
and Scientific Applications Manager
(614) 292-1091 • ktomko@osc.edu

To contact other OSC staff members,
please refer to the online directory at
osc.edu/staff-directory.

Ohio Supercomputer Center

1224 Kinnear Road
Columbus, Ohio 43212

P: (614) 292-9248
F: (614) 292-7168
support@osc.edu
www.osc.edu

/osc

/ohiosupercomputercenter

/oscnewmedia

/company/ohio-supercomputer-center

oh-tech.org/blog

Jamie Abel
OH-TECH Communications Director
(614) 292-6495 • jabel@oh-tech.org

Ian MacConnell
OH-TECH Creative Director
(614) 292-9319 • ian@oh-tech.org

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