Research Report 2014–15

Ohio Supercomputer Center

An OH·TECH Consortium Member

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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.

"Through the powerful systems and services of the Ohio Supercomputer Center, researchers across the state are able to achieve groundbreaking scientific research and industrial innovation."

— 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.

"In 2014, Ohio Supercomputer Center clients at Ohio's public research universities* accounted for $146 million—or nearly 19 percent—of the $780 million in active-award funding awarded to those universities from three of the largest federal research-funding agencies.**

We cannot say that OSC resources necessarily contributed to each of the identified grants, but it is clear that a significant segment of Ohio researchers rely upon OSC computational resources to advance their vital innovations and discoveries."

A Vision for OSC

Here at the Ohio Supercomputer Center, the gleaming hardware and sophisticated software are certainly important components of our contributions to discovery and innovation, but it remains the human element that lies at the heart of what we do.

First, the researchers: Last year, OSC awarded compute time that resulted in nearly 1,173 faculty, staff and student assistants across the state running simulations or analyses for 239 new research projects. This report highlights a sampling of Ohio's research endeavor; there are many more stories waiting to be told.

Second, the OSC staff: In 2014, OSC delivered more than 87 million CPU core-hours, for more than 2.2 million jobs using 975 terabytes of storage with 99.2 percent uptime. Our restructured management team has developed a sustainable, new business model that seeks collaborations with university and industry partners.

Third, statewide leadership: In early 2015, officials from across Ohio convened to dedicate our newest supercomputer system, and, through their support, we have been allocated capital funding for a 2016 system much larger than the total current OSC infrastructure.

We welcome researchers to tell us more about their computing needs and interests and encourage policymakers to learn more about how OSC is helping Ohio build on its legacy as a leader in discovery and innovation.

Pankaj Shah

Executive Director, Ohio Supercomputer Center & OARnet

* The public institutional members of the Research Officers Council of the Ohio Board of Regents

** Department of Energy's Office of Science, the National Institutes of Health and the National Science Foundation

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Center offers the critical services that facilitate discovery, innovation

"Our clients' most valuable resource is their time. We allow them to spend less time on infrastructure and more time on their research."

David Hudak, Ph.D.
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OSC Overview

Since the creation of the Ohio Supercomputer Center (OSC) in 1987, the center's staff has provided critical services that allow Ohio researchers, professors and students to achieve new levels of success, from empowering amazing scientific discoveries to partnering on remarkable industrial innovations. The center provides its clients with a wide array of invaluable assistance, from high-end supercomputing and storage, to domain-specific programming expertise, to intuitive and effective resource interfaces and school-to-college-to-workforce education and training.

Our mission is to empower our clients, partner strategically to develop new research and business opportunities and lead Ohio's knowledge economy. David Hudak, Ph.D., director of supercomputing services, offers some perspective on how OSC is supporting that mission:

Capacity

"We work with researchers who need computational and storage capacities that far outstrip what they can expect from machines in their offices or departments. There are many benefits in having access to a state-of-the-art, modern computer center that deploys large-scale systems that are professionally maintained and monitored. However, the bottom line is for researchers to be able to focus on their science and not on whether they've installed the latest software, what happens to their computers when the building loses power or any other operational issues. Our clients' most valuable resource is their time, and we provide sophisticated solutions that allow them to spend less time on infrastructure and more time using the infrastructure to do their research.

Reliability

We've built an extremely reliable and exceedingly usable high performance computing environment here at OSC. We have a production software stack that is meticulously developed and maintained by more than a dozen in-house experts. Regular maintenance windows allow us to refresh applications so clients have access to the latest, most reliable software in their fields. We're focused on issues like security updates, performance improvements and improved usability; there's a tremendous amount of work that goes into making our production environment as good as it is. I am grateful to our outstanding team for all their efforts.

Services

We offer clients domain-science expertise in computational science, as well as scientific fields like computational chemistry, numerical analysis, computer science, finite element analysis and computational fluid dynamics. We're also strengthening our ability to assist clients with their needs in data analysis, supporting such initiatives as Ohio State's Discovery Themes, the University of Cincinnati's business analytics program and Case Western Reserve University's data science and analysis programs.

Our clients are scientists with deep levels of expertise in their own fields of study—chemistry, physics, biology, pharmacology and so on—not HPC engineering. On top of that, our practitioners, more often than not, are graduate students who work for the scientists for a year or two—a very short learning curve. We're making our experts more available so they can provide customized solutions that bring that scientific work into our production environment and help clients get the most they can out of our services.

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

There's also hardware customization, as we're always looking for the right balance between specialization and commodity hardware. For example, we offer big-memory machines (one terabyte RAM) for those experiments and those codes that simply require a terabyte of RAM that cannot be split across multiple nodes. Also, we have nVidia K40 GPU accelerators and Intel Xeon Phi coprocessors in the Ruby Cluster, in addition to the nVidia K20 GPUs in the Oakley Cluster. If we don't have some particular feature that a researcher needs, I'd love to have a conversation to better understand that need and find out if others across the state have the same need.

Access

As I said, a researcher's most valuable resource is his or her time. OSC OnDemand was our first large-scale initiative at the production level aimed at making HPC easier to use; we are trying to redesign and simplify the interfaces with our computing systems. With myOSC, we're making a single location for managing all administrative functions. This way, if a client needs to work on a project, they go to OSC OnDemand; if they have to file a proposal, need to check status on a ticket or register for a training classes, they go to myOSC.

Organizational Focus

Over the last couple of years, we've reorganized the entire supercomputer services staff. The overall goal was to scale and sustain operations and improve the reliability and service levels we provide to our clients. We now have a scope and mission for each of four production teams: HPC Systems (led by Doug Johnson), HPC Client Services (led by Brian Guilfoos), Scientific Applications (led by Karen Tomko) and Web & Interface Applications (led by Basil Gohar). With just a few strategic hires left to make, we're well on our way to forming the team that can provide a potent blend of services and support of the highest quality. ”

CAPACITY

ISSUE:
Researchers need high-capacity computation and storage

SOLUTION:
OSC provides access to state-of-the-art large-scale systems

RELIABILITY

ISSUE:
Researchers want a highly dependable HPC environment

SOLUTION:
OSC represents an extremely reliable and usable HPC center

SERVICES

ISSUE:
Researchers are seldom HPC experts, yet require HPC resources

SOLUTION:
OSC offers deep staff expertise and a wide range of HPC solutions

OSC Impact July 2014 – June 2015

Production Capacity

87,000,000+
CPU core-hours delivered

2,200,000+
computational jobs run

975 TB
data storage space in use

99.2% uptime
(target: 96% cumulative uptime)

Client Services

25 universities
served around the state

1,173 people
ran a computing simulation or analysis

155 people
attended 10 training opportunities

239 new projects
launched by Ohio faculty

Research projects & new projects by institution, OSC 2014 – 2015

Critical Partnerships

The Ohio Supercomputer Center—renowned statewide, nationally and internationally for its ability to bring valuable contributions to collaborative efforts—plays a significant role in numerous critical partnerships. A couple of examples demonstrate this deep commitment: a coalition to investigate and combat harmful algae blooms and an initiative to deliver vital computational services to biomedical informatics researchers.

In 2015, following a three-day "no-drink" municipal water advisory to the 500,000 citizens of Toledo, Ohio, Department of Higher Education Chancellor John Carey organized his agency's Lake Erie R&D Initiative to find ways to effectively counter the harmful algae blooms plaguing Ohio lakes. Carey brought together research labs from a group of colleges and universities already engaged in water quality studies, several state agencies with a vested interest in a successful solution and scientists from NASA Glenn Research Center.

The Ohio Supercomputer Center is providing solutions for big data storage and warehousing for labs at the partnering research institutions: Bowling Green State University, Central State University, University of Cincinnati, Defiance College, Heidelberg University, Kent State University, The Ohio State University and University of Toledo.

OSC engineers adapted the AweSim industrial engagement program's simple, web-based dashboard interface to facilitate collaboration on data analysis for field biologists working on the problem. In addition, colleagues at OARnet recently installed a peering service that connects their statewide network with NASA's, allowing vast amounts of data to flow between the universities and the research center.

In addition to the challenges blue-green algae presents to water treatment facilities, these toxins present a serious threat to those communities that depend upon activities, such as tourism and most forms of water sports.

In Columbus, the Biomedical Informatics Department (BMI) within the College of Medicine at The Ohio State University Wexner Medical Center (OSUWMC) leads a robust and expansive informatics research, development, service and training program. This important, game-changing research depends heavily upon powerful and responsive computational resources.

OSC staff members are assisting BMI researchers in transitioning from several small, in-house computational cluster systems to the more sustainable and powerful infrastructure of OSC's Ruby and Oakley HPC systems. For the past few years, OSC has been providing system administrative and user support for the aging BMI systems, mirroring the BMI genomics databases, installing and supporting software required for analysis of genetic data of human disease and running PhemoLIMS, a lab notebook.

BMI efforts are complemented by the operations of OSUWMC's CTSA-funded Center for Clinical and Translational Science, an NCI-designated Comprehensive Cancer Center, and a recent $1 billion expansion of OSUWMC. BMI research is further impacted by investments from the university's $400 million Discovery Themes Initiative, which will bring in 500 new senior faculty members over the next 10 years to augment identified areas of research strength at the university.

OSC engages in numerous critical partnerships, incuding an effort to transition biomedical informatics (inset) researchers to high performance computing systems and an initiative to combat harmful algae blooms in Ohio waters.

(Inset) Photo credit: Department of Biomedical Informatics at The Ohio State University.
(Below) Photo credit: The National Oceanic and Atmospheric Administration (2012).

Team provides specialized support and education services

"My team is here to enable your science and, in whatever way that we can help, we want to."

Brian Guilfoos

Manager, HPC Client Services

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HPC Client Services

Client Services is the entry point for our user community. We provide the connections to the services that OSC offers its clients, and we do that in a number of ways. We manage the administrative functions associated with research done here. We also provide the technical support through a recently expanded 24/7 help desk. Our staff takes service requests in and processes those to solve those problems. We'll bring in the right subject-matter experts from around the Ohio Supercomputer Center to assist with each specific issue.

We also provide facilitation services. We'll sit down and talk to a researcher or research group about what their research goals are and how computing fits in and help connect them to the right resources here to accomplish their work. So whether the work is high performance computing or high-throughput computing or data-intensive work, we can point them to the right services and resources or bring in engineers from our interface group to work with a project. We consider the subject matter, workflow, and compute and data requirements to make recommendations on how to move forward.

Support from OSC Client Services is ongoing. If somebody changes tack a little bit in their research or they hit a wall, we continue that facilitation and engagement. Sometimes issues are larger than a technical problem and, even if a client is experienced, if they're taking on a new aspect of science that they haven't done before on our systems or perhaps haven't done at all, we provide guidance on how to proceed.

Training

Through the integration of a new training and education lead on staff, OSC will have a dedicated person to curate and guide our training programs to help clients build core competencies that they need to be effective while using our services. We also plan to continue the connection with XSEDE's national training programs as well.

As we've been working more with university CIOs and IT departments, we're trying to build an infrastructure that more directly connects with researchers. We are spinning up a new program with campus facilitators. This will involve people on campuses who know our services very well who will provide local technical and facilitation support and know who to contact at OSC to bring in additional help. This makes OSC training a little bit easier for someone who's not in Columbus. We will also ensure that we're connected with faculty around the state of Ohio who are teaching computational science.

My team is here to enable your science and, in whatever way that we can help, we want to. We're here to help even if you don't know if you need OSC. If you're having problems, but you don't know much about supercomputing, that's a perfect time to talk with us. We may have something that can help you even if you don't consider your issue a 'big supercomputing problem.'

We're seeing a lot of growth in areas that are not of our traditional user base, such as business and economics. I think it's interesting because it shows people are finding ways to leverage these services that are available to them and exploring domains that they would have thought were out of reach before. Talking about these areas helps get other people thinking about how they can grow their science.

Building a Supercomputing Foundation

Our on-site introduction workshop for OSC is Computing Services to Accelerate Research and Innovation. If you use computers in your research, you might be able to leverage OSC, and this workshop will begin that conversation. It provides an engagement opportunity so we can answer your questions locally, face-to-face.

We are also working to identify the core competencies of a basic, intermediate or advanced HPC user and creating a curriculum for each skill level. So, if you come to OSC and you don't know anything about supercomputing, we can tell you what you need to know to be able to log on and do something productive. If you want to jump to the next step and do a little bit more, we'll provide materials for you. We're building curriculum so we have a broad set of materials available for our user community.

Classroom Instruction Resources

We provide resources for classroom instruction as well. If you're an instructor who wants to use the supercomputer services in the classroom environment, we can provide user accounts for your students and a limited amount of resource units for the duration of the semester. We'll provide you with priority reservations on the system to ensure acceptable turnaround time during lab periods, enabling faster feedback.

Faculty Recruitment

Another service we provide is faculty recruitment. We can participate in the conversations that you have with faculty candidates and talk about the services we provide, as Ohio's shared supercomputing model could be different than what outside candidates might be used to. Simply contact OSC Help to begin the process.

Ralph Regula School of Computational Science

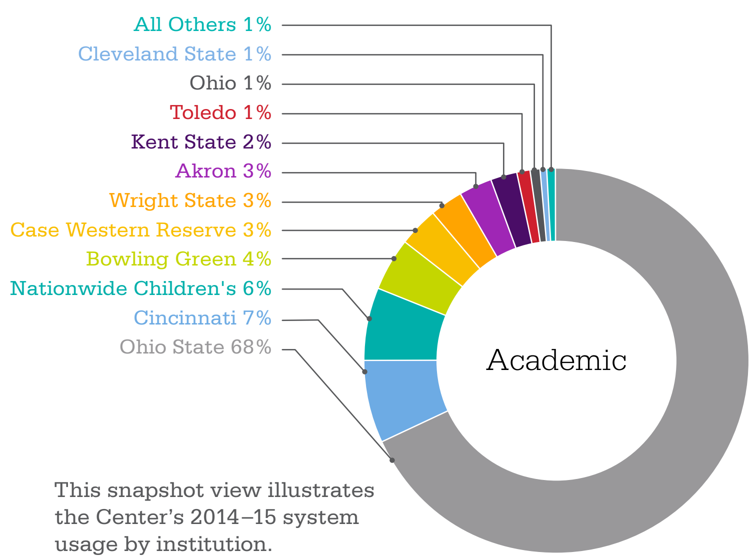
This collaborative, virtual program is a defined curriculum that leads to a minor in computational science at participating institutions. As we engage with computational-science instructors around the state, we keep these materials up to date and strengthen the collaboration among universities when it comes to computational-science education.

Summer Programs

We are developing a sustainable funding model to ensure our summer programs have a long future. We are working with faculty who are submitting National Science Foundation career-award proposals to fill their broader engagement requirement. We participate on these grants so they can help provide funding and expand the program to support kids.

We are also actively working to engage and provide better outreach to underserved youth. We're working to secure additional funding that will provide summer program scholarships to cover the cost of housing. We are working with Ohio State to provide coaching services in these communities to help students write better applications for the program since it is a blind review process. For Summer Institute, the program for high school students, we went from 16 students last year to 20 this year, and will continue to pursue opportunities to expand the program.

The focus for the Young Women's Summer Institute is to develop middle school girls' interest in computers, math, science and engineering. We do a lot of work to bring in faculty and graduate students from different disciplines to talk to attendees about careers in these fields. There's a lot of enthusiasm from faculty members and those graduate students who are really interested in participating to help expand this program as well. ”



This snapshot view illustrates the Center's 2014–15 system usage by institution.

Systems staff optimizes evolving OSC computing and storage services

A new system in 2016 "will exceed the peak performance of all the center's existing systems combined."

Doug Johnson
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HPC Systems Services

With the April dedication of OSC's newest cluster, the Ohio Supercomputer Center currently is offering researchers three mid-sized high performance computing (HPC) systems: the HP/Intel Xeon Phi Ruby Cluster, the HP/Intel Xeon Oakley Cluster and the IBM/AMD Opteron Glenn Cluster. OSC also is providing researchers with a storage environment with several petabytes of total capacity across a variety of file systems. With all of that already sitting on the floor at OSC's nearby data center, many upgrades and installations await OSC clients in 2016.

The Ruby Cluster

"The seven racks of the new Ruby Cluster house 240 nodes and provide a total peak performance of more than 140 teraflops. We look at Ruby as a transitional system that features newer hardware than Oakley and additional capacity. Since the Glenn Cluster will have to be turned off to make room for the 2016 system, the value of the Ruby Cluster only increases. It will provide additional computational capacity while we are physically removing the Glenn Cluster and before the new system is available. The software environment on Ruby will also be a good springboard to the next system.

Looking Ahead

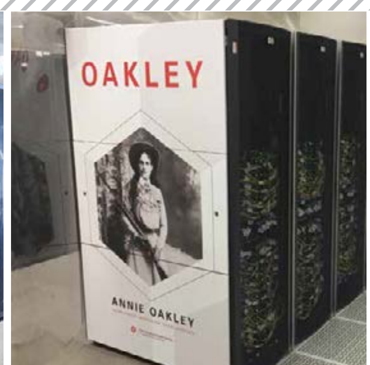
In 2016, the remaining racks of the Glenn Cluster are expected to make way for a new system that will exceed the peak performance of all the center's existing systems combined. Due to the significant increase in performance relative to the current systems, OSC will ensure that other facets of the infrastructure can keep pace with the new system.

We'll be making enhancements to our external network connections. The core router that OSC uses to connect to the Internet through OARnet will be upgraded to support a 40-gigabit-per-second connection to OARnet. We will also upgrade our peer connection with The Ohio State University to the same speed. Both upgrades are designed for an eventual move to 100-Gbps connections to match what's already available on the OARnet backbone.

The coming year will see upgrades of all the storage at OSC. This includes upgrades and replacements for users' home directories, project storage and global scratch-file systems. We will increase our total file system capacity to over five petabytes, with aggregate throughput performance of approximately 200 gigabytes per second. Other improvements have been made to our storage environment to respond to the needs of our user community. These included expansions to our backup systems to not only accommodate the additional storage, but to also provide user accessible archive to tape for long-term retention of data."

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 Xeon Phi Ruby Cluster.

High performance computing systems



	Ruby (2014)	Oakley (2012)	Glenn (Phase III, 2009)
Theoretical Peak Performance	96 TF +28.6 TF (GPU) +20 TF (Xeon Phi) ~144 TF	88.6 TF +65.5 TF (GPU) ~154 TF	34 TF +6 TF (GPU) ~40 TF
# of Nodes / Sockets / Cores	240 / 480 / 4800	692 / 1384 / 8304	426 / 856 / 3408
Cores per Node	20 cores/node	12 cores/node	8 cores/node
Local Disks Space per Node	~800 GB in /tmp	~800 GB in /tmp	~400 GB in /tmp
Compute CPU Specs	Intel Xeon E5-2670 v2 CPUs • 2.5 GHZ • 10 cores per processor	Intel Xeon x5650 CPUs • 2.67 GHz • 6 cores per processor	AMD Opteron 2380 CPUs • 2.5 GHz • 4 cores per processor
Compute Server Specs	200 HP SL230 40 HP SL250 (for NVIDIA GPU/Intel Xeon Phi)	HP SL390 G7	IBM x3455
# / Kind of GPU/Accelerators	20 NVIDIA Tesla K40 • 1.43 TF Peak double-prison • 2880 CUDA cores • 12 GB memory 20 Xeon Phi 5110p • 1.011 TF Peak • 60 cores • 1.053 GHz • 8 GB memory	128 NVIDIA M2070 • 515 GF Peak Double Precision • 6 GB memory • 448 CUDA cores	18 NVIDIA Quadro Plex 2200 S4 • Each with Quadro FX 5800 GPUs • 240 CUDA Cores/GPU • 4 GB memory/GPU
# of GPU / Accelerator Nodes	40 total (20 of each type)	64 Nodes (2 GPUs/node)	36 Nodes (2 GPUs/node)
Total Memory	~16 TB	~33 TB	~10 TB
Memory per Node / per Core	64 GB / 3.2 GB	48 GB / 4 GB	24 GB / 3 GB
Interconnect	FDR/EN IB (56 Gbps)	QDR (40 Gbps)	DDR IB (20 Gbs)

Virtual reality enhances training, aids understanding

Don Stredney

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Virtual Environments & Simulation

While virtual environments often are associated with gaming and entertainment, OSC's Interface Lab has translated the technology into effective training and assessment tools for use by various sectors such as the health care, automotive and manufacturing industries.

The Interface Lab explores the capabilities the virtual world offers to a variety of professional areas. Three of the lab's main focus areas include virtual temporal bone surgery, simulated hazard training for home health care and interfaces used for studies in distracted driving in collaboration with OSU's Driving Simulation Lab.

Driver alertness

"One thing we're doing with regard to the Driver Simulation Lab that has implications in everything we do—because it's basically looking at brain physiology—is development for software using the fNIR (functional Near Infrared Imaging) system. Using near infrared light, you wear a headband and there's optics on the headband that emit near infrared light that goes through the skull and into the cerebral cortex. So, fNIR provides, in near real-time, a low cost, non-invasive method to determine the location and procession of functional activity within the brain during specified tasks.

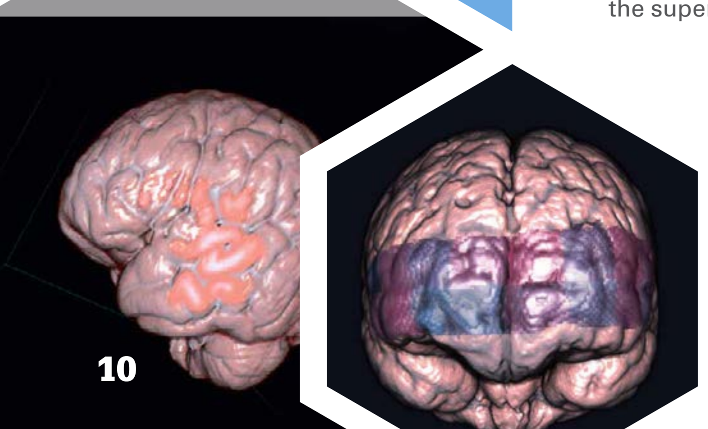
There's a lot of interest in distracted driving right now. One of the reasons people are distracted is they're bored, so they seek something to do while driving. We're focusing on the use of fNIR in studying attention during driving and surgical training. By integrating fNIR data with direct volume rendering, the group is developing a non-invasive, cost-effective tool for viewing and quantifying human performance. What we want to see is: Does the frontal lobe drop out at a certain point if you've been driving for a while?

This area of study has been many years in the making with my interest in brain science.

Going wireless

With recent upgrades, we're going to emphasize working toward shared virtual environments where individuals can move around freely without tethered devices. Our big goal is not only to create more innovative environments for research into how virtual environments can be used but also to use these to obtain better visual representations of a common model.

As we increase in complexity within industry, education and so on, the question becomes 'How do people understand what the situation is?' If it's a structural representation—whether it be an automobile, part or molecular modeling—what we want to do is put in their hands a robust set of tools that allows them to manipulate structures, visualize information very intuitively and use the power of the supercomputer for updates to steer equations and get results very quickly."



Functional Near Infra Red Spectroscopy (fNIR) is a low-cost, non-invasive method of study to determine the location and procession of functional activity during specified tasks by showing metabolic change in a localized region of the brain.

Photo credit: Brain data courtesy of the Allen Institute for Brain Science.

Software engineers lower the barriers for OSC clients

Karen Tomko, Ph.D.
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Top 10
Applications on the Oakley system for CY2014 are:

1. Gromacs
2. Matlab
3. Amber
4. Gaussian
5. OpenFOAM
6. Q-Chem
7. NAMD
8. Elk
9. VASP
10. LAMMPS

Scientific Applications

Karen Tomko understands the challenges software developers face, having worked directly on development teams in the past. One of the main barriers is finding ways to make sure the applications that get developed are available and working in a given system.

Tomko, interim director of research and scientific applications manager at the Ohio Supercomputer Center, works to ensure the process is a smooth one for scientific applications developers as well as researchers who require help installing existing software packages.

"In working with research groups that use the system, you start to see how that can really hold them up," Tomko said. "If they can't get over that hurdle, it doesn't matter if the hardware is up and running or how much hardware we have. They need their software to work to be able to utilize it."

In recent years, the HPC community has increasingly recognized the importance of easing the process of allowing researchers and developers to get their software up and working.

"It's becoming more acknowledged as a challenging aspect of maintaining these systems, and I think that's because our user base has broadened, which means the number of software packages we need to maintain has gotten larger."

Default software upgrades

"What we have done this year is our first software refresh on the Oakley and Ruby Clusters. The Oakley Cluster was set up in 2012 and the default software toolset was basically a 2012 version. So we're establishing all new updates for what the default software environment is for our users.

Our research scientists, who are mostly busy with the science aspects of their code, if they're not thinking about these things, will use the default ones and they're building on an older set of software. But there are changes. And it gets harder and harder to keep everything consistent if people are using older pieces of software. So updating them and making the updates the default encourages the users to move to the newer versions.

And, with that, they should see more robustness and reliability. They get a toolset that keeps up to date.

Additional support, tools

We've added to the staff. That's going to allow us to do more, some of it will be behind the scenes to make it easier to manage the software environment. And it gives us a little more capacity to work with specific research groups.

One of our main focus areas in this coming year is refining tools to track and understand software usage so we can make good decisions with respect to new purchases, what we should install and what we don't need to maintain anymore."

Access experts deliver app solutions, open-source OnDemand

"There's no magic going on behind the scenes; it's just normal technology at a larger scale."

Basil Gohar
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Web & Interface Services

For those intimidated by the thought of "talking" with supercomputers, Basil Gohar wants to help. As the manager of the Web and Interface Applications group, Gohar and his team have a big goal in mind: Deliver the benefits of powerful computing to users without perceived or actual complexities.

"There is an intimidation factor," said Gohar, whose group manages the way OSC HPC clients access OSC systems through the web. "People believe supercomputing involves very specialized hardware and you have to have a Ph.D. in computer science or be a mad scientist to actually do anything with it. There's no magic going on behind the scenes; it's just normal technology at a larger scale."

That technology is being used in numerous ways for OSC HPC clients. Two of the biggest highlights have been developing an online app store for the AweSim industrial engagement platform, along with setting the groundwork for the Open OnDemand web portal project.

App sharing

"Within AweSim, a lot of the work has continued from last year, and a big focus has been on sharing apps. We've enabled the AweSim app developers to actually share their apps through the AweSim dashboard, similar to what can happen in a mobile app store.

For example, say someone writes an application with a type of simulation for filling containers with a fluid. You can then upload a model for a gas can and how much fluid, say, water, oil or honey, you want to put in per second. You write an app that makes it easier for someone to make the calculations themselves and then you can share that app with someone, have them test it out, see if it's good or they can report bugs back to you. Then you report that out and they'll see those updates immediately.

You don't have to know the intricacies of the specific software being used—what's behind the scenes. You just need to know how to use a web site.

Open OnDemand project

Open OnDemand is going to be great because it's one of many open source projects that started at OSC and then went out and became very useful to a lot of people. It's an open source software that will allow people who run their own centers around the U.S. and world to be able to allow other researchers and students access to the system through a web interface rather than traditional command lines, terminals and shell access.

And, Open OnDemand will be modular so it will allow for additional features, like a web file browser, a virtual desktop manager, or even a cluster performance monitoring tool, to be configured and enabled as the site manager desires."

AweSim engages, provides solutions for businesses

"It doesn't matter what sector you are in, we can help."

Alan Chalker, Ph.D.

Director, Technology Solutions & Director, AweSim

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Industrial Engagement

It's staggering to consider the myriad ways in which the Ohio Supercomputer Center and the AweSim industrial engagement program benefit a wide array of industries. It is also hard to conceive how few leaders in these industries know what they could be gaining from the innovative cloud-based simulation application platform.

That's why Alan Chalker, director of AweSim, has worked diligently to get the word out about how modeling and simulation can assist all sizes of companies in all types of industries. Brand awareness efforts have paid off with 78 AweSim user accounts, more than 3,600 jobs run, 1,700 app launches and 1,100 unique logins into OSC systems.

Raising awareness

"We've had very good conversations with JobsOhio—Ohio's job creation and economic development entity—about OSC as a state resource they can use for retention, expansion and attraction. Jointly, we've created a list of companies to whom we want to say 'we think you are a prime candidate for making use of this.'

In some situations we're just building the market. In others it's, 'We haven't talked to you in a while; let's see if there's something we can support.' The bottom line is, we're here to help.

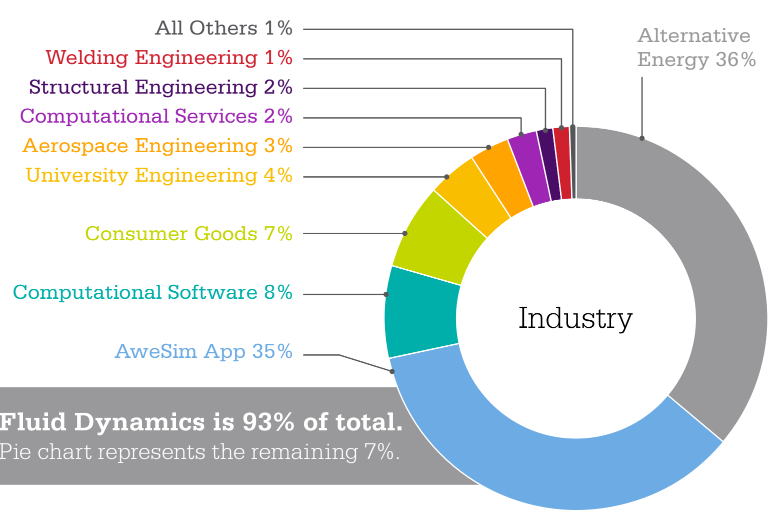
The benefits

The most important thing we have is expertise, both here and among our partners. With a network of more than 1,000 users all over the state, if I'm not able to solve an issue in-house, I can find somebody around the state who knows about it.

People ask: What's the real benefit? They might ask from a technical or business perspective. The technical is easy as some processes and products are too small, big or complex to understand. That's where modeling and simulation come in.

On the business side, it's proven that by using modeling and simulation you can get to market faster, reduce prototyping costs and tap into experts. Procter & Gamble has publicly stated when they bring modeling and simulation into a brand or product, on average they get a 7-to-1 return on investment. That's the compelling reason to adopt these technologies, no matter what business you're in."

This snapshot view illustrates OSC's system usage by type of commercial research organization.



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

Statewide Users Group

Since the first meeting of the Statewide Users Group (SUG) in November 1986—almost a full year before the official 1987 establishment of the Ohio Supercomputer Center by the Ohio Board of Regents (now the Ohio Department of Higher Education)—Ohio research practitioner-advisors have been providing OSC's leadership with sage program and policy advice. To that end, SUG established several standing committees to consider vital issues and meets as a whole twice a year to provide a forum for discussing current issues and trends and to present current developments in research.

The SUG Allocations Committee oversees a peer review grant process that allocates system resources to all academic users of the center. The Hardware and Operations Committee advises leadership on user needs and priorities for hardware configuration and acquisitions, as well as policy, procurement and operational issues. The Software and Activities Committee reviews software supported by the center for availability, clarity of documentation, quality of user interface, ease of use, logical development of the presentation, effectiveness, contribution to OSC resources and degree of restrictions. Eligible principal investigators of any OSC project are welcome to attend SUG general and committee meetings.

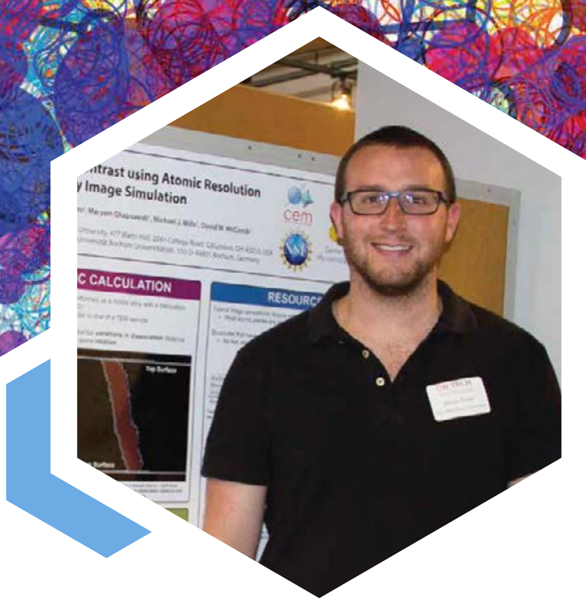
Guest speakers are a regular feature of SUG meetings. This past June, Jeff Graham, director of the Air Force Research Lab's HPC facility at Wright-Patterson Air Force Base, spoke to SUG members on "AFRL DSRC: Not just a DoD Supercomputing Resource Center." Graham was followed by Annika Peter, Ph.D., an assistant professor of physics at The Ohio State University, who presented "Exploring the Dark Side with Simulations."

In December 2014, SUG heard from Evelyn M. Goldfield, Ph.D., program director for the chemistry division at the National Science Foundation. As keynote speaker, Goldfield spoke on "NSF Support for High Performance Computing and Cyberinfrastructure." Invited Speaker Ray Leto, president of a local engineering service provider, shared his perspectives with "TotalSim USA and the Ohio Supercomputer Center." Earlier, at the June 2014 meeting, guest speaker Barry Dunietz, Ph.D., an assistant professor of chemistry and biochemistry at Kent State University, delivered a technical discussion titled "Two Tales on Computational Modeling of Charge Transfer Processes That Revise Understanding of Measured Spectra."

Beginning with the December 2014 meeting, SUG has hosted flash talk and poster competitions. OSC added this particular feature to the meeting as a way of placing more focus on the research needs and outcomes of the center's clients. The top entry in each category, as judged by a team of OSC staff, appears on the following pages.

SUG Executive Committee

Chair	Tom Beck, University of Cincinnati
Vice Chair	Hendrik Heinz, University of Akron (vacant as of August 2015)
Allocations Committee Chair	Christopher Hadad, The Ohio State University
Software Committee Chair	Rick Prairie, University of Cincinnati
Hardware Committee Chair	John Heimaster, The Ohio State University
Non-voting OSC Staff	David Hudak, Brian Guilfoos, Karen Tomko, Basil Gohar, Doug Johnson



June Poster Winner

Project Lead:
Bryan Esser,
The Ohio State University

Research Title:
Understanding dislocation core contrast using atomic resolution electron microscopy image simulation

Funding Source:
National Science Foundation

Bryan Esser, a graduate student majoring in materials science and engineering at The Ohio State University, took first place in the poster competition of the June 2015 meeting of OSC's Statewide Users Group. Esser also works as a graduate research associate at Ohio State's Center for Electron Microscopy and AnalysiS (CEMAS).

"Atomic resolution scanning transmission electron microscopy (STEM) is often used to analyze deformation mechanisms and properties," Esser explained. "Strong contrast has been observed around dislocation cores using medium-angle annular dark-field STEM, but not in high-angle conditions."

The research team to which Esser belongs conducted atomic-resolution image simulations at OSC using μSTEM, a software package for modeling the inelastic scattering of fast electrons. These simulations help to explain the nature of contrast variation as a function of scattering angles for thin-foil samples of these high-entropy alloys.

The research project is credited to Esser, as well as Timothy Smith, Maryam Ghazisaeidi, Ph.D., Michael Mills, Ph.D. and David McComb, Ph.D. (all of Ohio State), as well as Easo George, Ph.D., and Frederik Otto, Ph.D. (both of Ruhr University Bochum, Germany).

December Poster Winner

Project Lead:
Katharine Cahill,
The Ohio State University

Research Title:
Molecular docking study of organophosphorus pesticides with G3C9 and its variants

Funding Source:
National Institutes of Health

Katharine Cahill, a post-doctoral research associate specializing in organic chemistry and working in the Hadad Research Group at The Ohio State University, took first place in the poster competition of the December 2014 meeting of OSC's Statewide Users Group.

"Organophosphorus (OP) compounds are highly toxic chemicals capable of inhibiting the hydrolysis of the neurotransmitter acetylcholine by acetylcholinesterase," said Cahill. "Catalytic hydrolysis of OPs with enzymatic bio-scavengers, such as paraoxonase (PON1), is an active avenue of investigation towards the treatment of OP exposure."

G3C9 is a recombinant PON1 enzyme, which was developed for its improved solubility and has some effectiveness against OP pesticides. In this study, molecular docking simulations were performed at OSC on G3C9 and several of its variants. Docking analysis shows that, the V346A mutation significantly improves OP binding to the active site, compared to G3C9.

The research project was credited to Cahill, as well as her co-authors: Kiran Doddapaneni, Shameema Oottikkal, Thomas J. Magliery and Christopher Hadad, all of Ohio State.

June Flash Talk Winner

Project Lead:
Jason Brown,
The Ohio State University

Research Title:
A computational study of organophosphonate encapsulation in functionalized molecular baskets

Funding Source:
Defense Threat Reduction Agency,
National Institutes of Health

Jason Brown, a post-doctoral student specializing in organic chemistry and working in the Hadad Research Group at The Ohio State University, took first place in the flash talk competition of the June 2015 meeting of OSC's Statewide Users Group.

"Organophosphorus nerve agents (OPs) are a toxic class of compounds that have been used as pesticides and chemical warfare agents, and compounds for which there is a great need of effective therapeutics," Brown explained.

Gated molecular baskets conjugated to aliphatic amino acid functionalities have been examined for the binding and hydrolysis of the toxic nerve agent upon entering the bloodstream. Brown and the research group to which he belongs developed a computational protocol for the molecular baskets, including a Monte Carlo conformational search, molecular dynamics simulations and docking calculations, and ran the simulations on OSC systems.

In his talk, Brown acknowledged the contributions of Christopher Hadad, Ph.D., Jovica Badjic, Ph.D., Jeremy Beck, Ph.D., Ryan Yoder, Ph.D., Jeremy Erb, Ph.D., Paul Peterson, Ph.D., and Katharine Cahill, Ph.D. (all of Ohio State).

December Flash Talk Winner

Project Lead:
Matthew McMahon,
The Ohio State University

Research Title:
First PIC simulations modeling the interaction of ultra-intense lasers with sublaser with sub-micron, liquid crystal targets

Funding Source:
Defense Advanced Research Projects Agency

Matthew McMahon, a post-doctoral student specializing in physics and working as a graduate research associate with the High Energy Density Physics (HEDP) research group at The Ohio State University, took first place in the flash talk competition of the December 2014 meeting of OSC's Statewide Users Group.

"We recently introduced liquid crystal films as on-demand, variable thickness (50–5,000 nanometers), inexpensive targets for intense laser experiments," he said. "Here, we present the first particle-in-cell (PIC) simulations of short-pulse laser excitation of liquid crystal targets using the PIC code LSP, which is designed for large scale plasma simulations."

In order to accurately model the target evolution, McMahon and his research colleagues employed a low starting temperature and field ionization model. This was essential, as large starting temperatures lead to expansion of the target causing significant reduction of the target density before the laser pulse can interact. McMahon also described his group's investigation of the modification of laser pulses by very thin targets.

The project was credited to McMahon and his co-authors: Patrick Poole, Chris Willis, Ginevra Cochran, C. David Andereck and Douglass Schumacher, all of Ohio State.

Biological Sciences

Life: It's the common denominator that binds us all, and the enigma scientists have been trying to define and understand for centuries. From the deep recesses of a glacial cave to DNA in the human gut, the researchers featured on the following pages are harnessing the power of the Ohio Supercomputer Center to find answers to life's questions, wherever they may lie. While the microbes and genes they are working with may be microscopic, the implications of their research aided by high-performance computing could be huge.

Cell Communication

Buck, Zhang seek understanding of signals in neurological disorders

Researchers at Case Western Reserve University are continuing a 12-year investigation on how plexin, a protein found in human cell membranes, processes signals through the membrane to facilitate cell communication.

Plexins receive guidance cues from other proteins and transmit signals through the lipid membrane, regulating cell migration and targeting processes. However, if a signal is not transmitted correctly through plexin, studies have shown that this could result in serious neurological disorders. Biophysical scientists in the lab of Matthias Buck, Ph.D., are studying the signal transduction mechanism of a certain type of plexin that can become destabilized as part of an activation process.

Using Ohio Supercomputer Center services, Buck's lab has performed molecular dynamics simulations using both CHARMM and NAMD programs to understand the structure and dynamics of the transmembrane helixes of plexin and the intracellular and transmembrane domains of plexin in lipid membrane systems.

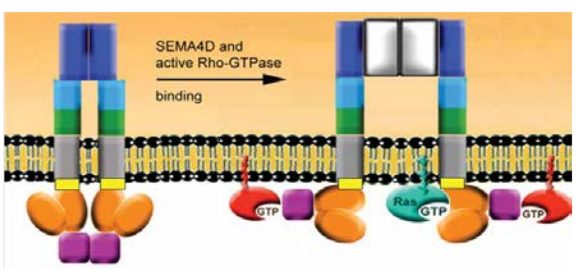
"In the first project, [resource units] were applied to characterize the dynamics of the transmembrane protein receptor in lipid membranes, which is critical for understanding the signal transduction process of plexin through the membrane," said Liqun Zhang, a previous postdoctoral scholar at Case Western; currently, she is an assistant professor in the Chemical Engineering department of Tennessee Technological University.

The initial structure of plexin was predicted with a CHARMM simulation and then virtually inserted into the cell lipid bilayer where further CHARMM simulations refined the possible structure of the protein. Based on the CHARMM simulations, consistent structures were predicted compared to the experimental structures.

"Based on this achievement we then used CHARMM-GUI software to insert the initial structure into the lipid bilayer, then applied explicit lipid and solvent CHARMM simulations to refine the structure," Zhang said.

Overall, three different plexin helix dimer structures were predicted. The results of this simulation were published in PLOS One.

Now, researchers are testing the function of the plexin structures within the cell membrane, with the long-term goal to understand the signal transduction process through the lipid membrane and in the cytoplasmic domain. They intend to continue the computational project in Dr. Buck's lab to give guidance to and synergize with experimental work performed in the lab. •



(Above right) Transmembrane and intracellular domains of plexin-B1 (in blue approaching the lipid bilayer in green). (Right) Schematic model for signal transduction via activation of plexin-B1 by a conformational change of the plexin-B1 dimer upon RhoGTPase binding to the RBD.

Project Lead: Matthias Buck, Ph.D., Case Western Reserve University
Research Title: Molecular dynamics simulations of plexin-b1 transmembrane plus intracellular domains
Funding Source: National Institutes of Health
Website: physiology.case.edu/research/labs/buck-lab

Antibiotic Resistance

Marsolo team researching techniques for early identification

Researchers at Cincinnati Children's Hospital Medical Center are using Ohio Supercomputer Center services as they zoom down to the genomic level to identify patients at risk of developing antibiotic resistance, a serious emerging health threat.

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. 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.

Partnering with David Haslam and Heidi Andersen, colleagues in CCHMC's Division of Infectious Diseases, the team obtained fecal samples from three cohorts: sick pediatric inpatients, healthy outpatient children and healthy adults. With data-processing help from OSC, Marsolo's team used a machine-learning approach known as support vector machines to analyze the 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.

With promising results from the initial study, the team is working with Drs. Haslam and Andersen on a larger prospective study. With a limited number of antibiotic drugs on the market, Marsolo's hope is the study will provide early measures for identifying sick patients most prone to developing infections, as the current process is quite slow.

"If you know ahead of time that they've got the multi-drug resistance, you can go for the more powerful antibiotics in the beginning and potentially treat them with more targeted therapy or isolate them sooner so that you can limit the spread of the infection," Marsolo said.

As far as a long-term "wish list," clinicians could possibly restore a normal intestinal environment in patients with an off-balance microbiome through targeted probiotics or even microbiome transplants.

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

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

Project Lead: Keith Marsolo, Ph.D., Cincinnati Children's Hospital Medical Center
Research Title: Novel techniques for identifying patients at risk for invasive infection via fecal metagenomics
Funding Source: Cincinnati Children's Hospital Medical Center
Website: cincinnatichildrens.org/bio/m/keith-marsolo

Metagenomic Data

Hamilton: Bacteria, archaea key to the persistence of complex life

While many of earth's species have come and gone throughout billions of years of changing environment, its oldest inhabitants have somehow managed to evolve and adapt, despite their simplistic structure.

The oldest forms of life on Earth, bacteria and archaea, have managed to evolve and adapt to Earth's changing environment over billions of years. As a result, bacteria and archaea could hold the answers to the persistence of complex life. Trinity Hamilton, assistant professor of biological sciences at the University of Cincinnati, is searching for answers in caves, hot springs and glaciers as she processes the metagenomic data of these microbial communities through the Ohio Supercomputer Center.

Two of the basic building blocks of life, carbon and nitrogen, seem to be plentiful on Earth, but these elements are actually unavailable for use by most organisms until microorganisms transform them into biologically available sources that our bodies can process. Hamilton is studying communities of these microorganisms and how they facilitate nutrient flow within small-scale environments.

"These are the kinds of things that happen on a much larger scale, and we don't fully understand them, so we've picked a more simple community to start to understand why these communities coexist," Hamilton said.

Hamilton and her team traveled to the Pacific Northwest to gather samples of supraglacial organisms that thrive on top of the ice and snow. While they knew carbon fixation, the process of converting inorganic carbon to organic carbon compounds, was occurring within these communities, they wanted to know which members of the communities were responsible. There are very few nutrients in ice and thus light might serve as the dominant form of energy, fueling photosynthesis. They are also studying samples of nitrogen-fixing organisms from hot springs in Yellowstone National Park.

On the darker side of things, the team is studying organisms that are found in caves where carbon and nitrogen cycling occur in the absence of light.

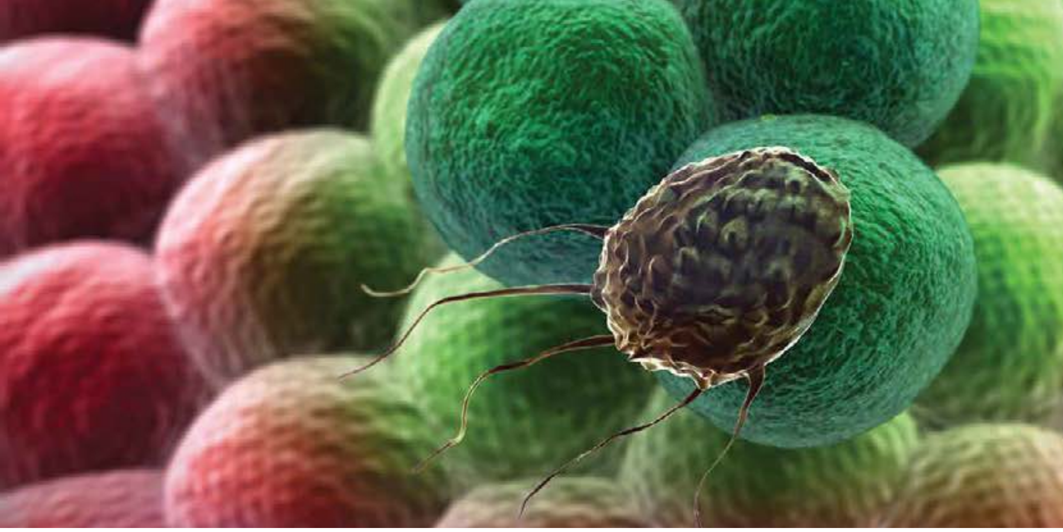
"This is very unique," Hamilton said. "There's no photosynthesis, which is one of the major sources of energy for ecosystems today."

Using high performance computing, Hamilton and her team look at all the functional genes encoded by these microbial communities with next generation sequencing. This gives them a fingerprint for bacteria and archaea, providing a better look at how these communities function to provide energy to the surrounding environment.

"This data, in combination with high resolution geochemical and geological data from natural systems, will aid in elucidating the role of biology in planetary evolution," Hamilton said. •

Sunset on Collier Glacier on the mountain of North Sister in Oregon.

Project Lead: Trinity Hamilton, Ph.D., University of Cincinnati
Research Title: Using next-generation sequencing to examine the global consequences of biogeochemical cycling
Funding Source: University of Cincinnati
Website: artsci.uc.edu/faculty-staff/listing/by_dept/biology.html?eid=hamiltt4&thecomp=uceprof



Targeted Therapies

Roychowdhury, team advise physicians on individualized treatment

"There is no routine cancer."

The powerful slogan of The Ohio State University Comprehensive Cancer Center – James Cancer Hospital and Solove Research Institute is a testament to the recent paradigm shift in the field of oncology. For years, a patient's cancer and treatment were characterized by location and stage. Now, researchers such as those in Dr. Sameek Roychowdhury's lab at OSUCCC – James are looking at tumors on a molecular level to understand the nuances in each individual's cancer. By processing genetic sequencing data through the Ohio Supercomputer Center, Roychowdhury and his team can advise physicians and patients on targeted, novel therapies for treatment.

When patients initially receive a cancer diagnosis, they are given the standard of care for their cancer type. If the standard of care fails and the tumor continues to grow or the cancer spreads, physicians often turn to clinical trials for more treatment options. Roychowdhury and his team are attempting to match patients with the most appropriate clinical trial, based on their genomics biomarkers.

"There are a lot of studies that require what we call molecular eligibility," said Julie Reeser, Ph.D., a clinical research coordinator with the Roychowdhury Lab. "So instead of being grouped by cancer, you're grouped by a genetic alteration that you have."

The lab performs a biopsy on tissue from referred patients either looking for the best clinical trial option or who have selected a trial and want to compare with results after treatment. Researchers use next generation sequencing, looking at 300 different genes and the changes that occur to these genes during treatment. They run this data through the supercomputer to be analyzed. Researchers then compare the cell line before it became resistant to a certain therapy and after to inform decisions on the next course of treatment for a patient. Though the pharmacological purpose of this study is ongoing, researchers are hoping to better understand why tumors develop resistance to certain drugs and to identify the driving mutations that provide molecular eligibility for targeted therapies.

"All the information helps other patients in some way," Reeser said. "The more we learn about it, the more discoveries we can make."

While clinical trials enroll patients for whom the standard of care was not successful, physicians can use the genetic information of patients with certain types of cancer to inform standard-of-care procedures. For these cancer types, there are certain genes that are known to have mutations that cause tumor growth, and so they can be treated with targeted therapies. These "smart drugs," as Reeser called them, are becoming more prevalent, but more research is needed on many different tumor types before they become the dominant therapy. The data collected in the Roychowdhury Lab will help inform this research. •

(Above left) Photo credit: Nihaochan (Own work) [CC BY-SA 4.0], via Wikimedia Commons

Project Lead: Sameek Roychowdhury, M.D., Ph.D., The Ohio State University
Research Title: Translational cancer genomics to characterize resistance to targeted therapies
Funding Source: The Ohio State University
Website: precisioncancermedicine.osu.edu

Advanced Materials

Ohio is proud to be known as a manufacturing powerhouse, backed by those using computational modeling for advanced materials research. Nanophysics, magnetic properties and HCP alloys are just a sampling of the advanced materials research projects OSC supports.

Magnetic Control

Windl group determines heat can be regulated by magnetic fields

Phonons — the elemental particles that transmit both heat and sound — have magnetic properties, according to a landmark study conducted by a research group from The Ohio State University and supported by the Ohio Supercomputer Center.

In the journal *Nature Materials,* the researchers describe how they employed a magnetic field to reduce the amount of heat flowing through a semiconductor by 12 percent. Simulations performed later at OSC identified the reason—a magnetic field induces a diamagnetic response in vibrating atoms known as phonons, which changes how they transport heat.

Heat and sound are both expressions of the same form of energy, quantum mechanically speaking. So any force that controls one should control the other.

"This adds a new dimension to our understanding of acoustic waves," said Joseph Heremans, Ph.D., Ohio Eminent Scholar in nanotechnology and a professor of mechanical engineering at Ohio State. "We've shown that we can steer heat magnetically. With a strong enough magnetic field, we should be able to steer sound waves, too."

The nature of the effect of the magnetic field initially was not understood and subsequently was investigated through computer simulations performed on OSC's Oakley Cluster by Oscar Restrepo, Ph.D., a research associate, Nikolas Antolin, a doctoral student and Wolfgang Windl, Ph.D., a professor, all of Ohio State's Department of Materials Science and Engineering. After painstakingly examining all possible magnetic responses that a non-magnetic material can have to an external field, they found the effect is due to a diamagnetic response, which exists in all materials.

The implication: In materials such as glass, stone, plastic—materials which are not conventionally magnetic—heat can be controlled magnetically if you have a powerful enough magnet. This development may have future impacts on new energy production processes.

"OSC offered us phenomenal support; they supported our compilation and parallel threading issues, helped us troubleshoot hardware issues when they arose due to code demands, and moved us to the Lustre high-performance file system," said Antolin, the expert for high-demand computations in Windl's group. Next, the group plans to test whether they can deflect sound waves sideways with magnetic fields.

Coauthors on the study included graduate student Hyungyu Jin and postdoctoral researcher Stephen Boona from mechanical and aerospace engineering; and Roberto Myers, Ph.D., an associate professor of materials science and engineering, physics and mechanical and aerospace engineering. •

An artist's rendering of a phonon heating solid material demonstrates research findings proving that acoustic phonons — the elemental particles that transmit both heat and sound — have magnetic properties.

Project Lead: Wolfgang Windl, Ph.D., The Ohio State University
Research Title: Phonon-induced diamagnetic force and its effect on the lattice thermal conductivity
Funding Source: U.S. Army Research Office, U.S. Air Force Office of Scientific Research, National Science Foundation
Website: windlgroup.engineering.osu.edu

Alloy Deformation

Ghazisaeidi studies HCP alloys for theoretical, industrial applications

The compelling need for energy efficiency in the transportation industry provides a strong motivation for the increased use of lightweight engineering materials such as titanium and magnesium alloys that will lead to weight reduction.

A majority of common metals have one of three different crystalline structures, based upon certain attributes of the metal's basic unit cells, which contribute different physical properties to each classification of structure. Some metals are ductile but very soft, others are less ductile but stronger, while still others are very strong but brittle. This last set is known as Hexagonal Close Packed, or HCP, and includes metals such as titanium, magnesium, cobalt, zinc and zirconium. A mixture of different metals, creating an alloy, yields an even different set of properties.

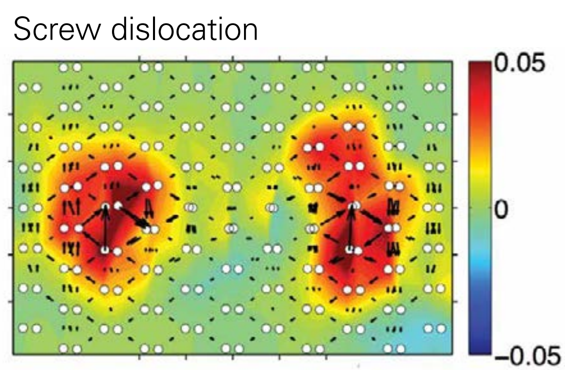
"Increasing both strength and ductility is the ultimate achievement for most structural materials," said Maryam Ghazisaeidi, Ph.D., an assistant professor of Materials Science and Engineering at The Ohio State University, who is leading a study of deformation in HCP alloys. "Traditional methods for strengthening rely on controlled generation of internal defects, and thereby increase strength at the cost of reducing ductility and toughness."

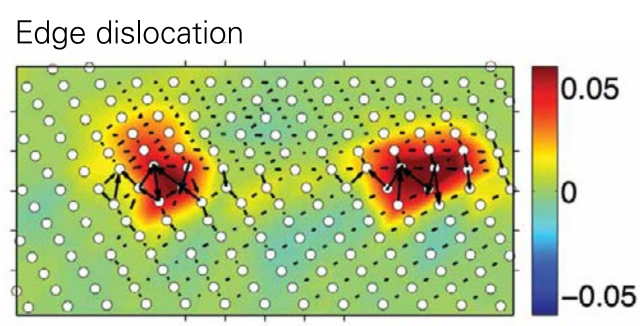
Various levels of ductility are observed in HCP metals and their alloys: from extensive ductility in titanium and zirconium to poor ductility in magnesium, zinc and beryllium. Ghazisaeidi believes understanding the mechanisms behind this divergent behavior is important from both theoretical and industrial application points of view.

"We aim to provide a scientific basis for a quantitative and systematic approach to design the strength and ductility of magnesium and titanium alloys through favorable alloying," she said. "The approach is based on electronic structure calculations of various deformation modes, including slip and twinning with an accurate account for chemistry change due to alloying."

The calculations are being performed on the HP/Intel Oakley Cluster at the Ohio Supercomputer Center by way of the density functional-theory code VASP, short for Vienna Ab initio simulation package. Electronic structure calculations of dislocations typically require large simulation sizes and accurate treatments of boundary conditions.

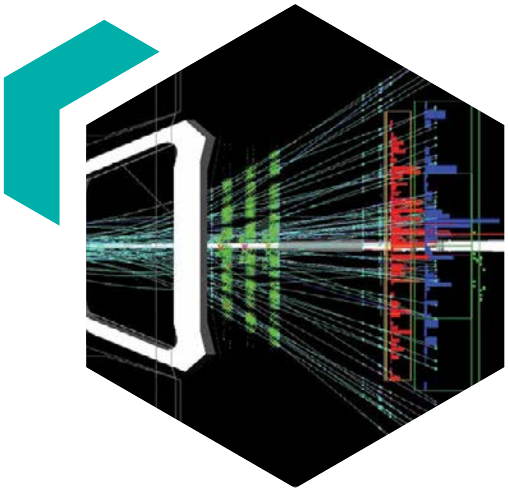
"Existing approaches to modeling material behavior generally rely on phenomenological constitutive relations that must be calibrated experimentally and therefore lack predictive capability," she explained. "Connecting the accurate atomic-scale study of deformation to the overall mechanical properties will potentially transform alloy design by replacing the trial and error approaches with quantitative predictive models." •

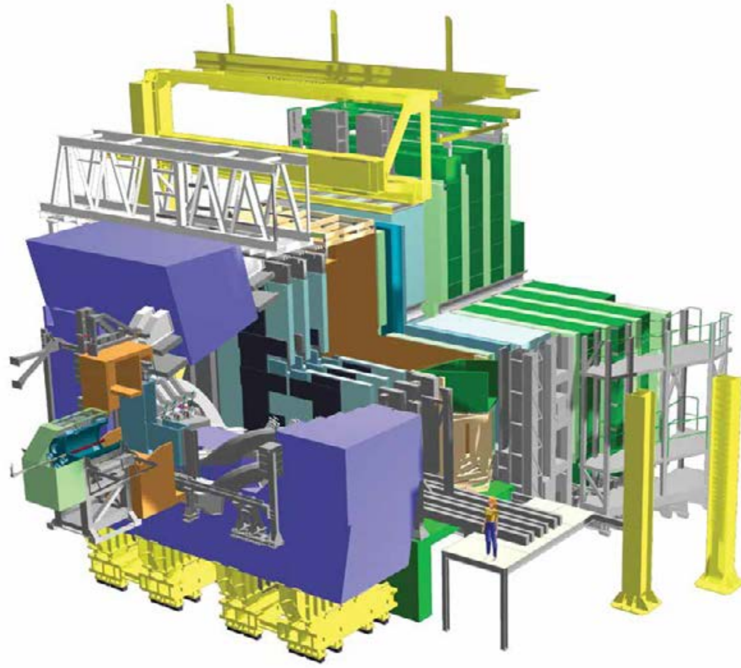




A study led by Maryam Ghazisaeidi, Ph.D., is investigating whether quantitative predictive models could replace existing trial-and-error approaches to modeling material behavior in hexagonal close packed metals and their alloys.

Project Lead: Maryam Ghazisaeidi, Ph.D., The Ohio State University
Research Title: First principles study of deformation mechanisms in HCP alloys
Funding Source: The Ohio State University
Website: u.osu.edu/ghazisaeidi.1/people





Flavor Physics

Sokoloff, fellow scientists chase post-Higgs questions with collider

The quest to understand the fundamental building blocks of nature and their interactions is one of the longest-running and most ambitious of human endeavors.

With the discovery of the Higgs Boson and other significant observations within the past decade, the Standard Model (SM) of sub-atomic particle physics has been validated as an accurate mathematical description of the strong, weak and electromagnetic forces.

However, Michael Sokoloff, professor of physics in the McMicken College of Arts and Sciences at the University of Cincinnati, is using Ohio Supercomputer Center services to help answer some of the remaining and, quite possibly, most interesting questions in the field:

"Why does nature express the symmetries embodied in the SM, and not other equally elegant symmetries? Why are there (even, are there) exactly three generations of basic building blocks (quarks and leptons)? Why are the masses of these building blocks so different from each other, both within a generation and between generations? What is the dark matter that pervades the universe? Does space-time have additional symmetries or extend beyond the three spatial dimensions we know? Are neutrinos, whose only SM interactions are weak, their own anti-particles?"

One of two principal paths used to address these questions at Europe's Large Hadron Collider is the LHCb experiment, where scientists study very high-mass particles, called quarks. These particles exist in six variations known as flavors, whimsically referred to as up, down, charm, strange, top and bottom, although the latter two are also known as truth and beauty. Currently the foremost flavor experiment in the world, LHCb will run for the next decade and involves more than 650 physicists representing 65 different universities and laboratories.

"We are using the LHCb detector to study the interactions of composite particles containing heavy quarks created by protons colliding with other protons," explained Sokoloff. "Large Monte Carlo samples of simulated data are required both for planning future operations of the experiment and for analyzing data after it is acquired."

Sokoloff requested 600,000 units of computational and storage resources on OSC's Oakley Cluster for LHCb collaborators. These resources should be sufficient to help Sokoloff and his colleagues understand how to optimize detector design and data selection strategies before data collection begins and how to understand the data they collect after the fact—all prerequisites to answering "the most interesting questions in physics." •

(Above left) The LHCb detector observes a proton-lead ion collision. (Above right) Each part of the LHCb specializes in measuring different characteristics of the particles produced by colliding protons. Collectively, each component gathers information and can single out particles that spray out from the collision point.

Project Lead: Michael Sokoloff, Ph.D., University of Cincinnati
Research Title: Flavor physics using the LHCb detector
Funding Source: National Science Foundation
Website: artsci.uc.edu/departments/physics/research/particle_experiment.html

The Kondo Effect

Ulloa research team investigates impact on quantum dots, valleytronics

Several years ago, a Physics World article posed the question, "Why would anyone still want to study a physical phenomenon that was discovered in the 1930s, explained in the 1960s and has been the subject of numerous reviews since the 1970s?"

Leveraging Ohio Supercomputer Center services, physicist Sergio Ulloa is doing just that—studying a well-known anomaly in condensed matter systems. These systems explain subtle physical aspects of phenomena as they change from one form, or phase, to another, such as melting ice.

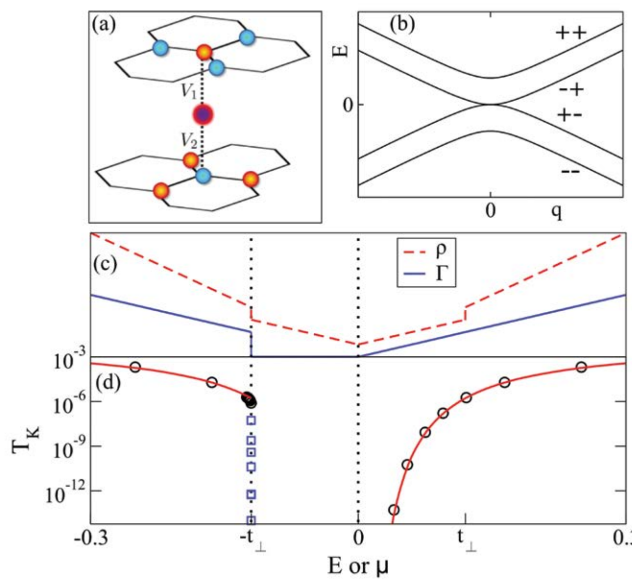
According to the article, this anomaly "arises from the interactions between a single magnetic atom, such as cobalt, and the many electrons in an otherwise non-magnetic metal." Over the years, scientists have found this very complex scenario, known as the Kondo effect, difficult to represent mathematically.

In 1933, Dutch physicist Wander Johannes de Haas and co-authors reported an unexpected rise in the resistivity of some gold samples at low temperatures. About 30 years later, in 1964, Japanese physicist Jun Kondo identified the cause of the phenomenon that was to bear his name. In 1974, Nobel Prize Winner Kenneth Wilson was able to first solve the Kondo model with a technique known as the numerical renormalization group, which Ulloa's group now employs.

"The appearance of different experimental systems and characterization techniques have resulted in a dramatic revival of the field in the last 10 years," explained Ulloa, professor of physics and astronomy at Ohio University. "Our theoretical and computational efforts continue studies of more challenging systems of increasing relevance to experiments. We explore new issues that arise as one is able to better control where and how the Kondo effect is produced."

Ulloa's research group is now studying the Kondo effect on systems involving quantum dots, tiny semiconducting "droplets" that can hold from one to a few electrons in a controllable manner and act then as man-made atoms. These and other quantum dots possess unique electronic properties and are employed in transistors, solar cells, LEDs and diode lasers. Metallic dots are also being studied for use in medical imaging and treatment.

Ulloa and his colleagues are also investigating how the Kondo effect impacts atom-electron interactions in other materials, such as molybdenum disulfide. These materials possess crystal symmetries that result in energy "valleys" that can be used to channel the flow of charge in a particular way. Trapping electrons within one valley or another might be used as a switch for "valleytronic" devices. •

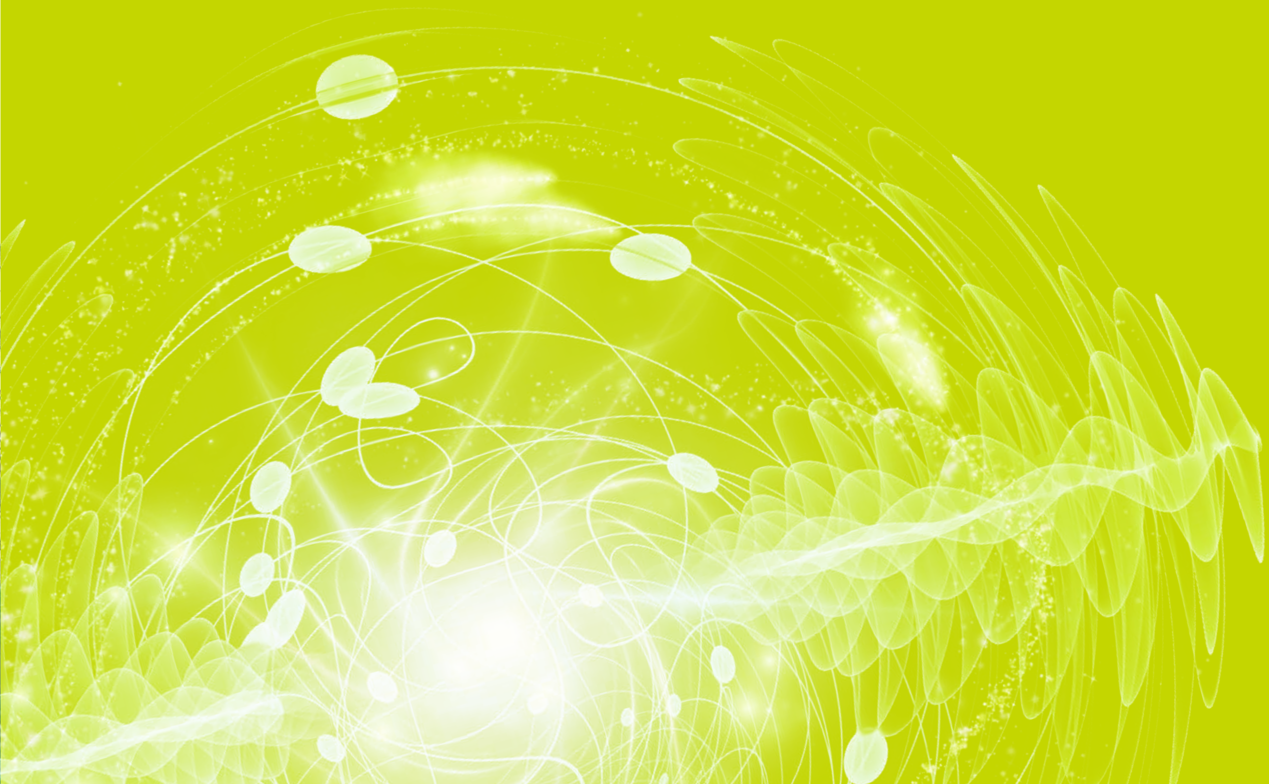


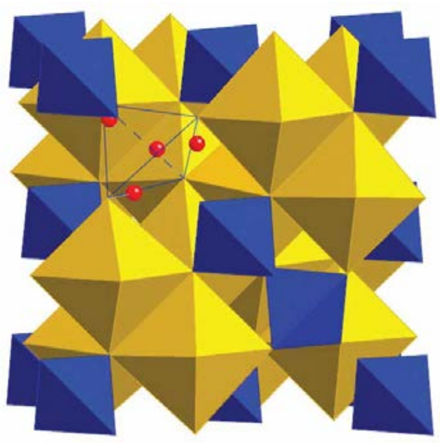
A research group led by Professor Sergio Ulloa, Ph.D., at Ohio University is studying quantum phase transitions into Kondo states by producing a magnetic impurity within a sample of graphene film two molecules thick. Here, the researchers model the lattice structure and diagram various properties of the graphene sample.

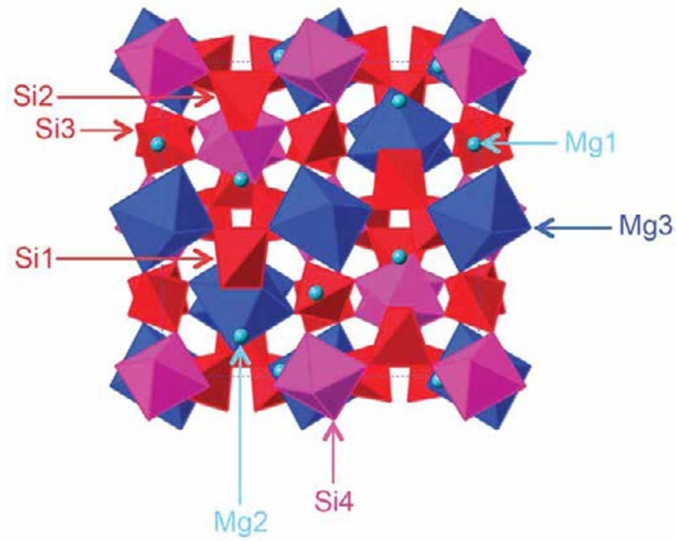
Project Lead: Sergio E. Ulloa, Ph.D., Ohio University
Research Title: Quantum phase transitions in Kondo systems
Funding Source: National Science Foundation
Website: ohio.edu/people/ulloa/News/News.html

Energy & Environment

The research featured on the following pages covers the ground hundreds of kilometers below us, satellites thousands of feet in the sky and the energy potential pulsing through the air around us. The Ohio Supercomputer Center meets the demands of energy and environment researchers as they model, simulate and analyze their way to improving our world.







Mineral Reservoirs

Panero group concludes earth's mantle holds vast amounts of water

Water, water everywhere, but it's all locked underground.

Wendy Panero, Ph.D., and The Ohio State University Mineral Physics Research Group have found that minerals within the earth's mantle hold a vast amount of water. The group is using Ohio Supercomputer Center resources to discover where and how much of this water could exist.

Panero's team focuses on the hypothesis that the earth created its own water. Hydrogen atoms are locked within solid minerals in the earth's mantle. Chemical reactions allow these hydrogen atoms to bond with oxygen, creating water molecules. Panero's team is using supercomputers to model the structure of these minerals and the energy cost of incorporating hydrogen atoms. They can then calculate how much hydrogen likely exists in a mineral as a function of pressure and temperature.

Researchers predict that the mass of water stored in the earth's mantle is approximately 50 percent greater than that on earth's surface.

"It's a lot of water," Panero said. "And it's completely inaccessible to humans—the earth has to give us the water from that depth through plate tectonics."

Many minerals undergo structural changes between 410 and 660 kilometers deep due to heat and pressure. If they contain more water than the new minerals can store, the rocks should melt at these depths, Panero said.

"What is kind of enchanting to think about, yet really difficult to look at in detail, is that those minerals that are stable between that 410 and 660 kilometer depth range can take on a huge amount of water," Panero said.

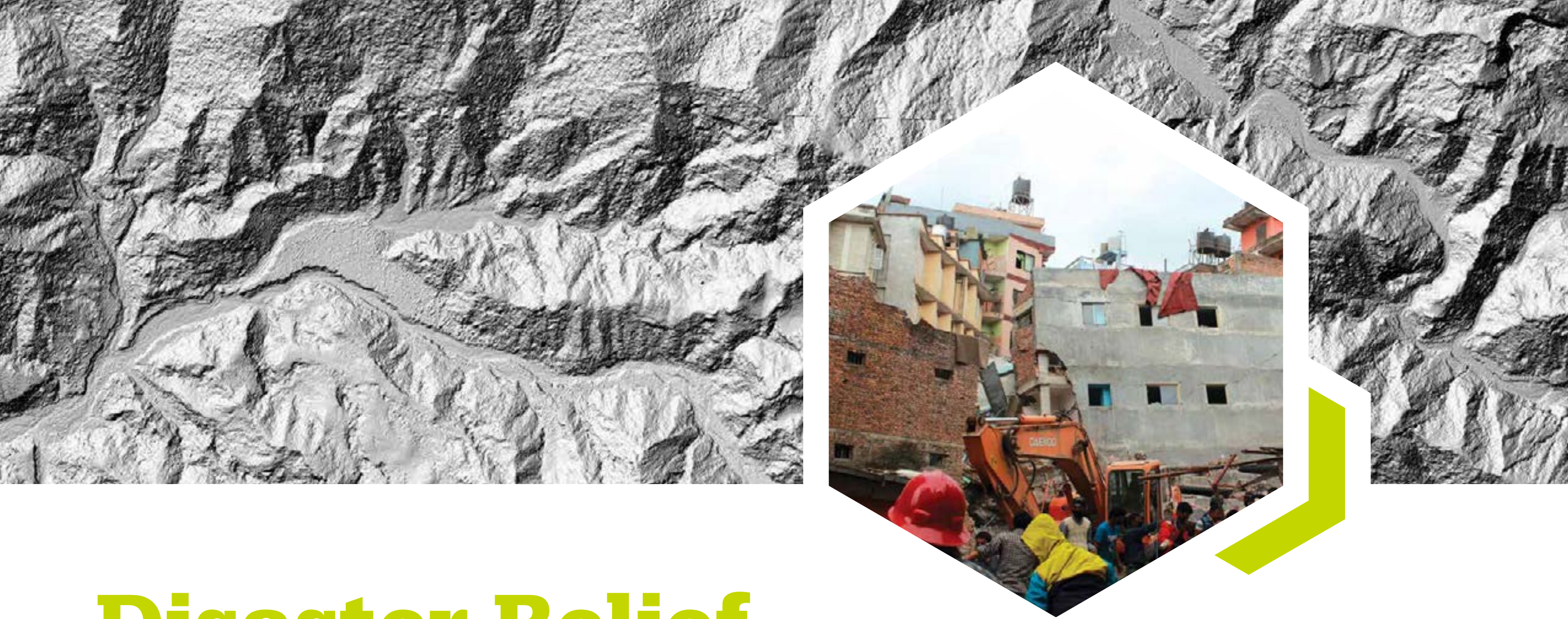
Panero's group has found that the minerals garnet and the lesser-known ringwoodite have the greatest potential to store water in the earth's mantle at 660 kilometers deep. Ringwoodite is the dominant mineral in the mantle at these depths and, luckily, can be synthesized in the lab. Garnet is of interest due to its stability in the earth's mantle down to 750 kilometers.

"The amount of water that garnet holds at that depth is going to be what tells us exactly how much water is in the earth because new data show us that the earth's mantle might be melting at 750 kilometers depth," Panero said.

The implications of this study extend out of this world. If hydrogen is a key ingredient for Earth, it could exist within the interior of other planets. Studies have suggested that water existed on the surface of Mars, but there is no explanation of its origins. Perhaps, trapped deep beneath the surface, the key to life exists. •

(Above) Atomic structure of ringwoodite calculations done with the Ohio Supercomputer Center. The red balls are hydrogen atoms surrounding the site of a missing silicone atom. The blue polyhedra are SiO_4 atoms and MgO_6 atoms are yellow polyhedra.

Project Lead: Wendy Panero, Ph.D., The Ohio State University
Research Title: Water partitioning at the base of the transition zone: No need for a lower mantle water filter
Funding Source: National Science Foundation
Website: u.osu.edu/panero.1



Disaster Relief

Howat, others transition glacier mapping to earthquake assistance

Researchers who normally use high-resolution satellite imagery to study glaciers used their technology 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—are working quickly to produce high-resolution, 3-D digital surface maps for use in the Nepali relief effort. The Ohio Supercomputer Center is providing 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."

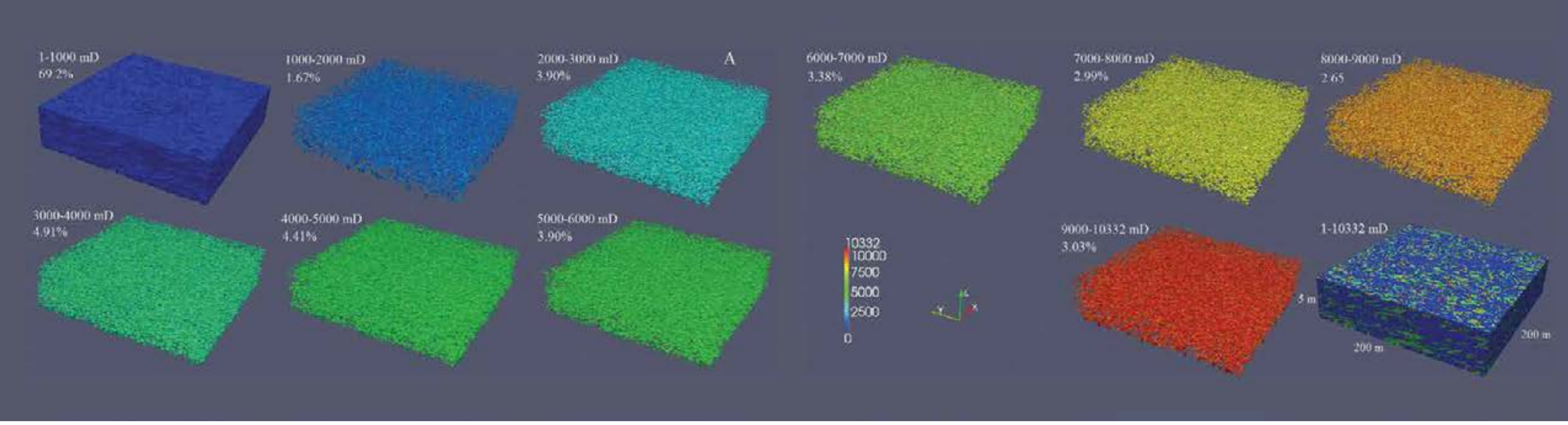
"To support this effort, we have granted the SETSM team priority queuing and an emergency allocation of up to 60,000 core hours for use of our flagship supercomputer system, the Oakley Cluster," said Brian Guilfoos, HPC Client Services Manager at the Ohio Supercomputer Center.

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 will distribute 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, starting this week, 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. •

(Above) A small section of a high-resolution shaded relief image of the Kathmandu Valley produced by Ian Howat and his colleagues following the April 2015 earthquake in Nepal.

Project Lead: Ian Howat, Ph.D., The Ohio State University
Research Title: Nepal earthquake elevation model
Funding Source: National Aeronautics and Space Administration
Website: u.osu.edu/setsm/author/howat-4



Carbon Injection

Ritzi, Gershenzon analyze safety of underground CO_2 sequestration

The Department of Energy supports pilot projects and basic research that evaluate the feasibility of capturing carbon dioxide created by industrial processes and power plants and injecting it into deep geologic formations for permanent storage, known as geo-sequestration.

This is part of evaluating strategies for reducing atmospheric emissions and mitigating accumulation of greenhouse gasses.

Robert Ritzi, Ph.D., Naum Gershenzon, Ph.D., and David Dominic, Ph.D., from Wright State University are studying the movement of CO_2 in the earth's subsurface to help inform this process for the Department of Energy and environmental industries.

In geo-sequestration, CO_2 is injected into underground reservoirs as a supercritical fluid, a substance with pressure and temperature above the liquid and gas phase separation point. After injection, it rises under buoyant forces. At the top of most reservoirs where CO_2 injection occurs is an impermeable seal or cap rock, which traps CO_2 until it dissolves or mineralizes. The integrity of the seal could be compromised by an undetected fault or fracture in the cap rock, so industry professionals look for additional mechanisms for trapping the CO_2. A number of candidate CO_2 reservoirs comprise sedimentary rock laid down by ancient rivers.

"It's not a new idea, but there is need for scientific qualification—what happens," Gershenzon said. "We want to be sure that this CO_2 will never affect groundwater and never goes back into the atmosphere."

Through three-dimensional models and flow simulations run through the Ohio Supercomputer Center, the researchers are showing that differences in the size of grains within this type of sedimentary rock cause capillary trapping of the CO_2 before it ever reaches the cap rock, providing added insurance that the CO_2 is permanently stored.

"What our research is showing is that the plume is being almost entirely, if not entirely, trapped by this residual trapping process in the reservoir, and the carbon dioxide is getting trapped even before it makes it to the seal, so that's a good thing," Ritzi said.

Their research has relevance in other areas. Facing an incessant demand for oil, the United States has recovered much of its easily accessible with traditional gravity drainage methods. To extract more oil, water and CO_2 are injected into oil reservoirs to sweep oil to the production well, in a process known as enhanced oil recovery, or EOR. The Wright State reservoir simulations are illuminating how formations in sedimentary rock affect flow patterns during EOR, providing insight into optimal strategies for improving oil recovery. A CO_2 sweep could end by leaving the injected CO_2 underground for permanent storage. •

(Above) Hydraulic properties of reservoirs vary with different sediment types and have highly non-linear relationships with the amount of water and oil saturation, requiring high performance computing to help solve the problem.

Project Lead: Robert Ritzi, Ph.D., Wright State University
Research Title: High performance computing to understand multiphase flow and capillary trapping processes in multiscaled and hierarchical sedimentary reservoirs
Funding Source: U.S. Department of Energy
Website: wright.edu/~robert.ritzi/research.html

Reactor Prototypes

Sun research team ponders odds of accident caused by air ingress

Compared to its centuries-old fossil fuel counterparts, nuclear power is a young player in today's energy sources.

Still, since the world's first nuclear power plant became operational in 1954, there have been three marked generations of nuclear technology. With the fourth on the horizon, nuclear engineers are designing a suite of safe, efficient and innovative systems, which they estimate to be operational within 15 years. Xiaodong Sun, Ph.D., associate professor at The Ohio State University's Nuclear Engineering Program, is ensuring one of these new systems is as safe as possible, using high performance computing resources to test prototypes.

One of the most promising Generation IV power plant designs is the Very High Temperature Reactor. Nuclear designers favor the helium-cooled, graphite-moderated VHTR design because of its inherent safety characteristics: helium is inert and remains a gas while the graphite core maintains structural stability at high temperatures. Though touted as one of the safest nuclear reactor designs, one variable could compromise this: air ingress. Previous studies have shown the graphite structure could lose up to 25 percent of its strength and 4.5 percent of its density due to an air-ingress event. Sun's work focuses on the impacts of air ingress to determine if the issue can be mitigated.

"Computer models have been developed to analyze this type of accident scenario," Sun said. "There are, however, limited experimental data available to understand the phenomenology of the air-ingress accident and to validate these models."

To test the phenomenon, Sun and his team, Emeritus Professor Richard Christensen, Ph.D., Doctoral Candidate David Arcilesi and Tae Kyu Ham, Ph.D., constructed a one-eighth-scale test model of part of a VHTR reactor system. Using ANSYS FLUENT, a computational fluid dynamics software tool, Sun simulates the air-ingress phenomenon through Ohio Supercomputer Center resources. The model facility will duplicate these FLUENT runs and the data obtained should validate the computational calculations.

So far, Sun's team has found the model provides reliable data, closely resembling the air-ingress accident that might occur in a full-sized prototype VHTR. They are currently testing the two modes of air ingress to determine under which conditions each could dominate. This information will be used to improve VHTR prototype designs and accident mitigation. Generation IV designs will maintain today's high level of safety while shifting from the current paradigm of mastering accidents to excluding accidents entirely. •

(Above) A one-eighth-scale test model of part of a very high temperature reactor system, including graphite core structures. So far, the model provides reliable data resembling true-to-life air-ingress accident scenarios.

Project Lead: Xiaodong Sun, Ph.D., The Ohio State University
Research Title: Computational analysis of air-ingress phenomenon in very high-temperature gas-cooled reactors
Funding Source: The Ohio State University
Website: mae.osu.edu/people/sun.200

Research Landscape

If you were to dive into the belly of a supercomputer, you would find yourself surrounded by a myriad of topics and results, like the swirling pages of a disassembled encyclopedia. The Ohio Supercomputer Center supplies strength to Ohio's basic and applied research across an impressive array of fields. Take a trip through the following pages for a sampling of what high performance computing can support.

Dark Matter

Peter, Kim comparing theoretical properties, observational evidence

To begin understanding dark matter in astrophysics, one must first step into a world where galaxies are considered small.

The is the world that Annika Peter, Ph.D., and graduate student Stacy Kim are discovering more fully at The Ohio State University's Center for Cosmology and AstroParticle Physics. Their research could better define the substance that comprises over a quarter of the universe.

While the particles that make up gases and stars are well known, scientists do not know what makes up dark matter—only that these are new, undefined particles. The dominant hypothesis is dark matter is made up of weakly interacting massive particles, or WIMPs. However, 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 its properties, astrophysicists look at how dark matter might interact with itself. Dark matter is gravitationally attractive and, by the WIMP theory, should settle into dense clumps. After observing the movement of stars within galaxies, researchers noticed stars were not orbiting as quickly as they should if dark matter were stable, as the WIMP theory suggests.

Peter and Kim are exploring a model called self-interacting dark matter. To do this, they are researching the "stickiness" of dark matter—if dark matter particles can collide with each other. To test the theory of collisionality, Kim is virtually smashing galaxy clusters together through the use of the Ohio Supercomputer Center.

"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.

Kim observes how dark matter and galaxies move when two galaxy clusters with equal mass collide. By looking at the distribution of galaxies and dark matter after a collision, Kim may be able to determine how "sticky" dark matter is.

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

"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. •

(Above right) 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.

Photo credit: NASA, ESA, and the Hubble SM4 ERO Team

Project Lead: Annika Peter, Ph.D., The Ohio State University
Research Title: Investigating the collisionality of dark matter with simulations of merging galaxy clusters
Funding Source: National Aeronautics and Space Administration
Website: physics.osu.edu/people/peter.33

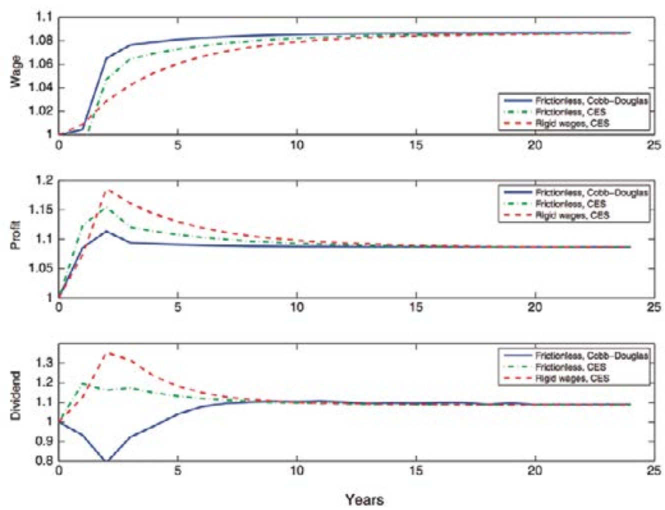
Market Performance

Lin, Favilukis partner to model equity premium puzzle adjustments

In most of the standard equilibrium models used to explain equity market performance, the volatility of stock market returns is far too low.

This muted volatility is closely related to the equity premium puzzle, a phenomenon whereby returns on "risky" stocks are historically much higher and more volatile than returns on "safer" government bonds.

Researchers are looking for ways to adjust the standard models to address these puzzling facts regarding the fluctuating prices of financial assets, such as aggregate stock market, portfolios with certain characteristics, etc. Xiaoji Lin, Ph.D., an assistant professor of finance at the Fisher College of Business at The Ohio State University, and Jack Favilukis, Ph.D., an assistant professor of finance at the University of British Columbia's Sauder School of Business, are leveraging Ohio Supercomputer Center resources to better understand and address some of these riddles.



"A seemingly unrelated characteristic of these models is that wages are too volatile and too highly correlated with output," explained Lin. "We show that the failure to match wage dynamics is closely related to the failure to explain financial data. Introducing sticky wages—a factor that accounts for workers' earnings adjusting slowly to changes in labor market conditions—brings the model close to the data for these diverse financial phenomena. To our knowledge, we are the first to capture quantitatively such a wide array of financial moments in a reasonably calibrated general-equilibrium model."

By introducing wage rigidity, Lin and Favilukis found they could greatly improve the model's ability to match financial data quantitatively. Within standard models, they feel, wages are far too volatile and procyclical relative to the data, and, therefore, act as a hedge for the firm's owners, making profits too smooth and dividends countercyclical. Thus, the equity volatility in the data is about four times that of standard models.

In Lin's adjusted model, the average wage is smoother because of infrequent wage resetting and a higher complementarity between labor and capital. Therefore, both profit and dividend behavior are similar to the data, and the volatility of equity returns is now 75 percent that of the data. The model addresses several other hard-to-explain features of financial data: high Sharpe ratios, low and smooth interest rates, time-varying equity volatility and premium, a value premium and a downward-sloping equity term structure. •

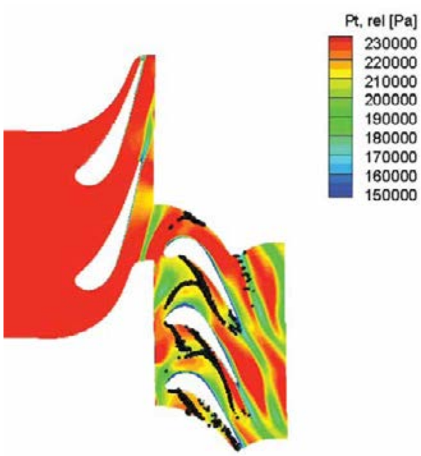
(Left) These plots illustrate the impulse responses of the aggregate wage, aggregate profit and aggregate dividend to a positive productivity shock that lasts one year.

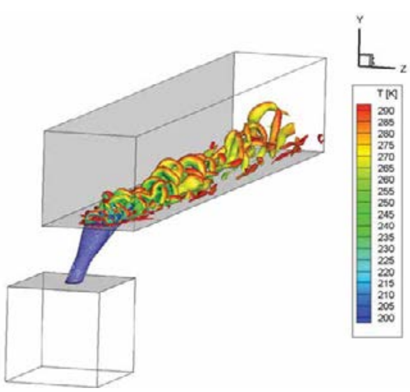
Project Lead: Xiaoji Lin, Ph.D., The Ohio State University
Research Title: Wage rigidity: A quantitative solution to several asset pricing puzzles
Funding Source: The Ohio State University – Fisher College of Business
Website: fisher.osu.edu/fin/faculty/lin

Jet Propulsion

Ameri group investigates dust's role in turbomachinery failures

For all the different moving parts that go into mechanical engineering systems, the gas turbine is a relatively simple design: a large rotor fitted with vanes is made to revolve by a fast-moving gas flow.





Perhaps then it could be expected that something as innocuous as dust can cause significant problems with the operation of these machines that provide propulsion for jet engines and power plants. A team of researchers at The Ohio State University is studying and modeling the deposition of particles on turbine passages to inform more reliable turbomachinery designs.

"Many of these questions are difficult to answer in the lab, so we simulate these phenomena," said Ali Ameri, Ph.D., a research scientist at Ohio State's department of mechanical and aerospace engineering.

Ameri and his team from the lab of Professor Jeffrey Bons, Ph.D., use the Ohio Supercomputer Center to run engine simulations using ANSYS FLUENT software as well as software the team has written.

Most engines are powered by combustion of fuel, usually petroleum or coal-based. The fuel is run through a high-pressure combustor, creating hot gas that flows at high speeds to rotate the turbine generating power. This power can be used to propel an airplane or generate electric power. The hot gas may contain particles of dust or ash, which can build up on the turbine blades and make them rough, increasing the heat transfer within the engine. These same particles can become lodged in cooling passages as well, interrupting the engine's ability to regulate internal temperatures and cool the turbine blades.

Using high performance computer simulations and software, Ameri and his team study everything from engine temperature and pressure to particle type and size to predict the most likely location of particle deposition within the turbines. Their work is helping to create more efficient engine models and designs that are less susceptible to the effects of unavoidable dust particles. While multiple iterations of their research have been published, their work is far from complete.

"It is ongoing work. As we learn what types of activities might affect the deposition, we include them in our models" Ameri said. "We are coming closer and closer to simulating this activity very well." •

(Left top) Simulation of flow through a turbine passage of a gas turbine showing the trajectory of ash particles. (Left bottom) Simulation of film cooling flow emerging from a shaped hole showing isosurfaces of temperature.

Project Lead: Ali Ameri, Ph.D., The Ohio State University
Research Title: Effect of hot streaks on ash deposition in an uncooled turbine vane passage
Funding Source: U.S. Department of Energy
Website: mae.osu.edu/people/ameri.1

Noise Generation

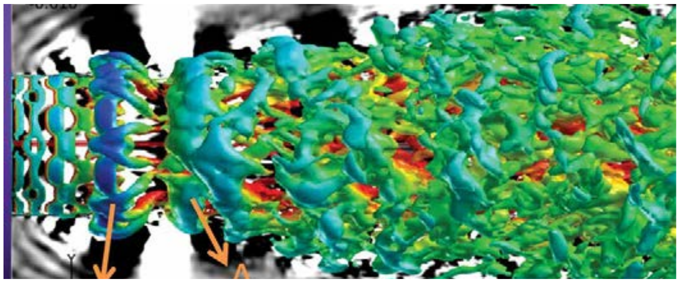
Gaitonde team modeling turbulent eddies within jet plumes

The noise from jet-engine exhausts can cause substantial hearing loss for crewmen and airport personnel and activate restrictive regulations and/or fees for airlines.

The large turbulent eddies within the jet plume—also known as large-scale coherent structures—produce the majority of the noise in the aft angles of the engine. However, the process by which these eddies generate noise is not well understood.

To gain insight into the noise-generation process, computational results from The Ohio State University's High Fidelity Computational Multi-Physics Lab (HFCMPL) are being coupled with experimental results from Ohio State's Aerospace Research Center (ARC). Plasma actuators at the jet exit are triggered at specific frequencies to create consistent large-scale coherent structures. This localization allows researchers to study the interaction of these structures with the surrounding air and the resulting noise signature.

Datta Gaitonde, Ph.D., a professor of mechanical and aerospace engineering at The Ohio State University and his team, are modeling excited jets using Large Eddy Simulations—a high-fidelity method of simulating time-accurate turbulent airflow—by leveraging the computing power of the Ohio Supercomputer Center's Ruby and Oakley Clusters.



"Our computational studies reproduced the experimental data very accurately," Gaitonde said. "But the real advantage of numerical results lies in their extraordinarily detail, which allows us to scrutinize the complex process by which coherent structures are generated and disintegrated to produce noise. This cannot be done in live experiments due to the invasive nature of measuring techniques that can obtain three-dimensional spatio-temporally resolved data."

Recent computations have shown the large-scale turbulent structures generated by the actuators are highly correlated to the near field i.e., the region immediately outside of the jet plume. Interactions between successive structures are quasi-linear and thereby result in a quasi-linear superposition of the resulting sound.

"Currently, to be able to further analyze the noise-generation process, we are focusing on the decomposition of the near field into acoustic components and non-noise fluctuations, also called hydrodynamic components," said Rachelle Speth, a graduate student working on the study with Gaitonde at HFCMPL. "This insight should aid in the development of revolutionary new control strategies."

Current interests of researchers at HFCMPL include jet noise, shock wave-turbulent boundary-layer interactions, scramjet flow paths in hypersonic flight and flows past wings. •

(Left) Simulations of flow and the resulting near-jet region help give Gaitonde's research team a visual understanding of phase-averaged pressure probes. Here, the white waves correspond to an increase in pressure, while the black waves correspond to a decrease in pressure.

Project Lead: Datta Gaitonde, Ph.D., The Ohio State University
Research Title: Near field pressure and associated coherent structures of excited jets
Funding Source: Air Force Office of Scientific Research
Website: hfcmpl.osu.edu

Industrial Engagement

The Ohio Supercomputer Center has a legacy of supporting industrial research and is empowered to do so at a high standard. By using simulation-driven design, small- and mid-sized manufacturers can supplement their physical product prototyping with faster, economical computer simulations. OSC also has the resources and capability to support even the largest of customers, witnessed by its partnership with NASCAR.

Racing Behavior

NASCAR, TotalSim model aerodynamics to boost safety, performance

Drive a car not originally built for racing around an oval track at 200 mph for a couple of hours, and you should begin to understand why stock car drivers would want the latest and greatest information on things, such as how their car will handle in close traffic on a banked curve.

Eric Jacuzzi, an aerodynamics and vehicle performance engineer at the R&D Center for the National Association for Stock Car Auto Racing, commonly known as NASCAR, has turned to the Ohio Supercomputer Center (OSC) to help drivers better understand performance factors that must be controlled to keep them competitive and safe.

"NASCAR has always realized the importance of aerodynamics, with specific sets of rules for the various tracks that the series runs on," said Jacuzzi in an article for the U.K. magazine Racecar Engineering. "Understanding the aerodynamic behavior of the cars in traffic is crucial to ensuring the cars do not become overly aero sensitive and limit the racing quality."

NASCAR first dove into leveraging computational fluid dynamics (CFD) in 2012, turning to TotalSim USA, an engineering services provider in Dublin, Ohio. TotalSim is a stalwart partner of OSC industrial engagement programs and possesses valuable CFD experience in every professional racing series in motorsports.

"Eric was trained by TotalSim on our software stack and OSC usage so he can now operate independently with only occasional software and other support from TotalSim," said Ray Leto, president of TotalSim.

Jacuzzi performs most of his work through a TotalSim-customized version of the open-source CFD software package OpenFOAM, designing grids of 50–120 million polyhedral cells for a single car run. A recent study featured a stationary lead car with a second car in a variety of trailing positions. Jacuzzi performed a series of 46 simulations that generated 500 gigabytes of data. The study yielded important clues on a myriad of racing and competition-related issues, such as drag advantage, cornering performance, underbody downforce deficit and sideforce loss.

"NASCAR will continue to work on improving car aerodynamics, while considering what magnitudes of forces work best at specific tracks and for tire supplier Goodyear," Jacuzzi said. "... continuing on the path of scientific analysis and attacking the problem analytically will ultimately yield the best result for fans, drivers and the series as a whole." •

(Above) Depending on the track, NASCAR race speeds can average up to 200 mph. In order to view how cars handle in close traffic and on banked curves, NASCAR and TotalSim use simulation studies to view aerodynamics through a variety of trailing positions.

Project Lead: Eric Jacuzzi, National Association for Stock Car Auto Racing
Research Title: Sprint Cup car's aerodynamic characteristics both alone and in traffic, based on extensive mapping of multi-car CFD runs
Funding Source: NASCAR R&D Center
Website: linkedin.com/pub/eric-jacuzzi/8/894/99a

Automated Modeling

Via Honda SIMCenter, Soghrati seeks to simulate billions of elements

A $5 million gift from Honda R&D Americas Inc. prompted the April 2015 launch of a center for virtual simulation and modeling of product performance and manufacturing processes in the College of Engineering at The Ohio State University.

Researchers at the Simulation Innovation and Modeling Center, or SIMCenter, research and apply computer-aided engineering techniques in the six identified thrust areas: solid mechanics, fluid mechanics, digital manufacturing, multi-physics, system integration and optimization. The Ohio Supercomputer Center provides the SIMCenter with co-location services and its researchers with access to high performance computing storage systems.

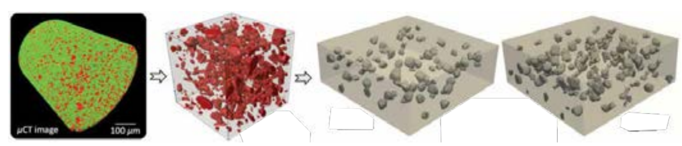
One Ohio State faculty member already leveraging the services of OSC and the SIMCenter, Soheil Soghrati, Ph.D., an assistant professor of mechanical and aerospace engineering as well as materials science and engineering, is studying the development and implementation of new numerical techniques for the automated modeling of problems with complex forms and structures, or morphologies.

"The finite element method (FEM), is one of the most widely used numerical techniques for the analysis and computational design of engineering structures and materials systems," Soghrati said. "With advanced methodologies, researchers can significantly decrease the development time of the computational model, which reduces both the labor cost and the probability of human error during this process. Moreover, for problems such as heterogeneous and composite materials, the intricate microstructure of the problem can prohibit the straightforward application of FEM."

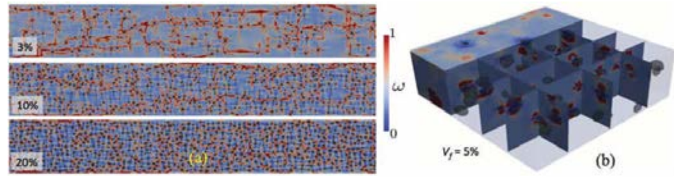
The first step of Soghrati's approach was to implement a more advanced numerical technique that sidestepped the burden of creating conforming finite element meshes, where adjacent elements share a whole edge or face forming the shape of the item being modeled. His research team recently developed a hierarchical interface-enriched FEM (HIFEM), which enables modeling multiphase problems with highly complex microstructures using finite element meshes that are completely independent of the shape.

The automated construction of HIFEM models, featuring up to 120 million elements, require the use of advanced computational geometry algorithms to determine the location of materials interfaces and evaluate the enrichment functions. The large number of geometric calculations required for creating such models cannot be treated efficiently without the parallel computing capacity, Soghrati explained. Thus, Soghrati's team developed a fully parallel computing paradigm for the automated treatment of such large-scale problems in multi-processor environments.

"The ultimate goal of this ongoing research is to further enhance the capability for automated modeling and simulation of problems with more than one billion elements," Soghrati said. •



Soheil Soghrati, an assistant professor at Ohio State University, is leading a study into the development and implementation of new numerical techniques for the automated modeling of problems with complex forms and structures, or morphologies. Two examples illustrate the application of his work: (above) a heterogeneous adhesive based on information extracted from micro-CT scans and (below) a heterogeneous adhesive depicted in 2D (left) and 3D (right) models, where ω indicates the extent of damage where 0=intact and 1=damaged.



Project Lead: Soheil Soghrati, Ph.D., The Ohio State University
Research Title: An automated computational approach for the treatment of problems with complex geometries
Funding Source: The Ohio State University
Website: acml.engineering.osu.edu

Turn-key Solution

Rescale delivers OSC high performance computing via the cloud

In the five years since inception, Rescale is making waves in the cloud-computing world.

With a team of industry thought leaders and domain experts, Rescale's high performance computing (HPC) cloud platforms combine leading engineering and science software with HPC hardware to provide users with a unified interface, enabling them to accelerate their analyses, leading to better product innovation.

Rescale has worked with the Ohio Supercomputer Center to make OSC resources available on-demand on the Rescale platforms. According to Tony Spagnuolo, vice president of sales at Rescale, "OSC provides some very unique capabilities and this turn-key solution available on Rescale's platform provides a compelling offering to commercial enterprises that are seeking greater agility and improved performance."

Founded in 2011 in the heart of San Francisco by Joris Poort and Adam McKenzie, Rescale has held true to its mission, "to provide highly powerful simulation platforms to the world's engineers, scientists, developers, CIO and IT professionals to develop innovative products, develop robust applications and transform IT into unified, agile environments."

Rescale is a company that delivers software platforms and hardware infrastructure to scientific and engineering companies focused on performing critical simulations. This hardware-software combination, which Joris and Adam developed from their experience as engineers within Boeing's 787 program, allows manufacturers to seamlessly run complex simulations without needing to make capital investment.

This pay-per-use model is ideal for both small and large companies that need to run critical simulations but lack the infrastructure necessary to meet the timing demands for the product development cycle.

Backed by an impressive list of high-profile investors, including Richard Branson, Jeff Bezos, and Peter Thiel, Rescale offers the largest available HPC network worldwide. According to Kenneth Wong in Desktop Engineering, Rescale's major contribution to large enterprises and midsized businesses is its ability to offer cloud-hosted HPC platforms "that scale up or down" according to dynamic demands along with a, "workflow designer to specify and set up commonly executed simulation exercises."

Along the way, Rescale has developed partnerships with industry-leading CAE software providers including Convergent Science, CD-adapco, Dassault Systemes and Siemens—offering more than 120 different software packages to date.

OSC's HPC infrastructure coupled with Rescale's intuitive and consolidated cloud platform enables engineers and scientists to leverage cloud resources to fully explore their design space and develop better products. •

(Above) Rescale's HPC cloud platforms allow users the ability to access science and engineering software through a unified interface. This accelerates analyses, which leads to better product innovation.

Project Lead: Tony Spagnuolo, Rescale
Research Title: Commercial simulation and HPC solution provisioning
Funding Source: Rescale
Website: rescale.com

SimApp Analyses

Kinetic Vision, Comet Solutions team up to improve product testing

As one of North America's largest manufacturers of rigid metal and plastic containers, BWAY Corporation is a global market leader in packaging solutions for large and small manufacturers and container distributors.

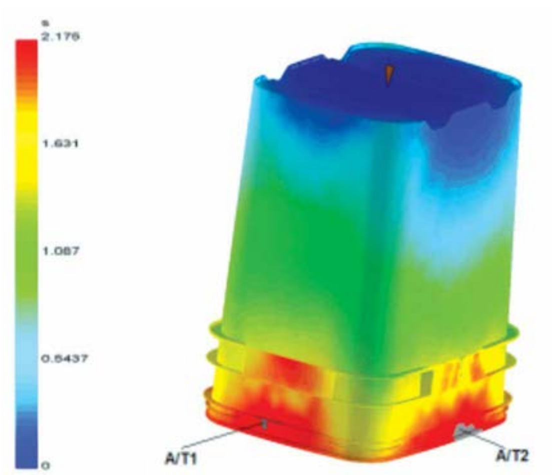
Traditionally, the company's engineers and designers have relied on outsourcing the analysis and simulation of new product designs. Because delegating such responsibility to outside resources is inefficient, time-consuming and costly, BWAY began a search for a solution to allow their product engineers to easily and expertly run these simulations.

BWAY found the solution through a partnership with Comet Solutions—a developer of simulation applications, SimApps™ that automate analyses, for various American and Asian manufacturing companies, including Intel, American Axle and Magna International. In collaboration with AweSim partner Kinetic Vision, a Cincinnati-based engineering service provider, the team created a BWAY-specific SimApp. This SimApp will interface with the AweSim platform at the Ohio Supercomputer Center, enabling it to be accessed by BWAY when needed for testing and analysis runs.

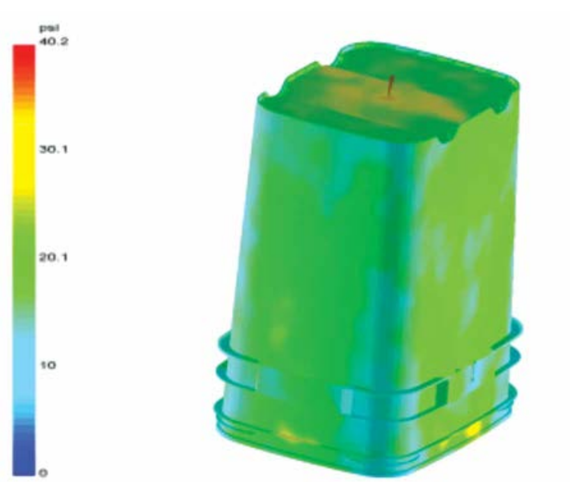
The key difference? Comet SimApps are proven to measurably reduce the high costs and slow time-to-market associated with extensive product testing. For example, leveraging a Comet SimApp allowed NASA to slash trade study time from a six- to eight-week process to just eight hours. Similarly, at Intel, Comet reduced an analysis process that typically took in-house experts up to two weeks to complete down to a process of less than 15 minutes. Furthermore, the work was conducted by Intel non-experts.

Speaking this summer at the NAFEMS International Conference of Simulation Process and Data Management, Comet's CTO, Malcolm Panthaki noted: "Simulation has been in the hands of too few for too long. Yet, all engineers and designers in the product development process could use simulation to answer questions and optimize designs during all design phases."

Comet Solutions' platform offered an easy-to-use template for rapid creation of a SimApp by Comet Solutions and Kinetic Vision. This SimApp has enabled BWAY end-users to perform fully automated simulations to "explore the design space of entire families of containers, analyzing them automatically," according to Comet. •



This "bucket crush test" illustration is an example of how Comet Solutions' simulation applications, or SimApps, allow manufacturers to automate various analyses. This allows engineers and non-expert designers the ability to run fully automated, on-demand and accurate tests inexpensively and quickly.



Project Lead: Daniel Meyer, Comet Solutions
Research Title: Development of SimApps for manufacturing designers and engineers
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