Ohio Supercomputer Center | Resources & Research Report 2014

Ohio Supercomputer Center
An OH·TECH Consortium Member

OSC and Our Vision

Here at the Ohio Supercomputer Center, we take great pride in providing powerful resources to help accelerate discovery.

The raw data tells part of our story: In 2013, the Ohio Supercomputer Center delivered more than 82 million CPU core-hours, for more than 3.3 million jobs. But behind these numbers lies the rest of our story: OSC exists to enable science.

Last year, OSC awarded compute time that resulted in nearly 950 faculty, staff and student assistants across the state running simulations or analyses for 194 new projects. This annual research report highlights a small sampling of Ohio's research capability; there are many more surprising innovations and dramatic stories waiting to be told.

The report also showcases, through first-person accounts, the perspectives of our talented staff members. Individually, OSC employees are subject-matter experts in parallel computing, computational chemistry, fluid dynamics and engineering – to name just a few. Collectively, they all are passionate about accelerating research and innovation through the powerful hardware, sophisticated software and myriad services of the Ohio Supercomputer Center.

As we look to the next year, our priorities will further support this foundation of research. We plan to acquire a $12 million high performance computing and storage system that should rank Ohio in the top 10 academic systems nationally. Additionally, we are actively seeking collaborators to co-invest in this state-of-the-art system as part of our evolving business model.

Our vision also includes growing our partnerships with research and industry communities. We welcome conversations with researchers regarding their computing needs, and we encourage researchers to participate in our steering organization, called the Statewide Users Group (SUG), to help us continue to be a powerful and targeted resource for Ohio. Together, we are working to empower you, the state's research community, to help Ohio retain its legacy as a leader in discovery and innovation.

We look forward to working with you toward these goals in the months and years ahead.

Warm regards,

Pankaj Shah
Executive Director

David Hudak, Ph.D.
Director of Supercomputer Systems

Karen Tomko, Ph.D.
Interim Director of Research

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

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On the Cover: An assortment of images from our research clients, both academic and industrial, provide a collage above the forboding landscape of the Greenland Ice Sheet (see page 27).

OSC Impact July 2013-June 2014:

- **Production Capacity**
  - 82+ million CPU core-hours delivered
  - Over 3.3 million computational jobs run
  - 835 TB data storage space in use
  - 98% uptime (target: 96% cumulative uptime)
- **Client Services**
  - 24 universities served around the state
  - 194 new projects awarded to Ohio faculty
  - 948 individuals ran a computing simulation or analysis
  - 330+ individuals attended 18 training opportunities

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CENTER PROVIDES SOLUTIONS TO FIT RESEARCH NEEDS

Since the center's creation in 1987, the Ohio Supercomputer Center (OSC) has worked to propel Ohio's economy, from academic discoveries to industrial innovation. The Center provides researchers with high-end supercomputing and storage, domain-specific programming expertise and middle 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 operations, offers some insights on how the Center is supporting that mission:

Capacity

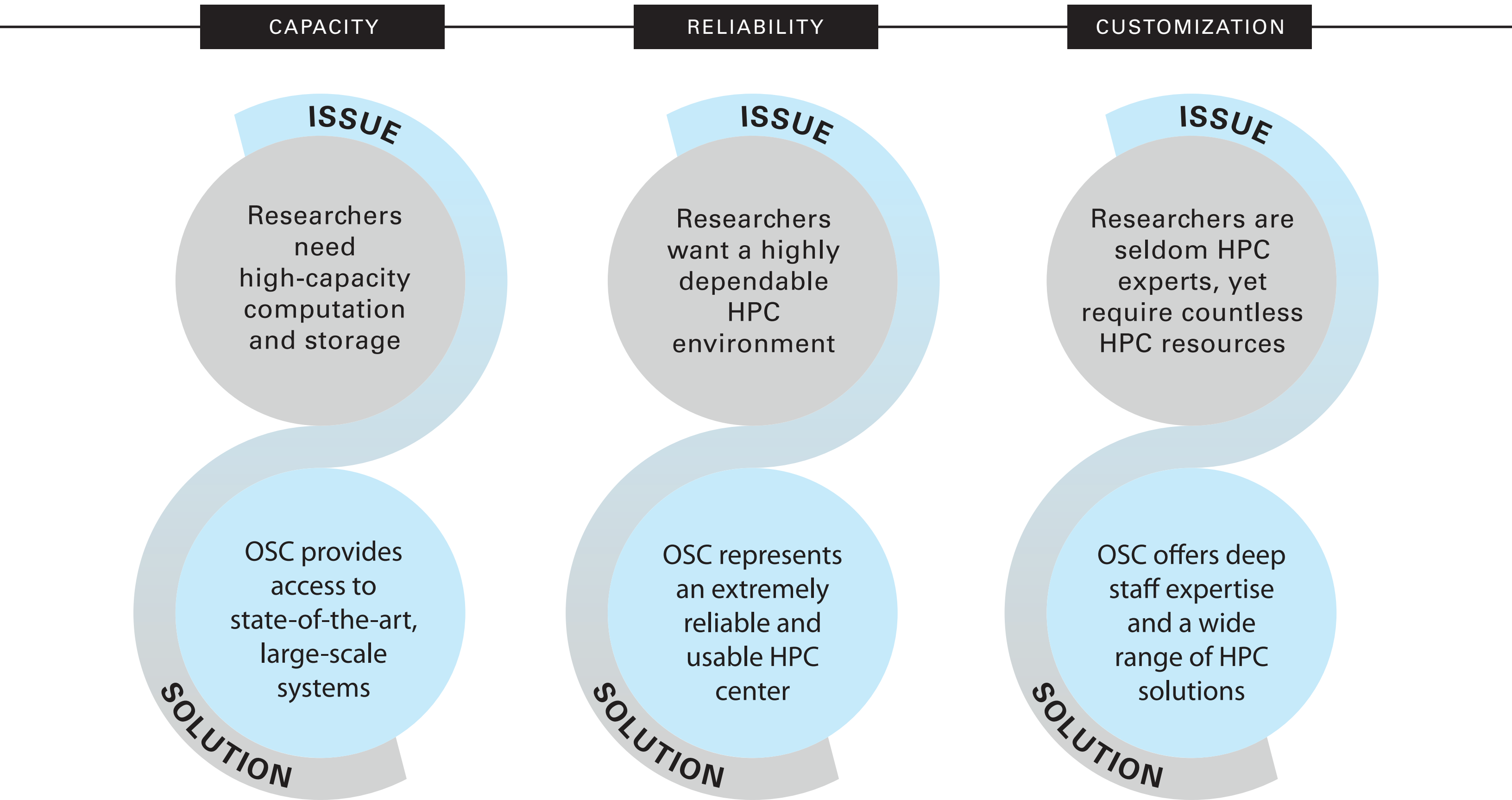
"We want to work with researchers who need computational and storage capacities that far outstrip what they can reasonably expect from the machines in their offices. There are all kinds of benefits in having access to a state-of-the-art, modern computer center that deploys large-scale system or systems that are professionally maintained and monitored. The goal here is for researchers to be able to focus on their science and not on whether they've installed the latest software or what happens when their computer's power cord gets unplugged. We also don't want researchers to have to look elsewhere just because they think we lack capacity. If we currently do lack the capacity to meet their needs, we have the ability to add capacity.

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 a dozen experts. We're focused on issues like security patches, performance improvements, latest versions, improved usability; there's a bunch of work that's gone into making our production environment as good as it is.

Customization

We offer clients domain science expertise in computational science, as well as in finite element analysis and computational fluid dynamics. 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. They use our systems for about a year and a half – not a long



learning curve. We're making our experts more available so they can provide customized solutions that bring scientific work into our production environment and to help clients get the most they can out of our systems.

There's also hardware customization, as we're always looking for the right balance between specialization and mass production. For example, we offer a few big memory machines, one-terabyte ram nodes for those experiments and those codes that simply require a terabyte of RAM that you just can't split up across multiple nodes. Also, we'll have Kepler GPU accelerators in the new Ruby Cluster to compliment the existing Tesla GPUs we deployed in the Oakley Cluster. And, we'll be deploying Intel Xeon Phi coprocessors in Ruby as well. 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 to find out if others across the state have the same need.

Partnerships

We're always looking to build deep research partnerships. We want to identify research communities that need common computational research support, for example, in analytics. For instance, if several analytics research centers are built up at Ohio State, then we stand up production environments and hire experts in support of the work that they're trying to do, rather than have them replicate that in each lab. We want to expand our staff in a strategic way to address client needs in support of our mission.

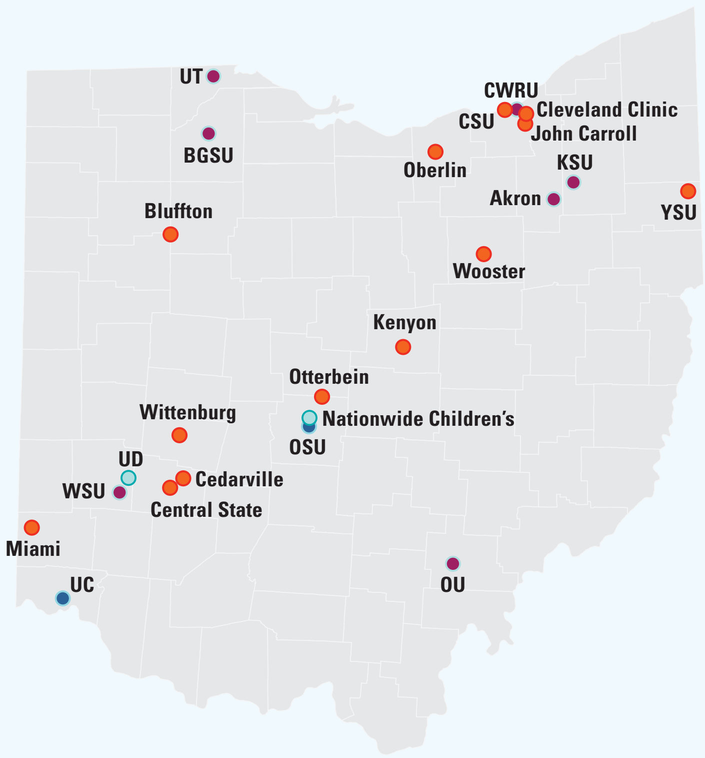
Access

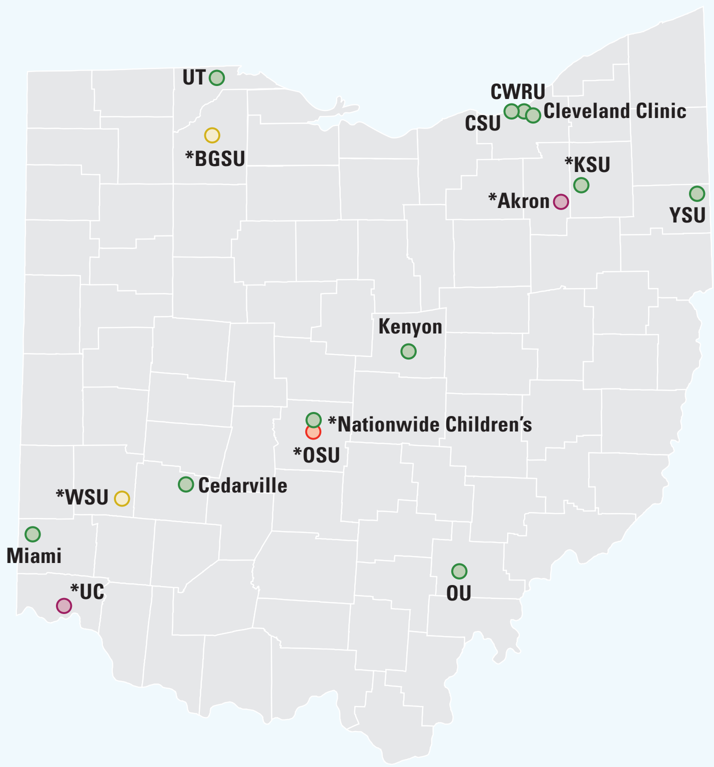
A researcher's most valuable resource is their time. OSC OnDemand was our first large-scale initiative at the production level aimed at making HPC easier to use; we are trying to redesign and simplify the interfaces with our computing systems. With MyOSC, we're making that the single location for managing administrative functions. This way, if you need to work on a project, you go to OSC OnDemand; if you've got a report to file or a ticket to resolve or software or training classes to access, you'll go to MyOSC.

Reorganization

Over the last year, we've pretty much reorganized the entire supercomputer operations staff. The overall goal was to scale and sustain operations and improve the reliability and service we provide to our clients. We now have a scope and mission for each of four production teams: HPC systems (Doug Johnson), HPC Client Services (Brian Guilfoos), Scientific Applications (Karen Tomko) and Web & Interface Applications (Basil Gohar). These four groups have now come together to more easily devise a "complete solution" to address a client's needs.

RESEARCH PROJECTS & PROPOSALS BY INSTITUTION, OSC: 2013-14





- 1-5 Projects
- 6-10 Projects
- 11-20 Projects
- 21+ Projects (UC 35, OSU 246)

- 1-5 Proposals
- 6-10 Proposals
- 11-20 Proposals
- 100+ Proposals (*Discovery Proposals)

Case study: Move the work to where the data is.

Hudak: In order to do the work that will be required by the new Honda Simulation Innovation and Modeling Center at Ohio State, the basic, scalable large computing is going to run at OSC. In order for the researchers to be productive, our systems team has installed and integrated eight Windows machines into the production environment at our data center. Researchers will be able to log in and do their preprocessing using the Windows applications that they already know and can use, then log into Oakley and submit the jobs to do the massive simulations, and, finally, log back into the Windows boxes to do the post-processing and visualizations. It was important that we "move the work to where the data is." These Windows machines, sitting within our production environment, can touch all of our storage systems, and all of the machines touch the same data – that's the model for today and into the future. Now, we're doing the same thing with one of our engineering service providers in the AweSim program – you open up a mesh and specify some weld passes, generate some data files, feed them into an FAE solver that will run on 30 or 40 nodes to generate a few dozen terabytes of simulation data, and then run that through another thermal processor. If you can have all that stuff happen and don't have to move the data around, it delivers a much, much faster time-to-solution.

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CLIENT SERVICES HELPS RESEARCHERS REACH OBJECTIVES

Supercomputers are powerful, yes. But they are only as powerful as the codes researchers write for them. Brian Guilfoos, HPC client services manager at the Ohio Supercomputer Center, understands that high performance computing isn't always intuitive and that education and training are essential services.

User Training

Faculty, staff and students can take advantage of everything from reference material on our website to web-based portals to in-person training. Workshop topics range from the very, very basic such as what OSC is, services provided and how to get an account, to more specific issues such as batch systems, scheduling or how to construct a job. We're also exploring asynchronous video training for people who are visual learners.

XSEDE (the Extreme Science and Engineering Discovery Environment) frequently partners with OSC, providing additional training opportunities. With XSEDE, a lecture happens in one location and is streamed to multiple sites, including OSC, with local teaching assistants.

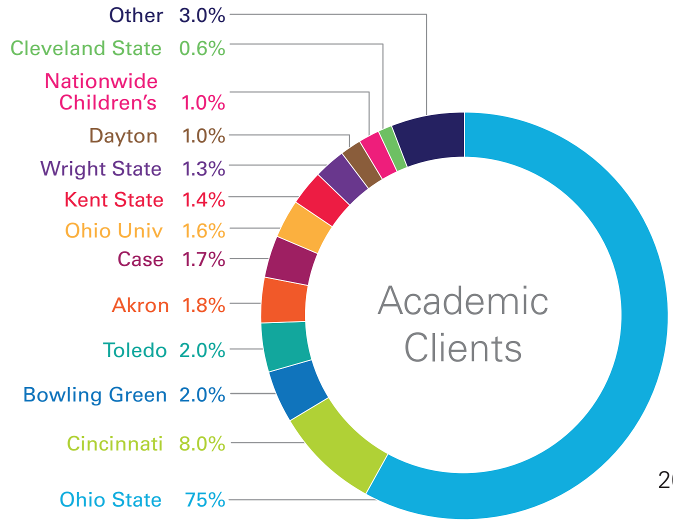
Support Services

OSC Help, which is staffed by the client services group, provides technical support and consulting. Researchers can contact us by phone or email during business hours, Monday through Friday.

Additionally, we look for proactive opportunities to assist our researchers. For example, the systems staff may notice a particular problem through their automated monitoring. If someone's code is not properly parallelized, it might cause all its threads to run on one host instead of across all the hosts in the job, which slows down the compute time. When we find those issues, we'll provide some guidance and assistance to adjust the code, so it runs more efficiently.

Staff Expertise

We're fortunate to have a number of staff with specialized domain knowledge. We have strengths in biological sciences and computational fluid dynamics. For issues such as finite element analysis, we also can engage subject matter experts in other departments. For the past two years, we've worked with University of Cincinnati IT to provide training opportunities for their research community. UC provides onsite logistics, and we provide the hands-on workshops. We want to collaborate more like this, to find people around the state who aren't OSC users but could benefit by using our services.



This snapshot view illustrates the Center's 2013-14 system usage by academic institution

Computational Science

OSC's education programs, led by Steve Gordon, senior education specialist, create a pipeline to build and sustain a computational science workforce, from middle and high school students, to internships to undergraduate education and in-career certification programs.

Ralph Regula School of Computational Science. This virtual collaboration offers students a program that leads to a baccalaureate minor or associate degree; the stackable workforce certification program provides workers with an opportunity to learn computer modeling and the underlying math and computer programming skills.

Student Internships. More than 30 undergraduate and graduate students gain real-world experience through a variety of internships at OSC and its partner organizations in the Ohio Technology Consortium.

Summer Programs. OSC's Summer Institute exposes Ohio's high school students to high performance computing and networking during the two-week residential camp. Likewise, the Young Women's Summer Institute helps middle-school girls develop an interest in computers, math, science and engineering.

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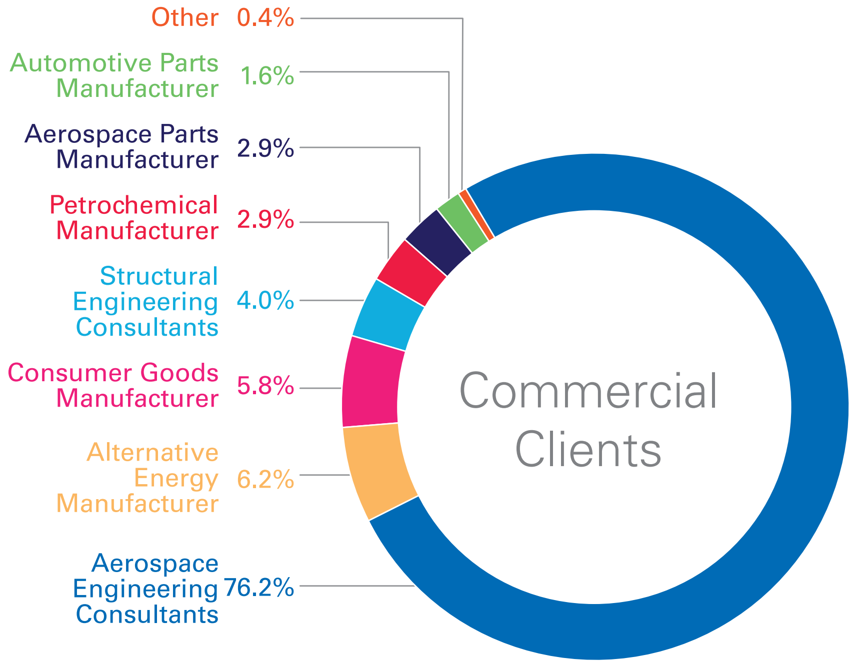
INDUSTRY CLIENTS GAIN ADVANTAGE WITH APPS, CYCLES

When the Ohio Supercomputer Center was established through a state operating budget bill in 1987, it was "intended that the center be made accessible to private industry as appropriate." Later that year, the Ohio Board of Regents created the Center "as a statewide resource designed to place Ohio's research universities and private industry in the forefront of computational research." Making this commitment to industry clearly understood is a challenge that Alan Chalker takes seriously as director of AweSim, OSC's latest and most innovative industrial engagement program.



OSC SYSTEM USAGE BY TYPE OF COMMERCIAL RESEARCH ORGANIZATION

Industrial Engagement

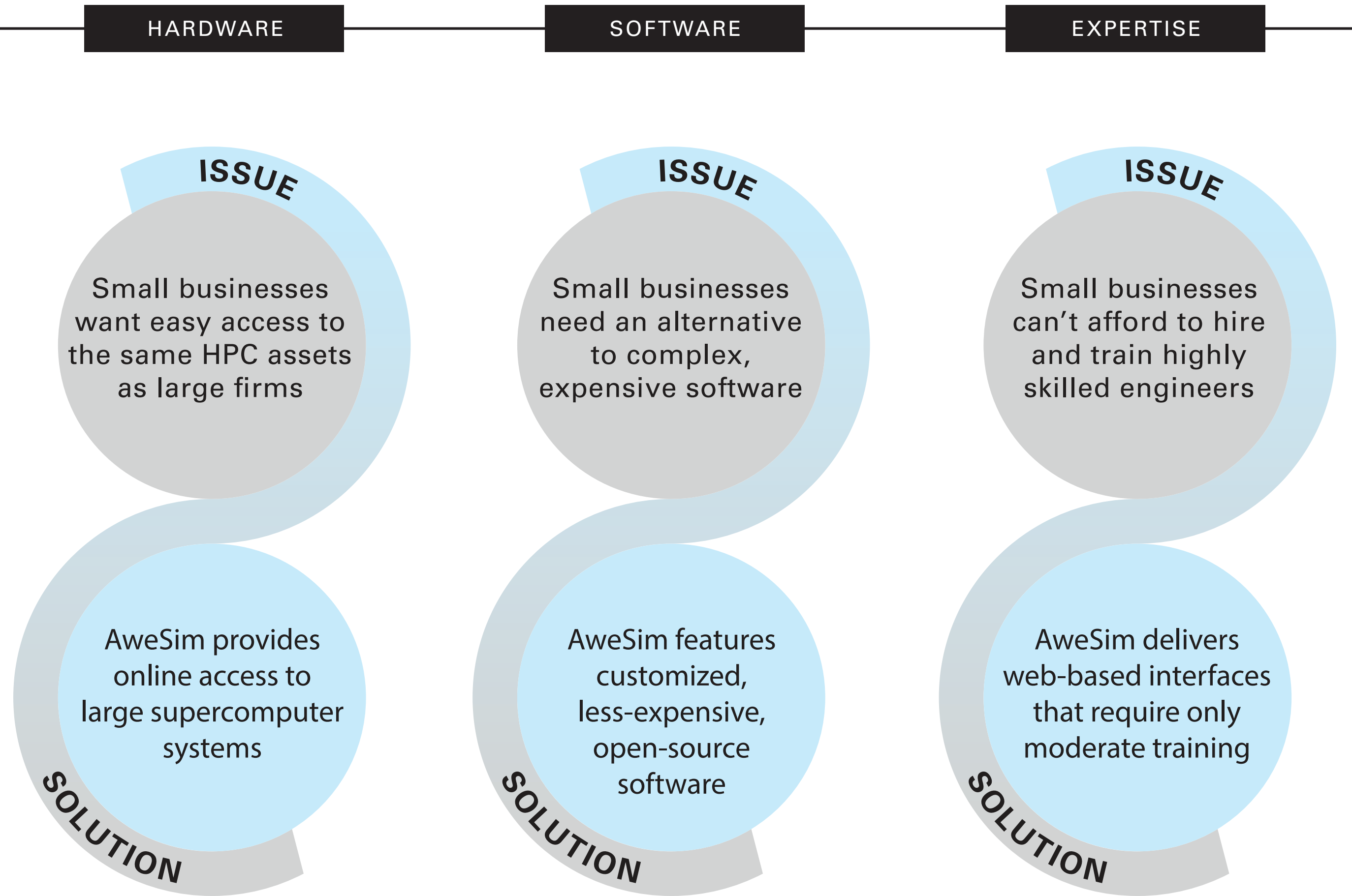
When I talk with potential commercial clients, I explain that we're located on a university campus as a matter of convenience, but, if you look, the mandate in our charter is to provide modeling and simulation resources to researchers, both academic and commercial. When I emphasize that, I see the light bulb go on. And, many of these people respond by saying, "Oh my gosh, that's really helpful because we've always thought of you like an academic center." We're not just sneaking in this industry stuff, we're empowered to do this at a high standard.

What we are fundamentally doing here is providing new and novel ways to benefit from computational science. OSC OnDemand is a great example of that; instead of coming in to the computers via some sort of command line or SSH protocol, you can access it from your web browser. We're constantly pushing the boundaries. It's not about the specific problem we're solving right now; it's about facilitating the process and making it easier for people to access and use these uncommon and valuable resources.

AWESIM
Virtual Designs. Real Benefits.

AweSim Manufacturing Apps

Small and mid-sized manufacturers are under constant economic pressure to deliver high-quality, low-cost products.



Simulation-driven design can help by supplementing their physical product prototyping with faster, less-expensive computer simulations. Based on these ideas, OSC and its partners have developed a strategy to help reduce the barriers faced by manufacturers trying to enter this market. With the financial support of Ohio's Third Frontier Commission and Development Services Agency, last year we launched AweSim, an innovative program to develop cloud-based manufacturing simulation applications sold through an e-commerce marketplace.

Since the launch, we've made very good progress developing the app kit, to the point that some of our engineering service provider partners are creating prototype apps. The app store website is up, featuring our initial apps for customers to test and utilize. We're also looking at a range of services, such as Software-as-a-Service, where customers who are interested in using a particular software package on our system only for a given amount of time can purchase a seat, say for two weeks.

We've worked a lot on the business model for AweSim and have narrowed our focus on some of the apps that we'll be developing. We also recently completed a comprehensive market survey that reached out to more than 8,000 small and mid-sized business contacts in Ohio, and we got back in touch with 300 respondents, who helped shape our understanding of the products our customer base wants.

Commercial Clients

Our regular commercial customers are coming to us primarily for access to our hardware, because they don't have anything like it, because what they have is saturated or because what they're doing could impact their operating environment. They're people who generally know modeling and simulation, but they need additional resources, typically hardware, but sometimes software or expertise.

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DEMAND KINDLES VAST UPGRADES TO HPC SYSTEMS

This is an exciting time to be a systems engineer at the Ohio Supercomputer Center. The Center is currently running three mid-sized High Performance Computing (HPC) clusters: the just-launched HP/Intel Xeon Phi Ruby Cluster, the HP/Intel Xeon Oakley Cluster and the IBM/AMD Opteron Glenn Cluster, as well as a storage environment with several petabytes of total capacity across a variety of file systems. If that wasn't enough, we're preparing for the acquisition in 2015 of a new system that will exceed the peak performance of all the existing systems combined. To compliment the new system, upgrades and expansions of OSC's storage and networking environments will be performed.

The deployments in 2015 will represent some of the largest increases in performance for the Center.

Ruby Cluster: Named for acclaimed actress, author and activist

The name of the Ohio Supercomputer Center's newest system pays tribute to actress, writer and civil rights activist Ruby Dee. Recent OSC systems have been named after Ohioans known as pioneers in diverse careers: The Glenn Cluster for astronaut and statesman John Glenn; the ARMSTRONG research portal for astronaut Neil Armstrong, the Csuri Advanced GPU environment for computer artist Charles "Chuck" Csuri, and the Oakley Cluster for legendary sharpshooter and social advocate Annie Oakley.

Born in Cleveland, Ohio, Ruby Ann Wallace grew up in Harlem. She graduated in 1945 from Hunter College with degrees in French and Spanish. Dee was married for a short time to Frank Dee Brown, before marrying actor Ossie Davis in 1948 and raising a family of three children together.

Dee debuted on Broadway in the late 1940s and then built a film career spanning several generations. Dee received numerous acting awards, including an Oscar nomination in 2008 for playing Mama Lucas in American Gangster.

Dee and Davis were very active in social and racial equality issues, first within the entertainment industry and then later throughout the Civil Rights movement of the 1960s.

In 1998, Dee and Davis celebrated their 50th wedding anniversary with the publication of a Grammy-winning dual autobiography. Dee and Davis remained married until his death in 2005, and Dee died in June of 2014.

Computers

"There's obviously a bit of a difference between the hardware we bought five years ago and the hardware we're buying today; the seven racks of the new Ruby Cluster house 240 nodes and provide a total peak performance of over 140 teraflops, compared to the remaining section of the Glenn Cluster, at roughly 425 nodes in 18 racks with a peak performance of about 40 teraflops. We look at Ruby as a transitional system that will feature newer hardware than Oakley and additional capacity. We like to think of Ruby as a stepping-stone for researchers to be prepared for the next large system at OSC.

As for the 2015 system, our target is somewhere in the range of 1 petaflop for peak performance. That's a big jump; we're not just doubling or tripling performance, we're looking at something that is close to an order of magnitude higher in performance than any individual cluster on the floor at OSC. That's going to really change the nature of the types of problems our systems can handle and the amount of throughput they can deliver. Since there is a good chance Glenn is going to have to be turned off in preparation for the 2015 system this increases the importance of the Ruby cluster. It will provide additional computational

	Ruby System (2014)	Oakley System (2012)	Glenn System (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	34TF +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 Disk 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-precision • 2880 CUDA cores • 12GB memory 20 Xeon Phi 5110p • 1.011 TF Peak • 60 cores • 1.053 GHz • 8 GB memory	128 NVIDIA M2070 • 515 GFlops Peak Double Precision • 6 GB memory • 448 CUDA cores	18 NVIDIA Quadro Plex 2200 S4 • Each with 4 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 IB (40 Gbps)	DDR IB (20 Gbps)

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 stepping-stone to the next system.

Storage

We've just completed a migration of data from 14 individual file servers and file systems into a single 1.1 petabyte file system. This architecture prepares us for future growth; we expect to increase capacity and performance of this new file system to 4-5 PB and 40-50 gigabytes-per-second to support the new system. Other improvements will be made to our storage environment based on the needs of our user community. These will include expansions to our backup systems to accommodate the additional storage, new high performance scratch file systems for working data, and new storage for user home directories.

Network

We're going to have a couple of areas of improvement in our network. We're going to replace the core router that OSC uses to connect to the Internet through OARnet. We're going to upgrade our OARnet connection to 40 gigabits per second, but we'll also have a backup router with a 10 gigabits per second connection to provide a redundant connection. We'll also upgrade our peer connection to OSU to a 40 gigabits-per-second connection. And, both of these upgrades are designed for an eventual upgrade to 100 Gbps connections to match what's already available on the OARnet backbone. We've also just upgraded the InfiniBand spine switches for our high speed interconnect fabric to allow for additional capacity, not only for the Ruby Cluster, but also for the next large system as well.

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SOFTWARE, STAFF PROVIDE CLIENTS WITH MAJOR VALUE

When we think of supercomputing resources, we automatically think of processors and petaflops. However, compute capacity is only one part of the equation; software is another important component. OSC maintains a variety of software packages – more than 70 currently installed – to support a wide range of scientific research areas, including the Mathematical and Physical Sciences, Engineering, Computer and Information Science/Computer Engineering, Biological, Behavioral and Social Sciences and Geosciences. Installed applications include CFD, FEA, molecular dynamics and quantum chemistry applications; linear algebra and parallel programming libraries and software development tools.

Individual Assistance

"We're willing to work with researchers, either helping them to install their own stack or to make it a publicly available resource, if it might be widely used. We have staff members who offer specialization domain expertise in areas like finite element analysis, computational fluid dynamics and computational physics, as well as some areas of specialized assistance, such as code optimization and tuning. We also provide appropriate development tools, such as compilers, debuggers and libraries, to support researchers who are writing their own HPC software. Our currently available software is listed on our website.

User Input

We would like to hear more from our users to help us identify the software needed in their research area, especially for emerging areas such as in the biosciences and data analytics for the social sciences. We'd welcome suggestions as we work towards having a good set of foundational packages – commercial and/or open-source – in place. By having these packages available here, we eliminate one barrier (that of obtaining and installing software) that individual research groups face and enable researchers to spend more effort focused on their simulation or data analysis problem."

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ENGINEERS DELIVER SMOOTH ACCESS TO POWERFUL SYSTEMS

The Web and Interface Applications Group controls the way in which OSC HPC clients access and use most OSC systems. The group works to enable easy access through whatever means clients find most comfortable, which still includes command-line interfaces for the old-school users, but, according to the group's manager Basil Gohar, also features more and more mobile devices – not just phones and tablets, but also watches, glasses and other wearable devices.

Industrial Engagement

"There is a huge variety of ways to access the HPC systems. Yeah, it basically all ends up being a batch job submission behind the scenes, but that job is just a means by which you send instructions to the HPC systems. How you compose those instructions could be as simple as inserting a small set of numbers into an algorithm. If you need to adjust those numbers, it's not necessary to go into SSH to do that. Just go into a web page or open a mobile app, type in the new numbers, submit them and get your results. Making it easy that way is our job.

The bulk of our time over the last year has been spent on the AweSim project. Working with our commercial partners has been, in my eyes, providing them with the access they need to accomplish their goals. We also support the general usage and maintenance of OSC OnDemand, which we plan to make a zero-install type of platform. We're looking at the interfaces that use the standard technology available to not require additional plug-ins and to avoid things that raise security issues, technology incompatibilities, firewall obstacles and so on."

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VIRTUAL REALITY KEY FOR EFFECTIVE TRAINING, TESTING

Below: Home health care providers are able to identify household threats to the health of patients, their family or themselves within a virtual training environment funded by the National Institute for Occupational Safety and Health.

Virtual environments, once seen only as a unique extension of gaming technology, now are considered essential tools for competitiveness, from healthcare to education to manufacturing. The Ohio Supercomputer Center's Virtual Environments and Simulation Group use this technology to create rich, precise, interactive simulations for training, assessment and remote collaborations.

"Our forte is surgical simulation," said Don Stredney, as he reflected on the advances of interactive simulations during his 20-plus years as director of the Interface Lab. "Our work on simulating temporal bone surgery for training is extensible to other areas, such as preoperative assessment and surgical planning, exploration of new surgical approaches, or applications beyond communication disorders.

Virtual Temporal Bone Project

We've accumulated well over 10 years of research on this National Institutes of Health RO1 project. (The project allows medical students and residents to practice delicate drill techniques on the skull, via a computer-based teaching system.)

We integrate the vast amounts of real-time multisensory data sets into a single, coherent simulation. The key is that we must execute what we are computing in real-time. It is fairly horrendous in terms of computation, but it has to be solved instantaneously for accurate training purposes. We've also been successful with remote rendering. This enables the visualization algorithms to be calculated at the Ohio Supercomputer Center, with just the resulting images delivered back to a hand-held device, such as an iPad.

We are establishing reliable, accurate and effective means of evaluating a student's technical skills using a simulator; this is a strong point of our work. By creating a composite dataset of the drill techniques used by our surgical partners at each of our 11 study sites around the United States, we established an "expert dataset" to use as a benchmark for evaluating residents.

Expanding Our Reach

We are collaborating with a variety of researchers within OSC and beyond to extend this technology.

For example, the University of Cincinnati's Ravi Samy, MD, is transferring temporal bone simulations to a robot, to test methods for improving the surgical precision. At The Ohio State University's College of Veterinary Medicine, researchers are looking at remote rendering as an option for students to study anatomy on demand, outside of the lab.

OSC's home health care training simulation, funded by NIOSH (the National Institute for Occupational Safety and Health) is being evaluated to help workers identify household risks for patients or health care workers themselves, such as mold, dangerous use of equipment or other injury producing events. Meanwhile, our Mammoth Cave project enables geology students, especially those with motion disabilities, to explore the geological structures of the cave.

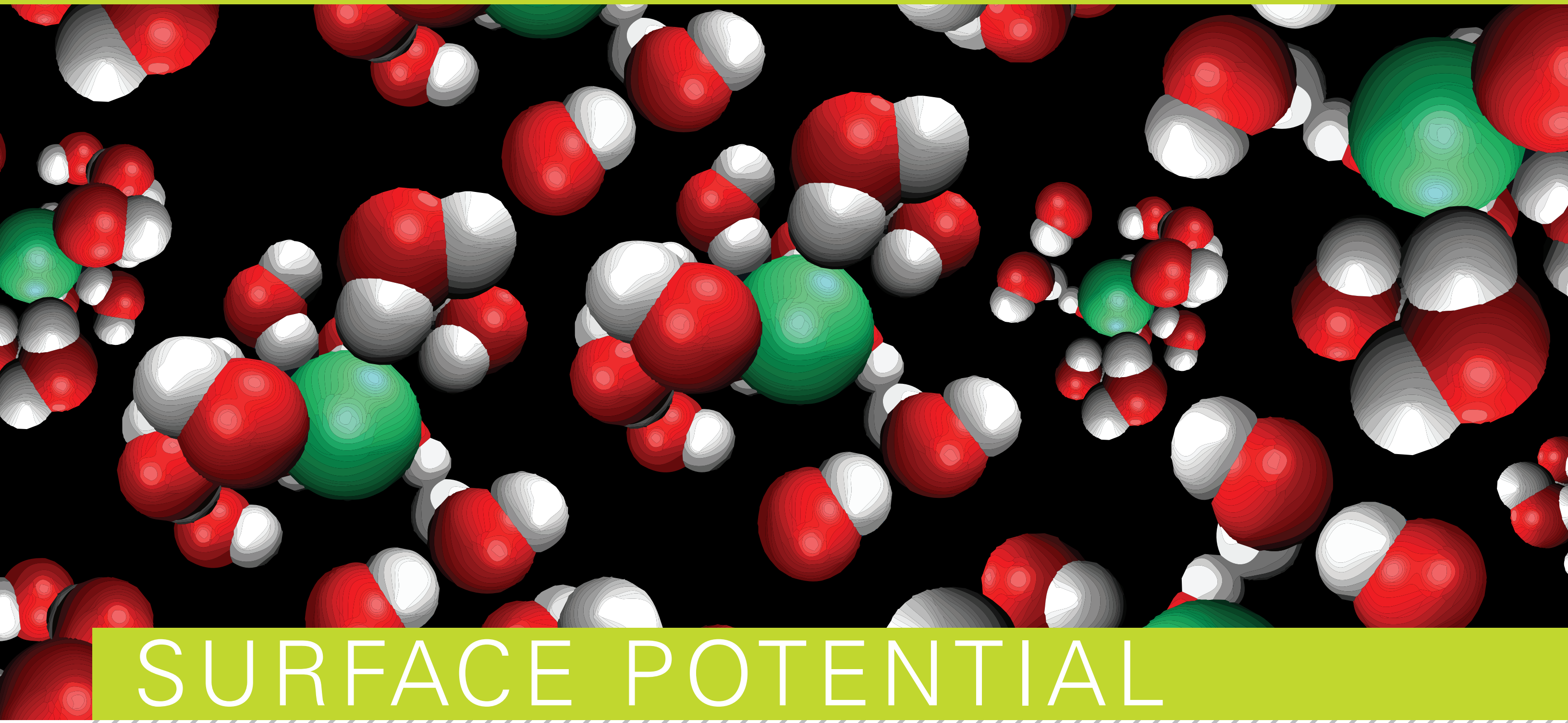
Finally, The Ohio State University Driving Simulation Laboratory studies how drivers use vehicle instrument panels and in-vehicle information systems. The lab was established through collaborations with Honda R&D Americas, oversight from Ohio State's Office of Research and technical expertise from OSC."

Ohio's bioscience researchers are using the Ohio Supercomputer Center to analyze vast amounts of genetic, molecular and environmental data to better understand human physiology, chemical processes and diagnose and treat diseases. The research stories on the following pages illustrate a sampling of these efforts, from finding the relationship between smoking and periodontal disease, to understanding how HPV causes cancer, and to calculating hydration thermodynamics.

BIOLOGICAL SCIENCES

"By combining classical simulations with quantum chemistry simulations, we are examining ion and water polarization and how it is calculated in hydration thermodynamics. The Ohio Supercomputer Center is an instrumental resource for these large-scale computing needs."

— Thomas Beck, Ph.D.
Professor, University of Cincinnati



SURFACE POTENTIAL

Beck enhances methods for gauging thermodynamics of ion hydration

Recent research suggests that long-standing methods for calculating the thermodynamics of ion hydration, while robust, are ambiguous regarding the inclusion of water's surface potential.

Why does this matter? Ions – molecules that have either a positive or negative charge – are at the center of chemical processes spanning electrical, biological, atmospheric and surfactant chemistries, to name a few. Water, the most important solvent for ions, is a polar molecule with positive and negative sides, which affects how the molecules align at the water's surface and can influence ion distributions and chemical reactions.

"From classical simulations, we know that a proper treatment of ion and water polarization is important to accurately calculate hydration thermodynamics," said Thomas Beck, Ph.D., a professor of Chemistry at the University of Cincinnati. "However, our quantum calculations show that the current classical methodologies can over-estimate the polarization state of the ions, particularly for anions."

People try to simulate ions in water by developing force fields, or a set of parameters and equations for use in molecular mechanics, and fitting them to experimental data such as the free energy values that may or may not include the surface potential. With inaccurate values, the models can be skewed.

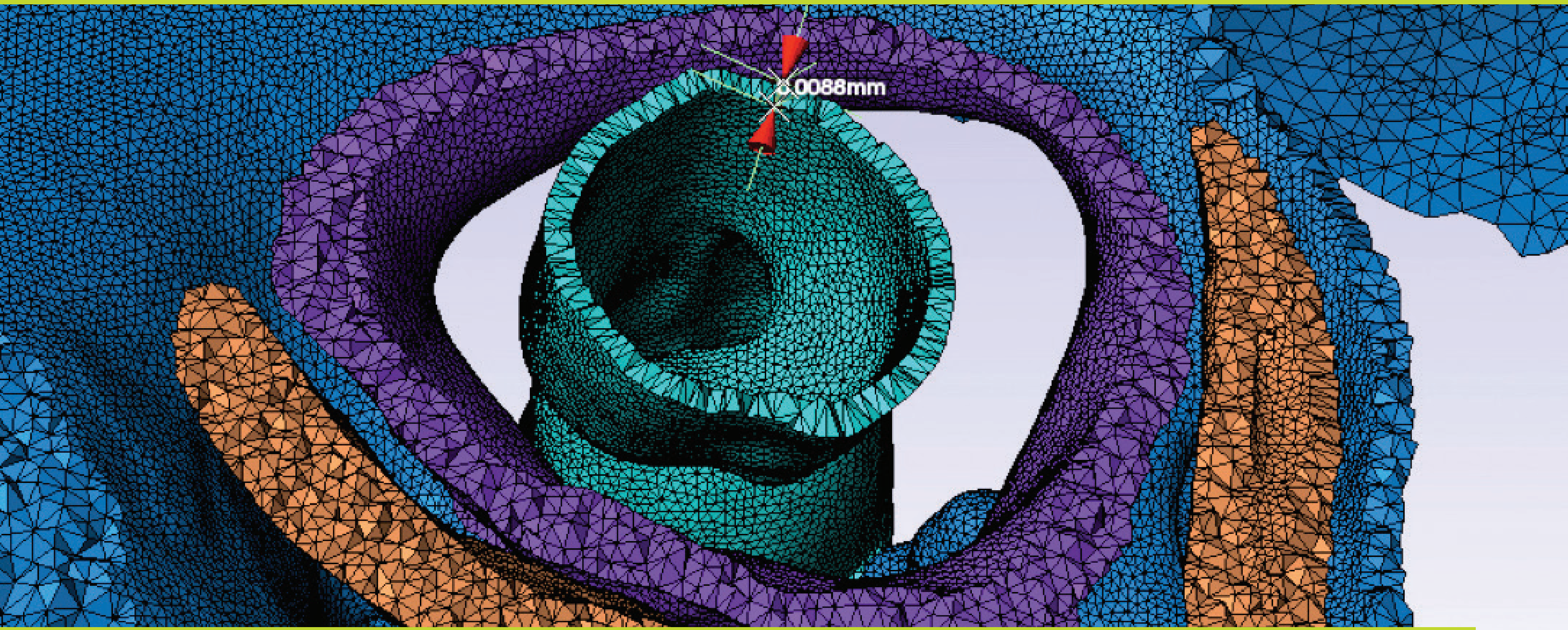
Because single-ion quantities are not directly accessible to bulk thermodynamic measurement, a variety of approaches work to identify the contribution of the individual ion. If the hydration free energy – the energy that can be converted to work – and enthalpy – the energetic contribution – are obtained for this ion (the proton), then the corresponding values for all other ions can be measured.

Beck examined these methodologies by conducting a theoretical analysis of existing experimental data; the re-analysis shows significant size dependence to the derived proton hydration enthalpy when employing an expanded ion data set that includes a range of complex molecular ions. He then leveraged Ohio Supercomputer Center systems to conduct high-level quantum modeling that examined the size dependence of hydration enthalpy differences for a sodium flouride ion pair between the small cluster and the converged bulk thermodynamic limits.

"People have debated whether the values estimated by previous experimental approaches included the surface potential," Beck said. "I think we proved that the current 'gold standard' experimental approach does. And, because we obtained a quantitative prediction for the surface potential that is outside the norm of what other people have set, it will surely stimulate discussion."

Above: Beck conducted high-level quantum modeling to determine how the molecules align at the water's surface and influence ion distributions and chemical reactions.

Project Lead: Thomas Beck, University of Cincinnati
Research Title: Computational studies of specific ion effects in water and ion channels
Funding Source: National Science Foundation
Website: http://homepages.uc.edu/~becktl/index.html



JOINT BIOMECHANICS

Castro, Nguyen gauge ant strength with eye to robotics, assistive devices

A recent study into the biomechanics of the necks of ants – which can amazingly lift objects up to 1,000 times heavier than its body – might unlock one of nature's little mysteries and, quite possibly, open the door to advancements in robotic engineering.

Engineers at The Ohio State University combined computational modeling at the Ohio Supercomputer Center with laboratory testing to determine the relationship between the mechanical function, structural design and material properties of the Allegheny mound ant (*Formica exsectoides*). The study focused on the ant's neck – the soft tissue component that bridges the stiff exoskeleton of the head and thorax and transfers the full weight of the ant's load carrying capacity.

"Loads are lifted with the mouthparts, transferred through the neck joint to the thorax, and distributed over six legs and tarsi that anchor to the supporting surface," explained Carlos Castro, Ph.D., Ohio State assistant professor of Mechanical and Aerospace Engineering.

To better understand the strengths and upper limits of the joint, the researchers reverse-engineered the biomechanical design by developing 3-D models of the ant's internal and external anatomy. The models were created by importing X-ray cross-section images (microCT) of ant specimens into a modeling program (Simpleware) to segment the model into components, convert them into a mesh frame model of more than 6.5 million elements, and assign material properties.

The model then was loaded into a finite element analysis program (Abaqus), an application that creates accurate simulations of complex geometries and forces. The simulations were run at OSC in conjunction with lab experiments that used a centrifuge to measure deformation of the neck joint under a range of calculated loads.

The experiments revealed that the neck joints could withstand loads of about 5,000 times the ant's body weight and that the neck-joint structure produced the highest strength when the head was aligned with the loading direction. The simulations confirmed the directional strength and indicated that the neck-to-head transition is the critical point for joint failure.

Former Ohio State student Vienny N. Nguyen, now a robotics engineer at NASA's Johnson Space Center, noted in her 2012 master's thesis on this research, "As we look to the future of human-assistive devices and ultra-light robotics, the development of 3-dimensional models for visual analysis and loading and kinematic simulation will also serve as tools for evaluating and comparing the functional morphology of multiple species and types of joints."

Above: A cross-section of an ant's neck joint helped researchers to study the strength of the small insect. The head exoskeleton is shown in blue, neck membrane in purple, esophagus in teal, and thoracic segments in orange.

Project Lead: Carlos Castro, Ph.D., The Ohio State University
Research Title: The exoskeletal structure and tensile loading behavior of an ant neck joint
Funding Source: National Science Foundation, The Ohio State University's Institute for Materials Research
Website: https://mae.osu.edu/labs/nbl/research

PERIODONTAL DISEASE

Kumar, colleagues uncover connection between smoking, periodontal risk

Fifty years after the surgeon general first reported on the harmful effects of tobacco, medical professionals continue to find more links between smoking and disease.

Recently, Purnima Kumar, an associate professor of Periodontology at The Ohio State University College of Dentistry, and her colleagues discovered a compelling cause-and-effect relationship between smoking and periodontal disease.

By combining advanced computational techniques and a novel scientific query, Kumar's research clarified the unusual composition of a smoker's biofilm, a collection of bacteria in the oral cavity that forms on moist surfaces in the body, including teeth and the spaces between teeth and gums. She also clarifies how the body recognizes and interacts with the novel bacteria. Kumar found that under their gingiva, smokers had many species that doctors did not know could be found in the oral cavity, and several species were systemic pathogens that usually cause diseases elsewhere in the body.

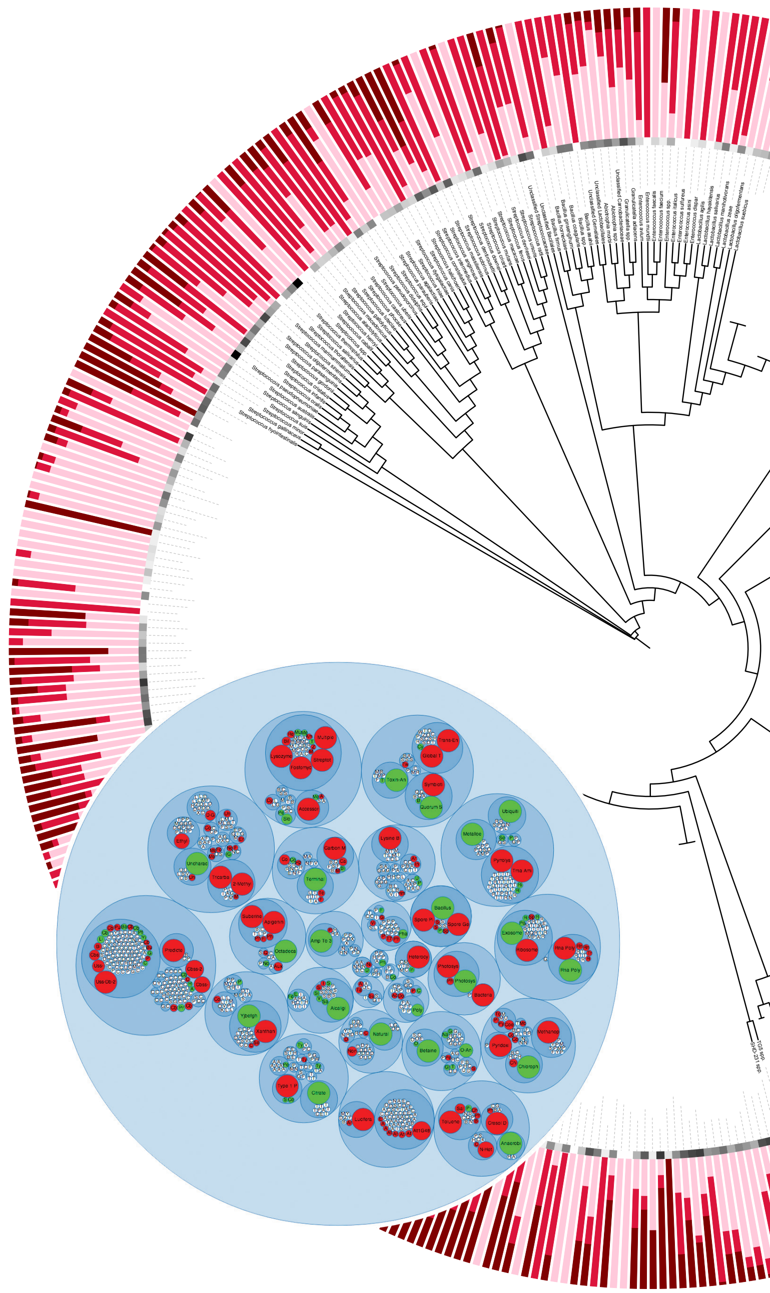
"We know that smoking increases your risk of getting severe periodontal disease and oral cancer," Kumar said. "Since bacteria outnumber human cells in our bodies by 10 to 1, and play such an important role in keeping us healthy, our research explores the ways that smoking can change the bacteria in the biofilm, from the moment they are acquired until the time the tooth is lost to disease."

As part of the initial research, the team investigated DNA and RNA sequences to identify the bacteria and learn what genes they express to survive and cause disease. The Ohio Supercomputer Center provided the computing power needed to analyze these immense datasets of molecular information.

Kumar is building on these preliminary investigations by combining large-scale clinical study designs with open-ended, as well as targeted, molecular approaches. This will bridge the gap between purely clinical studies and in vitro experiments, both of which have limited abilities to replicate disease in humans.

Patient samples will be processed for whole-cell genomic data using next generation shotgun sequencing and analyzed using a variety of computationally intensive tools. Ultimately, the results of this study will provide a timetable for administering periodontal therapy following smoking cessation.

"We have to be very aggressive in treating patients who smoke," Kumar added. "We need to see them more often and watch their periodontal tissue because they are high-risk individuals for periodontal disease. That's the message we carry to clinicians – these are our most vulnerable patients."



Above: To better understand the impact of smoking on gum disease, Kumar conducted DNA and RNA sequence analysis at the Ohio Supercomputer Center. These graphics illustrate the results.

Project Lead: Purnima Kumar, Ph.D., The Ohio State University
Research Title: Tobacco smoking and perturbations in the subgingival microbial ecosystem
Funding Source: National Institute of Dental and Craniofacial Research, R01DE022579
Website: dent.osu.edu/perio/research_kumar.php

HPV CANCER GENESIS

Symer, Akagi find DNA insertion loops likely spur cancer development

Human papillomavirus (HPV) causes about 610,000 cases of cancer worldwide, accounting for about 5 percent of all cancer cases and including virtually all cases of cervical cancer. Scientists have long known that certain types of HPV cause cancer, but they don’t completely understand all the steps that are involved.

For example, while the HPV cancer-causing genes E6 and E7 are known to be essential for the development of cancer, they are not sufficient to cause cancer. Additional alterations in host-cell genes are necessary for cancer to develop. Recently, a team of researchers at Ohio State’s Comprehensive Cancer Center identified a new way by which HPV might spark cancer development – by disrupting chromosomal DNA with repeating loops when the virus is inserted into host-cell DNA as it replicates.

“Our sequencing data showed in vivid detail that HPV can damage host-cell genes and chromosomes at the sites of viral insertion,” said David Symer, M.D., Ph.D., assistant professor of Molecular Virology, Immunology and Medical Genetics at Ohio State’s Comprehensive Cancer Center – Arthur G. James Cancer Hospital and Richard J. Solove Research Institute (OSUCCC – James).

Keiko Akagi, Ph.D., a bioinformatics expert and research assistant professor of Molecular Virology, Immunology and Medical Genetics at OSUCCC – James, leveraged the computational capabilities of OSC’s Oakley Cluster.

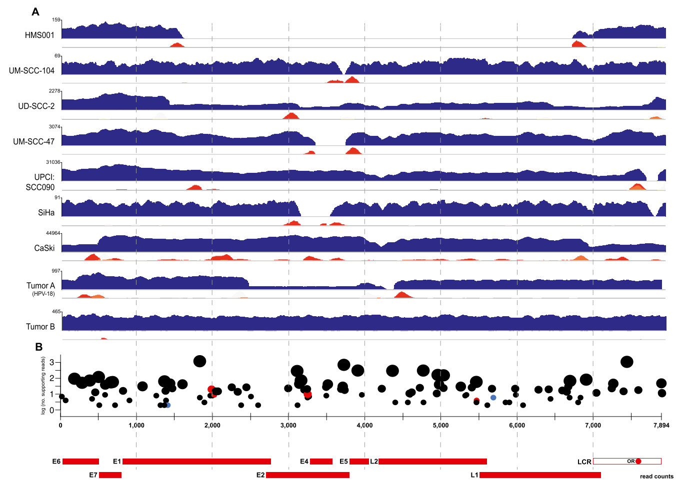
She studied whole genome sequencing data and other datasets to examine the DNA sequences of ten cancer-cell lines and two head and neck tumor samples collected from patients. Each sequence represented fragments of the roughly three billion chemical units within the human genetic instruction set.

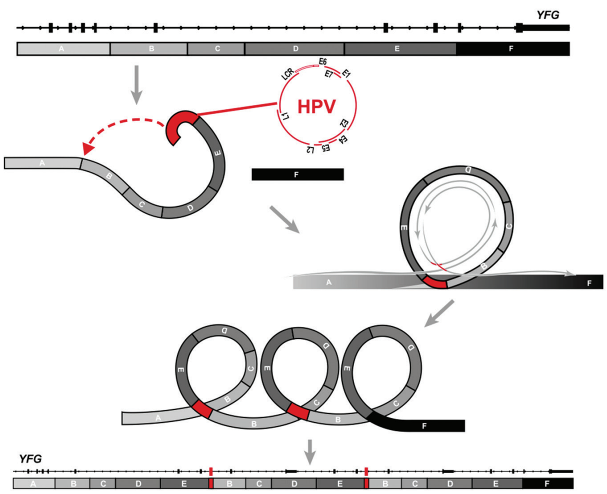
“HPV can act like a tornado hitting the genome, disrupting and rearranging nearby host-cell genes,” Symer said. “This can lead to overexpression of cancer-causing genes in some cases, or it can disrupt protective tumor-suppressor genes in others. Both kinds of damage likely promote the development of cancer.”

“We observed fragments of the host-cell genome to be removed, rearranged or increased in number at sites of HPV insertion into the genome,” said Maura Gillison, M.D., Ph.D., professor of Medicine, Epidemiology and Otolaryngology and the Jeg Coughlin Chair of Cancer Research at OSUCCC – James. “These remarkable changes in host genes were accompanied by increases in the number of HPV copies in the host cell, thereby also increasing the expression of viral E6 and E7, the cancer-promoting genes.”

Left: Histograms for various cancer samples of the HPV virome in human cancers.

Right: Focal amplifications and rearrangements explained by “looping” model.





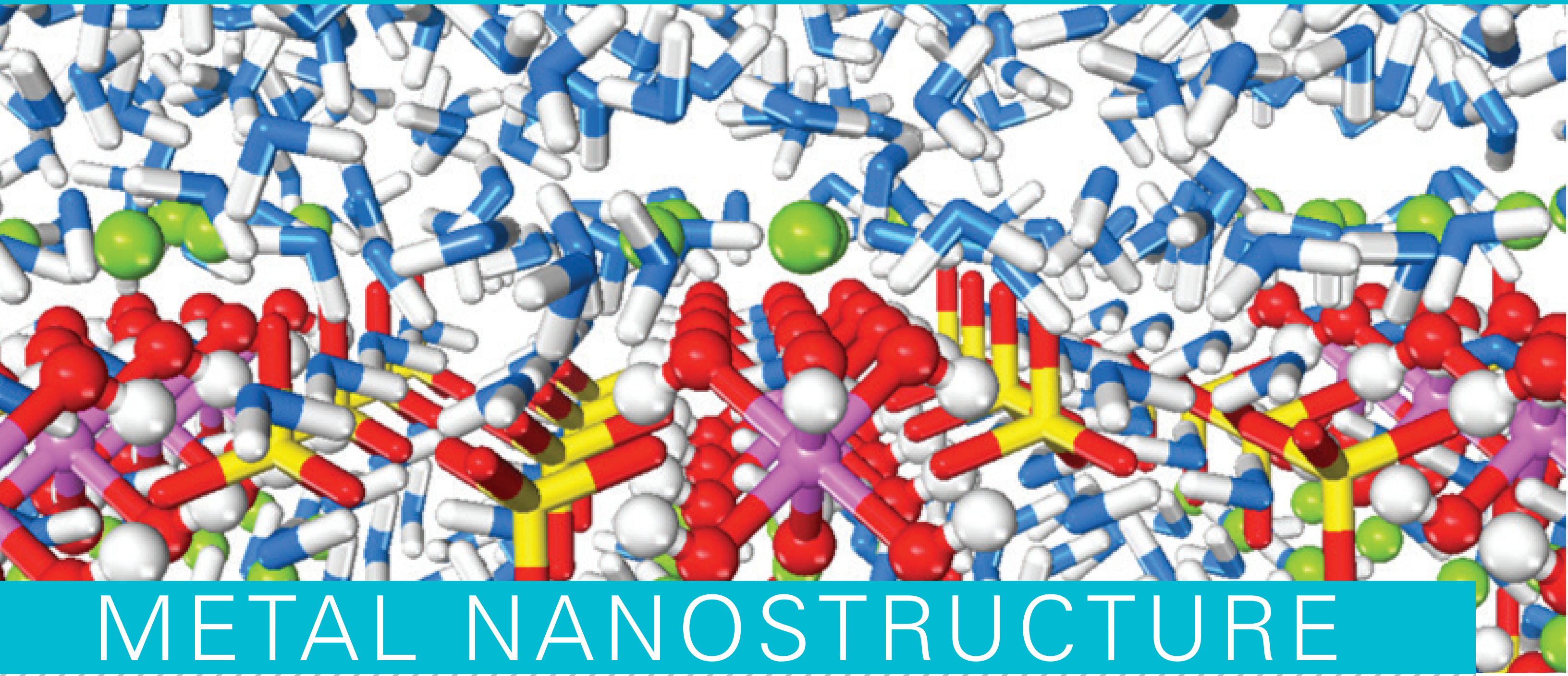
Project Lead: David Symer, M.D., Ph.D., The Ohio State University
Research Title: Genome-wide analysis of HPV integration in human cancers reveals recurrent, focal genomic instability
Funding Source: The Ohio State University, Oral Cancer Foundation, National Institutes of Health, National Cancer Institute
Website: http://medicine.osu.edu/mvimg/directory/medical-genetics/symer-david-md-phd/Pages/index.aspx

Computational modeling often lies at the crux of advanced materials research, a vital process in a state known as a manufacturing powerhouse. For example, the Ohio Supercomputer Center is powering studies to develop new applications for fuel cells, better cancer treatment drugs and thermal imaging sensors. These projects, described on the following pages, are just a few of the advanced materials research projects supported by OSC.

ADVANCED MATERIALS

"We are combining highly accurate synthesis and characterization tools with the computational resources of the Ohio Supercomputer Center to better understand alloy nanoparticles. The insights we gain can be applied to improve fuel cells, batteries, automotive catalysts, sensors and biomarkers."

Hendrik Heinz, Ph.D.
Associate Professor, University of Akron



METAL NANOSTRUCTURE

Heinz group models alloy catalysts that may enhance fuel cells, sensors

Scientists at the University of Akron, in collaboration with partners at UCLA, are investigating the unique properties of metal alloy nanostructures – materials measuring 1-1000 nanometers in length – that have potential applications in the manufacture of fuel cells, batteries, automotive catalysts, sensors and nanoeletronic devices.

More specifically, the research delves into modeling alloy catalysts that drive the electricity-generating chemical reactions within fuel cells by employing smaller amounts of the expensive metal platinum, which could accelerate the world's transition to emissions-free passenger vehicles and mobile power generation. Recently, it has been discovered that the reactions can be greatly enhanced and the costs lowered by introducing cheaper metals, such as iron, cobalt, nickel, copper, chromium or maganese, into the platinum.

Further, the research group believes that highly accurate synthesis, characterization and computation tools to predict internal atomic structures and the chemical properties of alloy nanoparticles at realistic length scales also can be applied to improve magnetic information storage, biomarkers and catalysts for other reactions.

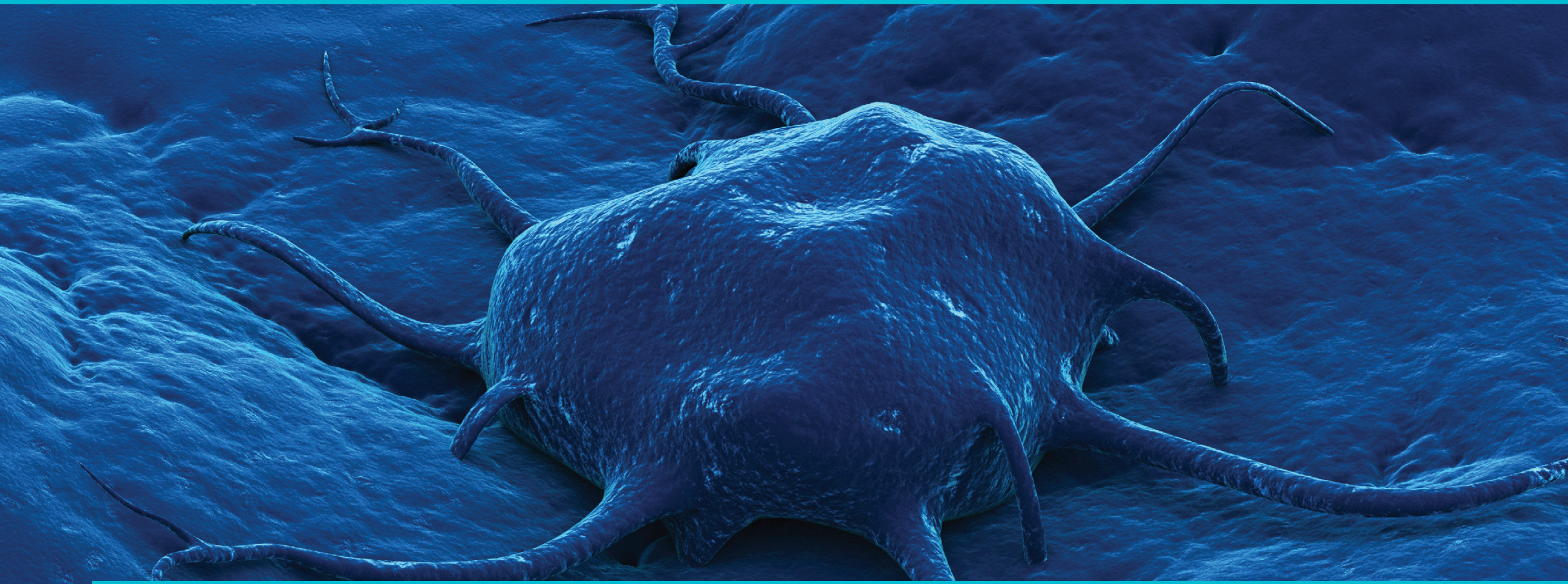
"The performance space of nanoalloys is exponentially higher compared to pure-metal nanostructures from routine synthesis methods," explained Hendrik Heinz, Ph.D., associate professor of Polymer Engineering at the University of Akron. "By accessing Ohio Supercomputer Center systems to create multi-scale simulations and develop force fields of revolutionary accuracy at length scales of 1 to 100 nanometers, we aim to close the wide gap between experimental capabilities and missing theoretical understanding of growth mechanisms, shape control and catalytic performance."

The coordinates of all atoms in the synthesized nanostructures will be monitored using a powerful electron microscope to feed computer models, validate interatomic potentials and predict 3-D atomic ordering and chemical reaction rates. To improve catalytic properties, the researchers are closely connecting the unique chemistry challenges of alloy synthesis and testing, characterization challenges to resolve 3-D atomic structures and annealing transitions, and computational challenges in multi-scale simulations and development of models. The outcome will be a full understanding of alloy nucleation and growth, atomic ordering and quantitative engineering of the reactivity from first principles.

Ultimately, the three research groups in this collaborative effort hope to achieve a full understanding of alloy nucleation and growth, atomic ordering and quantitative engineering of the reactivity from first principles and to share insights into new force fields and computational algorithms by distributing them as open-source data through research websites and software repositories.

Above: In order to understand and design corrosion-resistant alloys, Heinz conducted atomistic simulation, guided by experimental results, to determine phase changes upon heating, oxidation, and aqueous corrosion.

Project Lead: Hendrik Heinz, Ph.D., University of Akron
Research Title: Design and testing of nanoalloy catalysts in 3D atomic resolution
Funding Source: National Science Foundation
Website: www.poly-eng.uakron.edu/heinz.php



CANCER-FIGHTING DRUGS

Collins seeks new, less-toxic metal complexes to combat colon cancer

In 1978, the Food and Drug Administration approved cisplatin, a platinum-based compound, for clinical use. Cisplatin today is widely recognized as an effective cancer-treating drug, but it also is known to cause many severe side effects, such as kidney damage, nervous system impairment, nausea and vomiting. Thus, there is a strong interest in developing similar, new drugs that are less toxic.

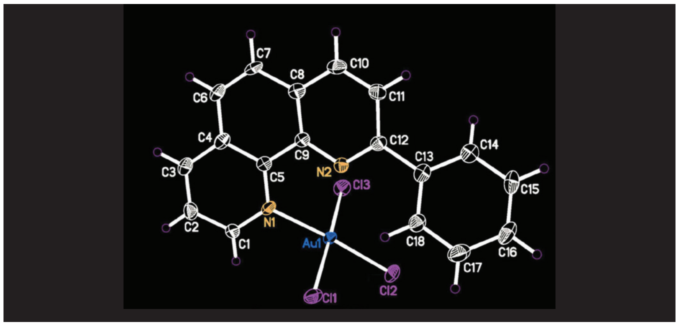
"Numerous studies are focusing on the development of other metal complexes – those containing metal centers such as ruthenium, copper and rhenium – with potential application as biological sensors and/or drugs for photodynamic therapy for cancer," said Sibrina Collins, Ph.D., assistant professor of Inorganic Chemistry at the College of Wooster.

As part of a recent study, Collins' research group used Ohio Supercomputer Center resources to help investigate the structure and anti-tumor behavior of an inorganic compound, namely [Au(pnp)Cl3] (pnp = 2-phenyl-1,10-phenanthroline), against colon cancer cell lines.

"At the College of Wooster, the Senior Independent Study requirement allows our chemistry majors to make important intellectual contributions to faculty research," Collins said. "Thus, training students is an important component of my research efforts."

The objective of the research in the Collins Group is to develop a detailed understanding of the molecular structures, electronic structures, photophysics and reactivity of a selection of late transition metal complexes and exploit this understanding to design effective anticancer agents.

Recently, Collins and her colleagues investigated the structure of several late transition metal complexes containing gold(III), copper(II) and palladium(II) containing the pnp organic ligand. They found that the gold complex adopted a monodentate bonding motif, where only one atom in the ligand binds to the metal and the molecular planes produced angles similar to other trichloridogold(III) complexes noted in scientific literature.



Above: The research group investigated the structure and anti-tumor behavior of an inorganic compound against colon cancer cell lines. Here, the molecular structure shows the atomic labeling scheme and 50 percent probability displacement ellipsoids.

Project Lead: Sibrina Collins, Ph.D., College of Wooster
Research Title: In-house and synchrotron X-ray diffraction studies of 2-phenyl-1,10- phenanthroline, protonated salts, complexes with gold(III) and copper(II), and an orthometallation product with palladium(II)
Funding Source: College of Wooster, Elizabeth Ralston Presidential Endowment for Faculty Development Award, William H. Wilson Research Fund, and Henry Luce II Fund for Distinguished Scholarship
Website: http://www.wooster.edu/bios/scollins/

MICROSCOPIC STRUCTURE

Drabold examines the physics of chemical elements for potential uses

A research group at Ohio University has been studying the physics of chemical elements in the oxygen family that lack a crystalline structure, elements known as amorphous chalcogenide materials. Chalcogenide materials containing traces of silver – a state referred to as "doped" – make rigid, fast-ion conductors, useful in applications such as solid oxide fuel cells and as a novel computer memory material. They are also working on thermal imaging sensors used in "night vision" applications.

The OU group analyzed amorphous titanium dioxide (TiO_2), revealing the microscopic structure – essentially a chemically ordered continuous random network, but with interesting twists such as the existence of two distinct local environments for titanium. Furthermore, while amorphous TiO_2 has well known photo-catalytic properties in nanophase form, the group is looking for similar characteristics from the amorphous phases of the material.

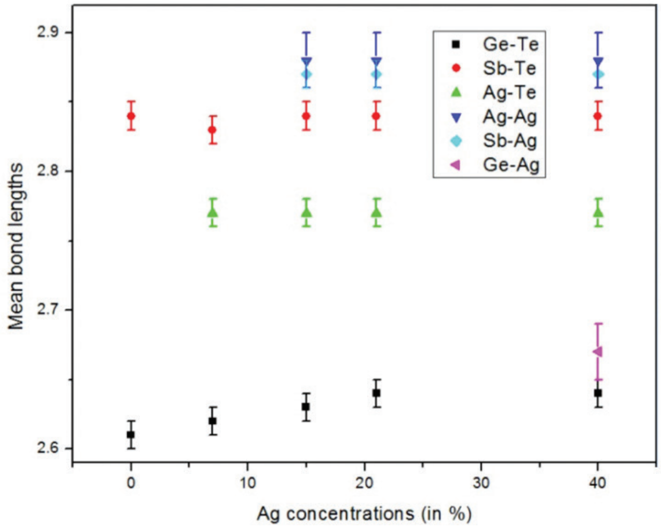
The researchers also are looking at two prime candidates for sensors and memory components: germanium-selenide (GeSe) and germanium-sulfide (GeS) hosts doped with up to about 40 percent of silver (Ag).

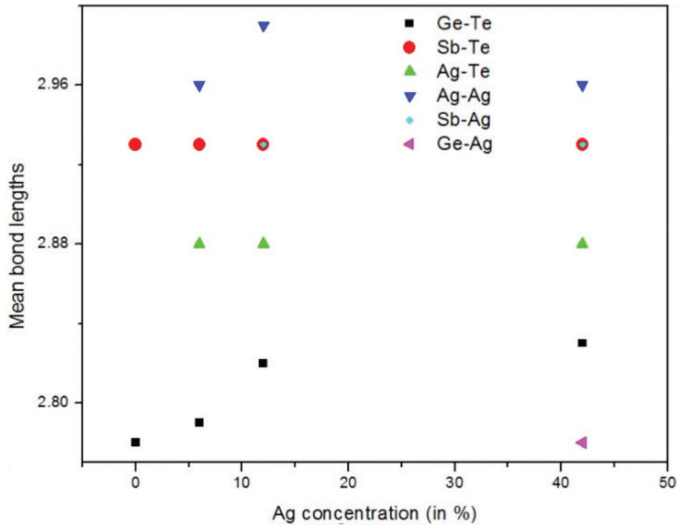
"Experimentally, it is known that the GeSe system has significantly better ionic mobility than the sulfide, which is interesting and unexplained," explained David Drabold, Edwin and Ruth Kennedy Distinguished Professor of Physics at Ohio University. "We have shown that, despite the great similarities in S and Se chemistry, the Ag tends to be trapped in more restricted environments in the sulfide."

The group also is investigating chalcogenide-based "phase-change memory," which at least one telephone manufacturer has begun to deploy in some of its cell phones. Here, they've found that crystalline germanium-antimony-tellurium (GeSbTe) alloys have a much higher electrical conductivity than those in amorphous states, forming the basis of on/off contrast required for memory applications.

"In a speculative but potentially important line of research, we have begun to use our Ohio Supercomputer Center resources to look at a system that is essentially a hybrid of the two types of chalcogenide memory materials: we are performing the first simulations of GeSbTe:Ag materials – GST with silver," Drabold said.

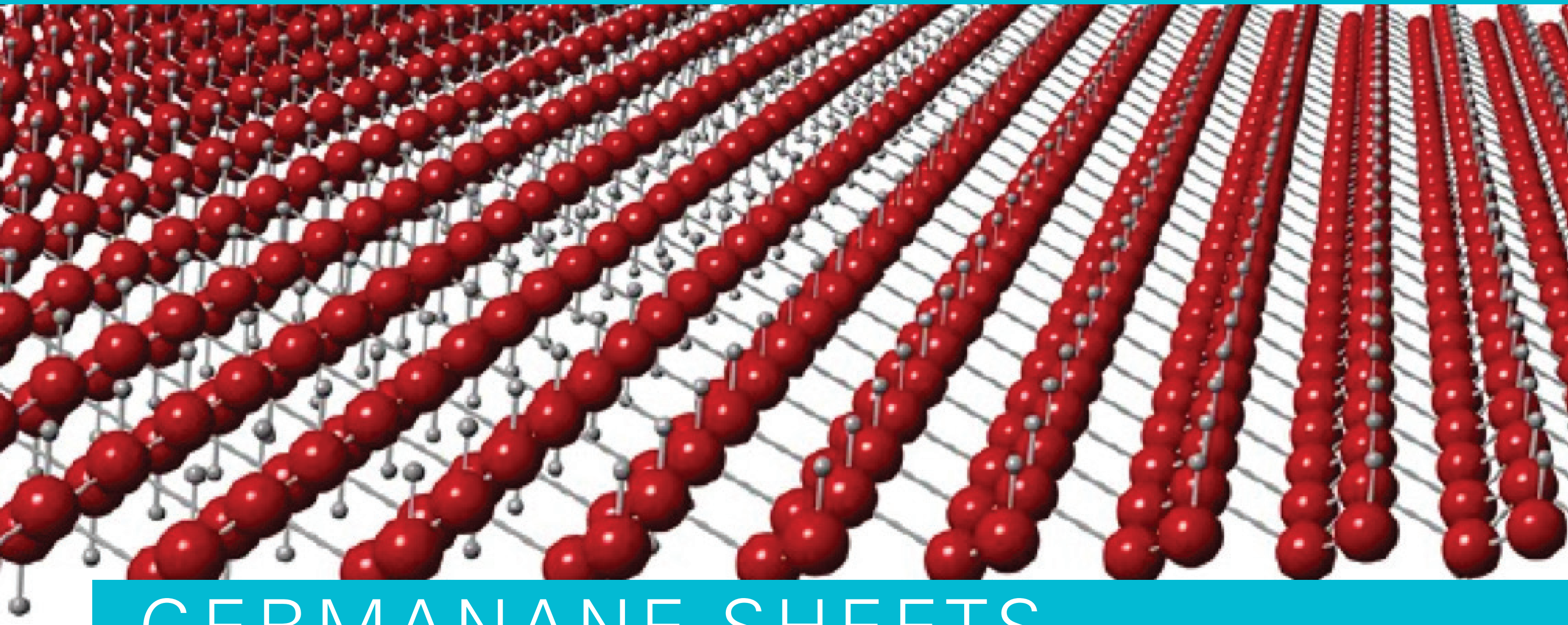
The group has learned that these materials maintain their semiconducting character with up to 50 percent Ag content. They are studying the topology of the network and silver dynamics, as well as the peculiar ability of the system to maintain its semiconducting character to very high metal concentration.





Above: Drabold's group is performing the first simulations of GeSbTe:Ag materials – GST doped with silver. The charts above provide a direct comparison between the coordination statistics found in experiment (top) and theory (bottom).

Project Lead: David A. Drabold, Ph.D., Ohio University
Research Title: Simulations of complex chalcogenide and oxide materials
Funding Source: National Science Foundation, Army Research Office
Website: http://www.phy.ohiou.edu/~drabold/



GERMANANE SHEETS

Windl, colleagues study properties of one-atom-thick, layered materials

Just one decade ago, researchers first isolated graphene, a carbon film only one atom thick – essentially a semi-metallic material so thin that it presents only two measurable dimensions, length and width. Despite its lack of depth, graphene is extremely strong and superconductive; scientists and manufacturers already have filed patents for various applications that leverage the remarkable properties of this material.

"Graphene-based materials have been proposed for many applications, ranging from transparent conductors to thermal interface materials to certain transistor-like devices," said Wolfgang Windl, Ph.D., professor of Materials Science Engineering at The Ohio State University. "Graphene's success has shown not only that it is possible to create stable, single-atom-thick sheets from a crystalline solid, but that these materials have fundamentally different properties than the parent material."

Windl and experimental collaborator Joshua Goldberger, Ph.D., from Ohio State's Chemistry department, observed that there exists an entire periodic table of crystalline solid-state materials from which scientists may be able to create single-atom or few-atom polyhedral thick 2-D layers, with each material having different electronic, mechanical and transport properties. However, most of the layered materials studied to date have been composed of neutral or ionic layers and lack the ability to modify the surface properties of industrial materials.

As single-layer materials are entirely surface area, their properties and reactivity profoundly depend on the underlying substrate, the local electronic environment and mechanical deformations. Windl's group predicted, based on density-functional calculations, that single layers of silicon, germanium and other similar materials terminated with hydrogen or other functional groups should have stability, tunable electronic properties by modifying the terminating molecules and record-breaking conductivity in the semiconductor world.

Goldberger's research group then mechanically deposited germanane sheets as single and few layers onto silicon dioxide/silicon surfaces. Subsequently, Windl's group predicted that substituting the hydrogen with methane molecules, the material should have strongly different optical properties, which Goldberger's successful synthesis of the material confirmed.

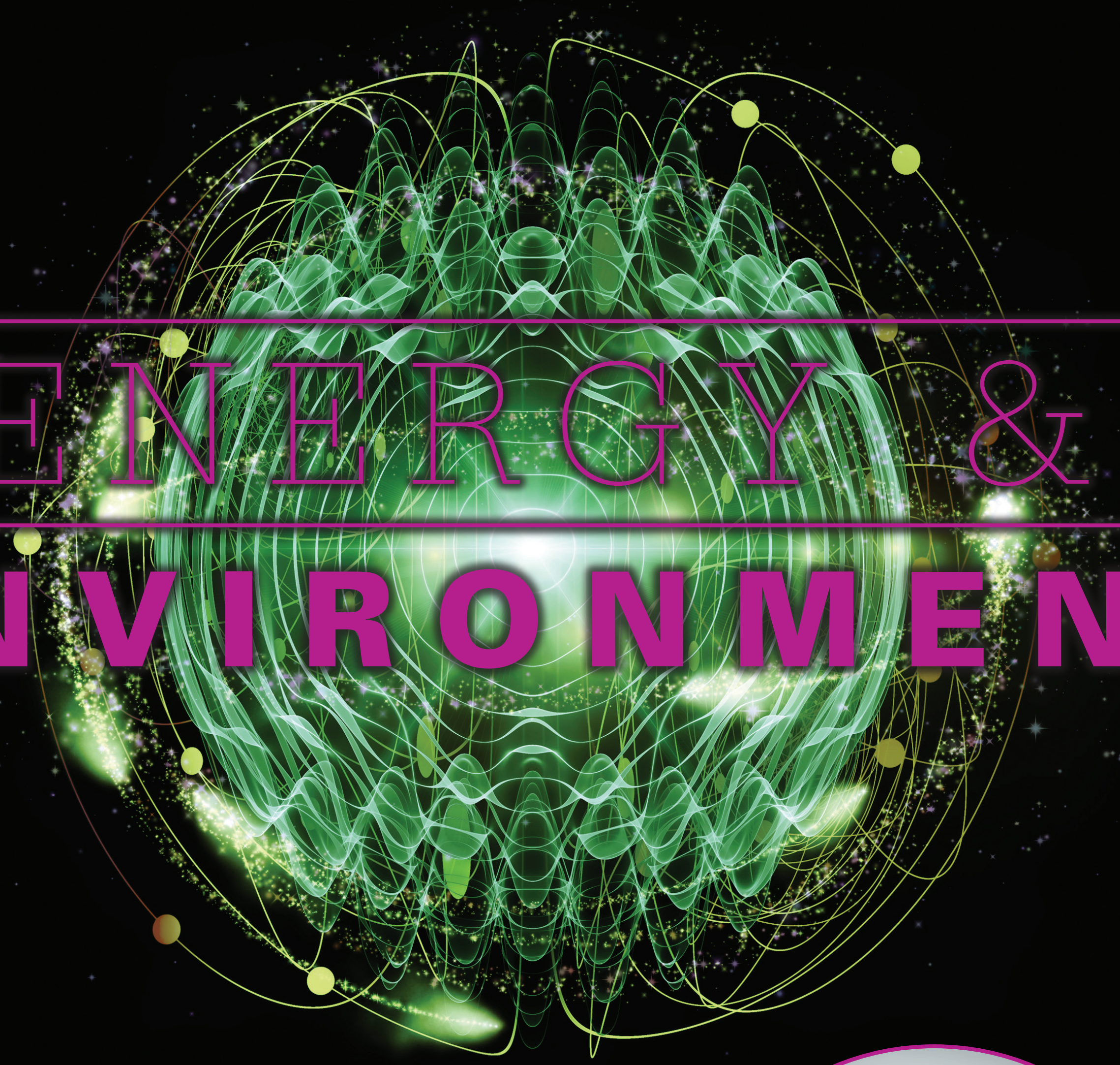
"We now have created gram-scale, millimeter-sized crystallites of hydrogen-terminated germanane – a single-atom layer of the element germanium – and have characterized for the first time their long-term resistance to oxidation and thermal stability, a necessary prerequisite for any practical application," Windl said. "This material represents a new class of covalently terminated graphane, a tunable relative of graphene that has great potential for a wide range of optoelectronic and sensing applications. This opens a new world full of opportunities significantly beyond graphene."

Above: Windl and Goldberger synthesized for the first time millimeter-scale crystals of a hydrogen-terminated germanium multilayered graphane analogue (germanane, GeH) from the topochemical deintercalation of CaGe2.

Project Lead: Wolfgang Windl, Ph.D., The Ohio State University
Research Title: Computational design of metallic glasses
Funding Source: Army Research, National Science Foundation
Website: https://mse.osu.edu/people/windl.1

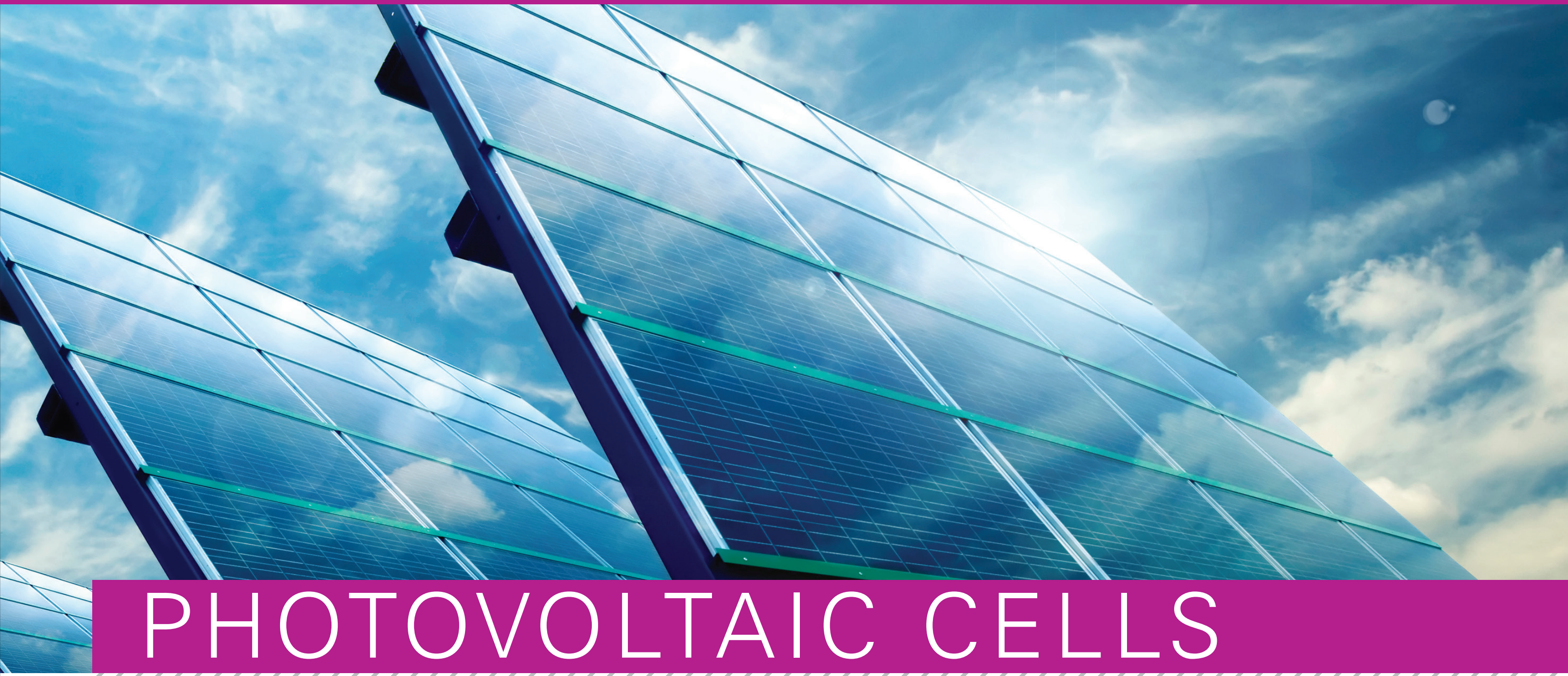
Harness solar energy, efficiently and effectively. Create a first-of-its-kind, 3-D model to study climate change. Conserve endangered plants. Complex global energy and environment sustainability problems often require significant demands for computational modeling, simulation and analysis. The Ohio Supercomputer Center supplies the researchers working toward these important outcomes – featured on the following pages – with the resources they need to power their data-rich projects.

ENERGY & ENVIRONMENT



"Our goal is to develop unique semiconductors that can be made into polycrystalline thin films that are electronically as good as single-crystal thin films. This is a new grand challenge of our time."

— Yanfa Yan, Ph.D.
Professor, University of Toledo



PHOTOVOLTAIC CELLS

Yan researching sustainable methods of clean solar electricity generation

With more than 120 terawatts of solar power irradiating the earth, photovoltaics offers the promise of essentially limitless energy for powering society. The reality, though, depends on whether the cost of the technology can be made competitive with more traditional carbon-based sources.

To that end, Yanfa Yan, a faculty member at the Wright Center for Photovoltaic Innovation and Commercialization and an Ohio research scholar endowed chair at the University of Toledo, is researching sustainable methods for clean solar electricity. In particular, he's combining two independent research focuses: efficiencies of solar cells and solid-state lighting devices, based on epitaxial single-crystal thin films; and efficiencies and cost reduction, based on polycrystalline thin films, by specifically investigating the theoretical properties of lead-halide-based perovskites.

Perovskites are a broad class of crystalline minerals that only in the past five years have been used to convert solar energy to electricity. Since then, the efficiency of perovskite solar cells has climbed from 3.8 percent to 19.3 percent, a pace of improvement unmatched by any other solar technology.

"To improve the cost metric, it is crucial to both dramatically reduce solar module fabrication cases, as well as improve device efficiencies. Lead-halide-based perovskites have burst onto the scene with a relatively quick demonstration of efficiencies, and simple low-temperature, low-cost processing," Yan said. "Despite these attractive features, some limitations need to be addressed before this approach is suitable for commercialization."

Specifically, the device efficiency at the cell level needs to be improved to more than 20 percent in order for the promise of an ultra-low-cost technology to be realized, the toxic heavy metal lead needs to be replaced with a less toxic alternative, and the stability of the materials and devices towards moisture, air and temperature needs to be established and improved.

Yan and his team are leveraging the computing resources at the Ohio Supercomputer Center to evaluate the structural stability of proposed non-lead perovskite photovoltaic absorbers, as well as their electronic and optical properties. They'll also, through theoretical models, calculate the defect physics in wide-bandgap perovskites, and examine the structure and effects of extended defects, such as dislocations and grain boundaries in photovoltaic materials.

"Our goal is to develop unique semiconductors that can be made into polycrystalline thin films that are electronically as good as single-crystal thin films," Yan said. "This is a new grand challenge of our time."

Above: Yan is investigating methods for developing highly efficient yet low-cost solar cells based on polycrystalline thin films, by specifically investigating the theoretical properties of halide-based perovskites.

Project Lead: Yanfa Yan, University of Toledo
Research Title: Theory of photovoltaic materials
Funding Source: Ohio Research Scholar Program, University of Toledo
Website: astro1.panet.utoledo.edu/~yyan/y_research.html

FOREST MANAGEMENT

Sohngen team create model series to assess impact of biofuel production

Biofuels, fuels derived from plant materials, have the potential to reduce the United State's dependency on fossil-based fuels. Brent Sohngen, professor of Agricultural, Environmental and Development Economics at The Ohio State University, and his colleagues have developed a series of land use and management models that assess, among many issues, the impact of using forests for biofuel.

With the help of the Ohio Supercomputer Center, Sohngen is building on these previous models to more accurately analyze whether forest-based biofuels are carbon neutral. The results have significant economic implications for the forestry sectors, as the Energy Independence and Security Act (EISA) of 2007 directed the US Environmental Protection Agency to approve biofuel pathways only for carbon-neutral feedstocks.

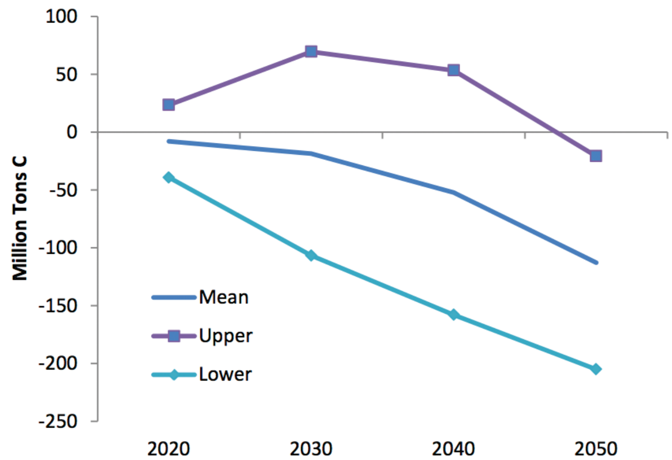
Sohngen's preliminary assessment of the EISA 2007 laws were inconclusive. The average result suggests that forests emit carbon under the biofuel mandate scenario, which would eliminate wood products from being used in biofuel production. However, many of the key parameters used in the models are derived from statistical analyses, which are considered uncertain. At the 95 percent confidence level, the results included significant positive changes – making forestry products candidates for biofuels.

Because this situation clouds the confidence-level government policy makers have in the results, the EPA asked Sohngen to develop confidence bands for the results from the global forestry and land-use model.

To do that, Sohngen and his graduate students created a Monte Carlo simulation method for the model, using information on uncertainty in the elasticity parameter used in the land supply functions and in the parameters used in the forest growth and yield parameters. (A computerized mathematical technique, Monte Carlo simulation allows people to account for risk in quantitative analysis and decision making.) The global model includes more than 200 regions and management types, providing for significant heterogeneity.

"Biofuel pathway analyses have traditionally ignored uncertainty," Sohngen said. "We've created one of the first methods to integrate uncertainty analysis, and it is the first implementation of Monte Carlo analysis in this type of land use modeling.

"Monte Carlo analysis with the global forest and land use modeling system routinely require eight to 15 hours on a desktop computer to obtain results. In order to make independent draws on over 1,000 parameters in the model, we need to solve a large number of scenarios. We benefit substantially by having access to the Ohio Supercomputer Center to run many of these computationally intensive scenarios simultaneously," Sohngen said.



Above: Net carbon change in forests due to the EISA 2007 biofuel mandate and 95 percent confidence intervals based on a Monte Carlo simulation analysis.

Project Lead: Brent Sohngen, Ph.D., The Ohio State University
Research Title: Global land use modeling
Funding Source: US Environmental Protection Agency Office of Transportation and Air Quality
Website: http://aede.osu.edu/our-people/brent-sohngen

LANDSCAPE CONNECTORS

Bohrer, colleagues confirm gaps, corridors enhance forest seed dispersal

A team of field ecologists has concluded that woodland corridors connecting patches of endangered plants not only increase dispersal of seeds from one patch to another, but also create wind conditions that can spread the seeds for much longer distances. The idea for the study emerged from modern animal conservation practices, where landscape connectivity – the degree to which landscapes facilitate movement – is being used to counteract the impacts of habitat loss and fragmentation on animal movement.

Gil Bohrer, Ph.D., an assistant professor in the Civil, Environmental & Geodetic Engineering department at The Ohio State University, and colleagues led by Ellen Damschen, Ph.D., an assistant professor of Zoology at the University of Wisconsin, wondered if similar interventions might aid plants that rely upon wind currents.

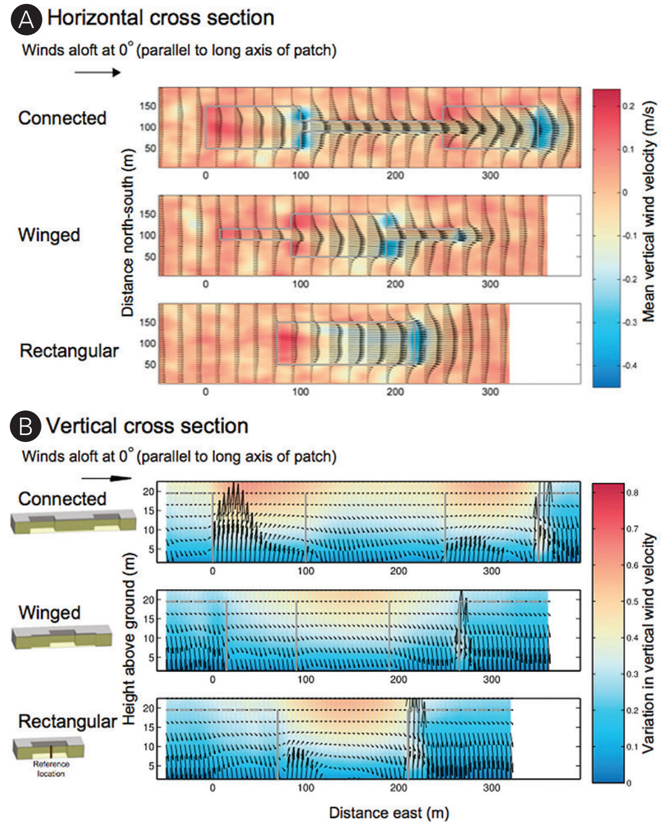
The field experiment involved connecting open patches of land by cutting gaps and corridors out of a longleaf pine plantation in South Carolina. A network of sensors was erected to provide observations on wind speed, turbulence, temperature and humidity. Seed traps sampled seed arrival at many points in and around the gaps, and hundreds of artificial seeds made of black-light fluorescent yarn were released and recovered in several controlled experiments.

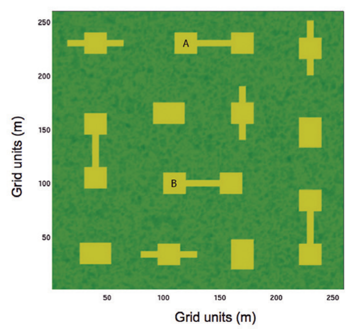
These very large experimental efforts provided a novel dataset of observations of seed movement and wind in patch-corridors landscapes, which scientists leveraged to generate a virtual and complete environment. Bohrer ran the dataset through a high-resolution atmospheric model that he had developed on Ohio Supercomputer Center systems.

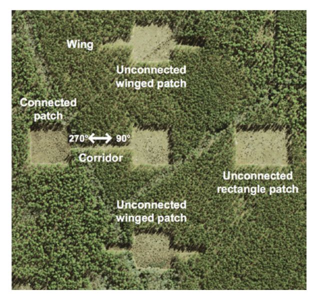
"The massive simulations used the Ohio Supercomputer Center to provide a detailed understanding of how corridors change the movement of the wind, and seeds that disperse with it, through a forest," Bohrer said.

The model resolves the wind flow and includes the effects of canopy leaves and tree stems on the wind. The simulations include a virtual domain of roughly 6.5 million pixels, each representing a volume of air (or air mixed with forest leaves) of about 10 cubic meters. It also represented millions of dispersing virtual seeds. The model calculated the movement of the air and virtual seeds 20 times per second, over four hours.

"We found that corridors could affect the wind direction and align the wind flow with the corridor, that they accelerate the wind and provide preferable conditions for ejection above the canopy, where long distance dispersal could occur," said Bohrer.







Top (A & B): In a study of how forest corridors could impact seed dispersal, Bohrer created a computer model to determine cross-sections of wind dynamics and seed ejection probabilities. The arrows correspond to horizontal wind speeds and directions. **Bottom:** Bohrer created a simulation domain (left) with a five-meter resolution, and an aerial photograph (right: Damschen/UW-M) reveals the experimental landscape used in the study.

Project Lead: Gil Bohrer, Ph.D., The Ohio State University
Research Title: How fragmentation and corridors affect wind dynamics and seed dispersal in open habitats
Funding Source: National Science Foundation, Department of Agriculture, Washington University
Website: http://www2.ceegs.ohio-state.edu/~bohrer.17/

GREENLAND ICE SHEETS

Howat, Noh build algorithm to generate digital surface model mosaics

Using the computing power at the Ohio Supercomputer Center, researchers at The Ohio State University are constructing a first-of-its-kind, time-stamped, high-resolution digital surface model of the Greenland Ice Sheet.

The vast body of ice – which covers roughly 80 percent of Greenland's surface – is of particular scientific interest. With record melting in recent years, the ice sheet is likely to contribute substantially to sea level rise.

"Digital surface models such as the one we are creating for the Greenland Ice Sheet will be transformational in glacier and climate-change related studies," said Ian Howat, associate professor at Ohio State's School of Earth Sciences. "It will provide a complete benchmarking map of the ice sheet that can be compared to both past and future measurements from various altimetry data."

Current digital surface maps, which create 3-D representations of the terrain's surface from elevation data, have resolutions of only 10's to 100's of meters, with a vertical accuracy comparable to the resolution. Additionally, they lack a definite time stamp, hindering comparative studies.

This new model builds on previous work by Howat and his Byrd Polar Research Center colleague Myoung-Jong Noh. They successfully demonstrated that their Surface Extraction from Tin-based Search Minimazation (SETSM) algorithim could automatically generate high-quality digital surface model mosaics over large regions, at very fine resolutions. Using data from Worldview 1 and 2 satellites, which take new photos of any place on Earth every 1.1 days, the algorithim retrived high-quality elevation data over a range of terrains, from very high relief mountain areas to flat expanses of the ice sheet.

"Our test data production revealed a major benefit of our approach: the high-resolution imagery enables surface extraction over relatively featureless expanses of ice and snow, including the interior of glaciers and ice sheets," Howat said.

SETSM's search minimization strategy enabled this result, in tandem with the very high spatial resolution and 11-bits-per-pixel of the Worldview imagery, which captures subtle features such as wind patterns in the snow and variations in grain size.

"This is a major breathrough because conventional imagery and digital surface model extraction methods fail in these areas." Howat added. "When our project is complete, we will have constructed a 3-D model of the Greenland Ice Sheet that will provide a major data set for polar and climate-change related studies."

Above and Cover: Howat's team applied their software to produce a complete Digital Surface Model of the Greenland Ice Sheet and its periphery at two-meter resolution. The process produced this visualization of the crevassed, tidewater glaciers of the Uummannaq region in coastal Greenland.

Project Lead: Ian Howat, Ph.D., The Ohio State University
Research Title: Demonstration of SETSM Phase 2: A 2-m Digital Surface Model of the Greenland Ice Sheet
Funding Source: National Aeronautics and Space Administration
Website: www.bprc.osu.edu/~ihowat

Analyze social networks. Understand the cosmos. Recognize facial expressions and speech patterns. Ohio's strengths in basic and applied research run broad and deep, spanning a multitude of academic organizations. The Ohio Supercomputer Center supplies the researchers working in these various fields of study – sampled on the following pages – with the computational power they need.

RESEARCH LANDSCAPE

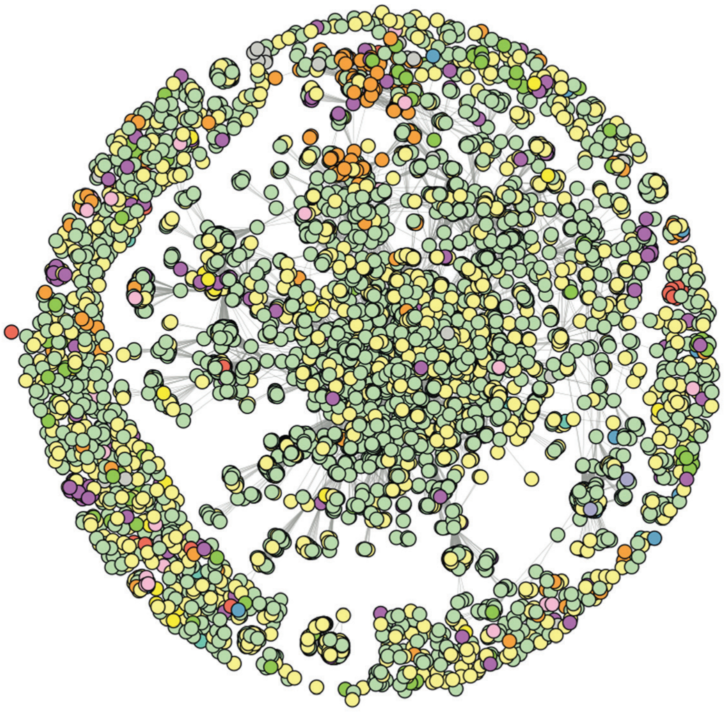
"We are leveraging Ohio Supercomputer Center resources to refine a popular statistical tool by accounting for random effects in the formation of networks. Precise modeling could improve analytics that have become increasingly vital to public health and the social sciences."

Janet M. Box-Steffensmeier, Ph.D.
Professor, The Ohio State University

NETWORK ANALYSIS

Box-Steffensmeier team tweaking model to account for randomization

The analysis of biological and social networks has become increasingly important in recent years. Inferential and predictive statistical models that analyze networks have been put to use in such areas as epidemiology, public health, molecular biology and the social sciences.



$$\Pr(\mathbf{y} \mid \mathbf{x}, \theta, \mathcal{Y}) = \frac{\exp\{\theta^T \Gamma(\mathbf{y}, \mathbf{x})\}}{\sum_{\forall \tilde{\mathbf{y}} \in \mathcal{Y}} \exp\{\theta^T \Gamma(\tilde{\mathbf{y}}, \mathbf{x})\}},$$

$$y_{ij} = -3.25\text{edges}_y + 0.75\text{gwesp}_{ij} + 0.25 \times \mathbf{1}(\text{group}_i = \text{group}_j) + \gamma(\sigma_i - \sigma_j).$$

$$\Pr(\mathbf{y} \mid \cdot) = \frac{1}{\kappa} \exp\left\{\theta^T \Gamma(\mathbf{y}, \mathbf{x}) + w_i + w_j\right\},$$

Above: This graph displays the network mapping of all interest groups, color-coded by industry area, that signed amicus briefs on Court per curiam or full opinions from 2000 to 2009.

Yet, while network analysis continues to attract a great deal of attention from scholars and the broader public, the quantitative study of networks remains in the early stages of development. Only recently have the statistical theory and computational techniques been developed to rigorously analyze many types of networks, but there remain significant gaps in the statistical tools that limit their usefulness to scientists.

A research group from The Ohio State University is seeking to improve the well known and widely used Exponential Random Graph Model, or ERGM, by adding a randomization effect – called a frailty term – to account for heterogeneity when modeling network formation.

"ERGMs provide a means of incorporating both structural network characteristics and individual-level traits in models that try to explain the network as a whole," said Janet Box-Steffensmeier, Ph.D., the Vernal Riffe Professor of Political Science at The Ohio State University. "However, while ERGMs offer important advantages over other methods of modeling network data, the approach currently lacks a method of incorporating unexplained heterogeneity, whether unmeasured, unobserved or unimagined, into these models. This is an important gap that limits the applicability of ERGMs in many areas of potential interest."

The first goal of the project has been to refine the statistical model by introducing individual (or group) random effects in order to model that heterogeneity in the propensity for individuals in the network to form ties. The second goal of the project has been to evaluate the statistical properties of the proposed model and to apply the model to well-known health behavior and social science data sets. The researchers leveraged Ohio Supercomputer Center systems to evaluate the model with a series of Monte Carlo experiments, which is a standard workhorse approach to assessing the performance of complex models in computational statistics.

"The significance of the project is that it will help fill a gap in the ERGM literature, allowing researchers to draw correct inferences in a broader set of circumstances," said Box-Steffensmeier. "And, for our own purposes, we are specifically interested in analyzing the diffusion of smoking and obesity in large social networks."

Project Lead: Janet M. Box-Steffensmeier, Ph.D., The Ohio State University
Research Title: Modeling unobserved heterogeneity in network formation with the frailty exponential graph model
Funding Source: National Science Foundation
Website: http://polisci.osu.edu/faculty/jbox/

FACIAL EXPRESSION

Martinez groups investigates methods to codify compound emotions

Understanding the different categories of normal facial expressions of human emotion is essential for scientists and doctors in order to gain insights into human cognition and affect, as well as for the design of computational models and perceptual interfaces. Past research on facial expressions of emotion – as far back as Aristotle – focused on the study of six basic categories of emotion: happiness, surprise, anger, sadness, fear and disgust. However, many more facial expressions of emotion exist and are used regularly by humans.

A research group led by Aleix Martinez, Ph.D., associate professor of Electrical and Computer Engineering at The Ohio State University, is investigating several important groups of expressions, known as compound-emotion categories. Compound emotions are those that can be constructed by combining basic component categories to create new ones. For instance, happily surprised and angrily surprised are two distinct compound-emotion categories.

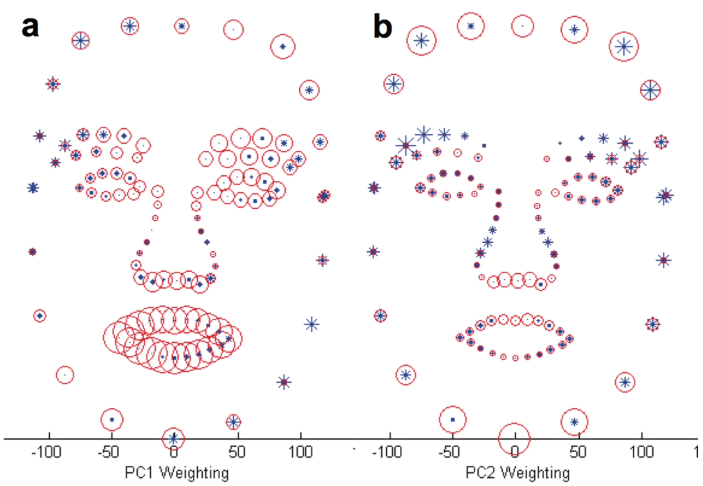
Martinez and his colleagues leveraged computational systems of the Ohio Supercomputer Center to analyze 5,000 facial-expression images of 230 subjects, categorizing the images by which facial muscles the participants used. The Facial Action Coding System (FACS) codifies facial expressions by action units, or muscles or groups of muscles that go into making facial expressions – such as lip parts (for showing disgust), showing teeth (for expressing happiness), mouth stretch (for fear), or eyelid tightening (for anger).

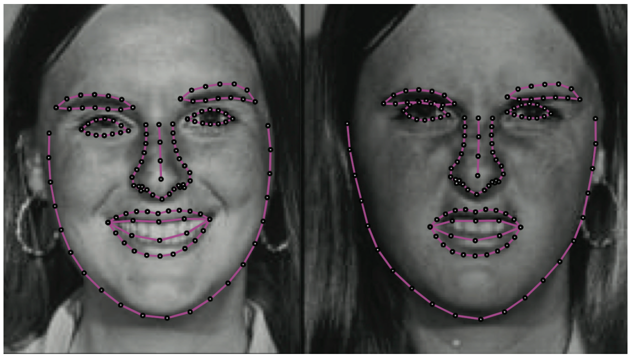
"Our current work defines 21 distinct emotion categories," Martinez explained. "An FACS analysis shows the production of these 21 categories is different from, but consistent with, the subordinate categories they represent. For example, a happily surprised expression combines muscle movements observed in happiness and surprised."

The long-term goal of the research is to understand how emotions and other facial cues – such as identity and grammar in sign languages – are encoded and interpreted from images and, thus, how these facial movements encode the communication signal.

"The main applications are in the understanding of what goes wrong in these computations in patients with certain conditions, such as depression, post-traumatic stress disorder or autism, as well as in the implementation of computational systems that can emulate this capacity," said Martinez.

The results of this proposal also will be useful to design computer algorithms that can do recognition of emotions. Face recognition is of primary importance in many areas of computational intelligence – ranging from human-computer interaction to content-based retrieval.

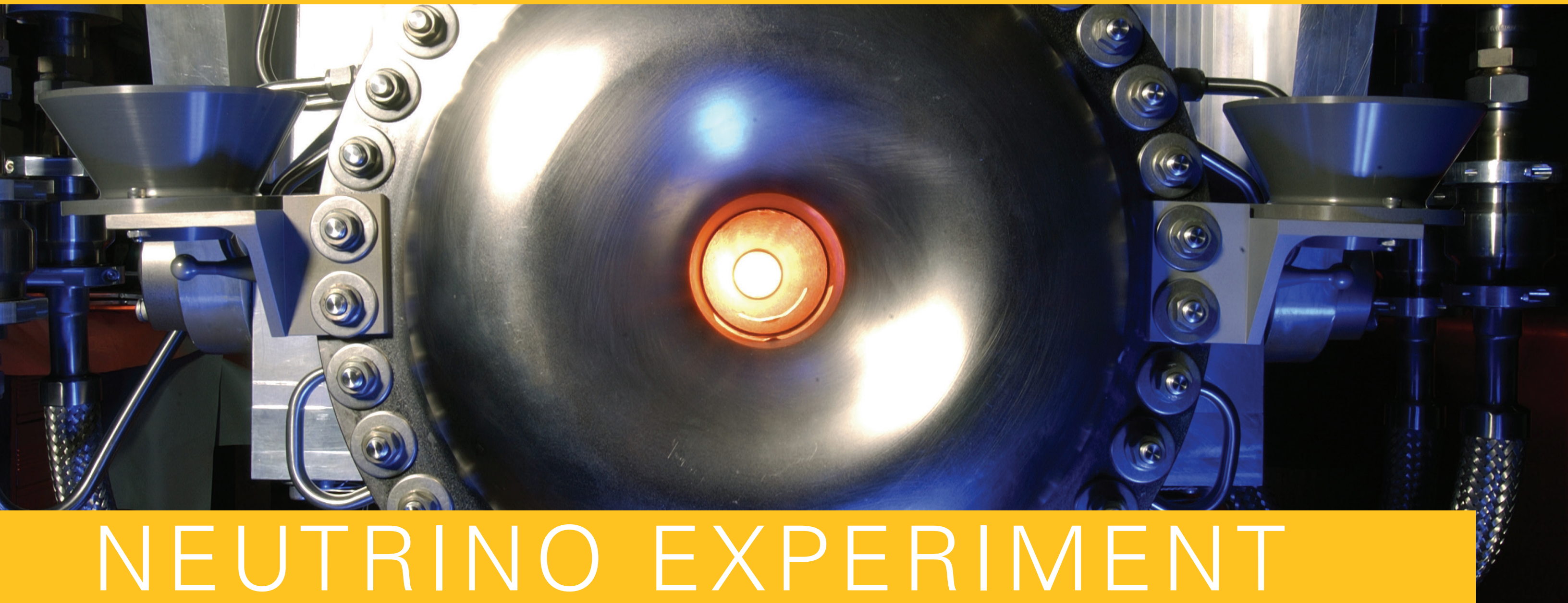




Left: These graphs indicate weighting of dimensions that most affect the perceptions of emotions in the image set; in this case, the graphs represent the dimensions for a.) sadness and b.) anger.

Right: Examples of shape-based recognition using a shape detection algorithm.

Project Lead: Aleix Martinez, Ph.D., The Ohio State University
Research Title: Face recognition: Computational modeling
Funding Source: National Institutes of Health
Website: http://www2.ece.ohio-state.edu/~aleix/



NEUTRINO EXPERIMENT

Sousa, other scientists evaluating behavior of elusive cosmic particle

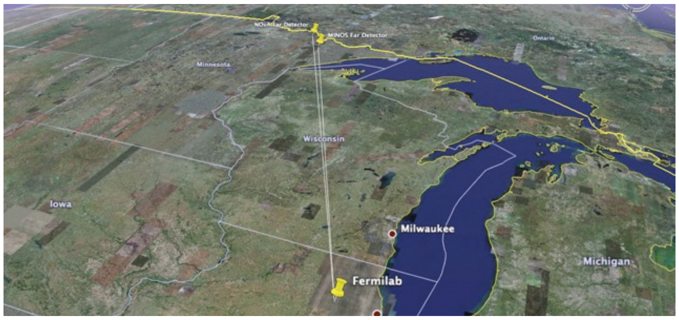
A researcher at the University of Cincinnati is leveraging the compute and storage resources of the Ohio Supercomputer Center to simulate the behavior of elusive cosmic particles. The research team is studying the behavior and nature of neutrinos and the particles' role in the balance between matter and antimatter.

Alexandre Sousa, Ph.D., an assistant professor of Physics at UC, is one of 208 scientists and engineers from 38 institutions from seven countries participating in the Department of Energy's Neutrinos at the Main Injector (NuMI) Off-Axis ve Appearance, or NOvA, experiment. Sousa is coordinating the development and validation of neutrino interaction simulations in the NOvA detectors and has been working with OSC staff to configure the Center to become what is now one of the experiment's primary locations for developing and generating simulations.

Each second, more than a trillion neutrinos from the sun and other celestial objects pass through the average human body. While neutrinos are a billion times more abundant than the particles that make up stars, planets and people, they so rarely interact with other particles that they are very difficult to detect.

In the NOvA experiment, researchers are using particle accelerators to send intense beams of neutrinos straight through the earth between massive particle detectors at Fermilab in Batavia, Ill., and even larger ones 500 miles away at facilities in Ash River, Minn. For six years, the detectors will capture and record the interactions of the neutrinos, creating massive amounts of data that researchers will use to study neutrino properties, especially the transition of one type of neutrino into another. Even with these large detectors, researchers will be challenged to detect actual neutrinos and will turn to simulations built upon sparse actual results to estimate outcomes for larger numbers of neutrinos. These simulations are equally fundamental in comparing the observed data with our own theoretical knowledge to measure neutrino properties and perhaps uncover unexpected surprises.

"The generation of NOvA simulated data involves several steps and multiple software packages," explained Sousa. "First, we will simulate the neutrino beam as it travels along its path and through the detectors. Second, we will simulate the neutrino interactions for each parent neutrino and its daughter particles. And, third, we will convert the detector energy depositions into digital signals analogous to the ones that will be produced during real data taking."



Top: The NuMI horn that scientists use to focus and steer a beam of particles that eventually decay into neutrinos.
Bottom: Scientists will detect a small fraction of the neutrinos in a near-detector at Fermilab and in a larger far-detector in Minnesota. The particles will complete the 500-mile interstate trip in less than three milliseconds.

Project Lead: Alexandre Sousa, Ph.D., University of Cincinnati
Research Title: A massively parallel computing approach to the generation of NOvA simulations
Funding Source: Department of Energy
Website: http://www.physics.uc.edu/~asousa/research.html

SPEECH SEPARATION

Wang, researchers train computers to hear through background noise

Machine-based speech separation, often referred to as "the cocktail party problem," refers to the problem of using computers and other devices to separate target speech from interference caused by background noise. Monaural speech separation, accomplished from input made with a single microphone or other source, is central to many real-world applications, such as robust speech and speaker recognition, audio information retrieval and hearing aid design. However, despite decades of effort, monaural speech separation remains one of the most significant challenges in signal and speech processing.

Traditional speech separation algorithms have fallen into two categories: speech enhancement and beamforming. Speech enhancement is primarily a signal-processing based approach that estimates the target speech based upon broad statistics of speech and noise, while beamforming utilizes a sensor or microphone array.

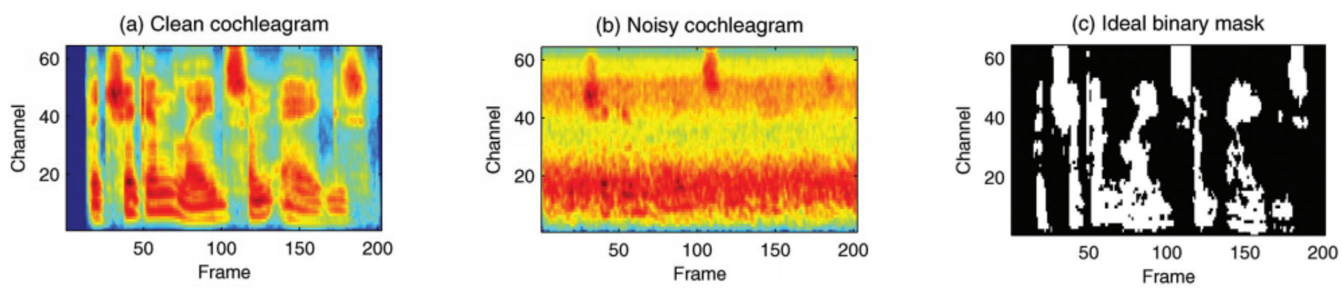
More recently, however, researchers have begun to use high performance computing to formulate speech separation as a binary classification problem – dividing the elements of a given set into two groups. With such a formulation, considerable advances have been made in computational auditory scene analysis on monaural speech separation.

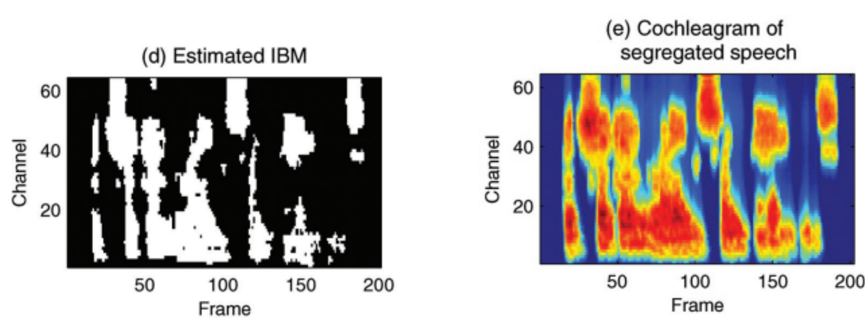
By utilizing resources at the Ohio Supercomputer Center, a research team headed by DeLiang Wang, Ph.D., professor of Computer Science and Engineering at The Ohio State University, already has made significant progress in identifying two important components of the supervised learning task for speech separation. First, the researchers identified a set of complementary discriminative features that works well for speech separation, and, second, they identified deep neural networks as better choices than many other alternatives.

"We are now systematically studying the use of deep neural networks for feature learning and classification for the purpose of speech separation," said Wang. "Specifically, we are training the classifiers on a large number of acoustic conditions in order to separate speech from a variety of noises."

To improve generalization of the system to unseen acoustic environments, the researchers employ a large number of speakers and noises.

"We've managed to obtain significantly improved generalization performance through training on hundreds of hours of audio data," explained Yuxuan Wang, an Ohio State doctoral student who is leading the research. "Solving the resulting large-scale machine learning problem is greatly facilitated by the Ohio Supercomputer Center."

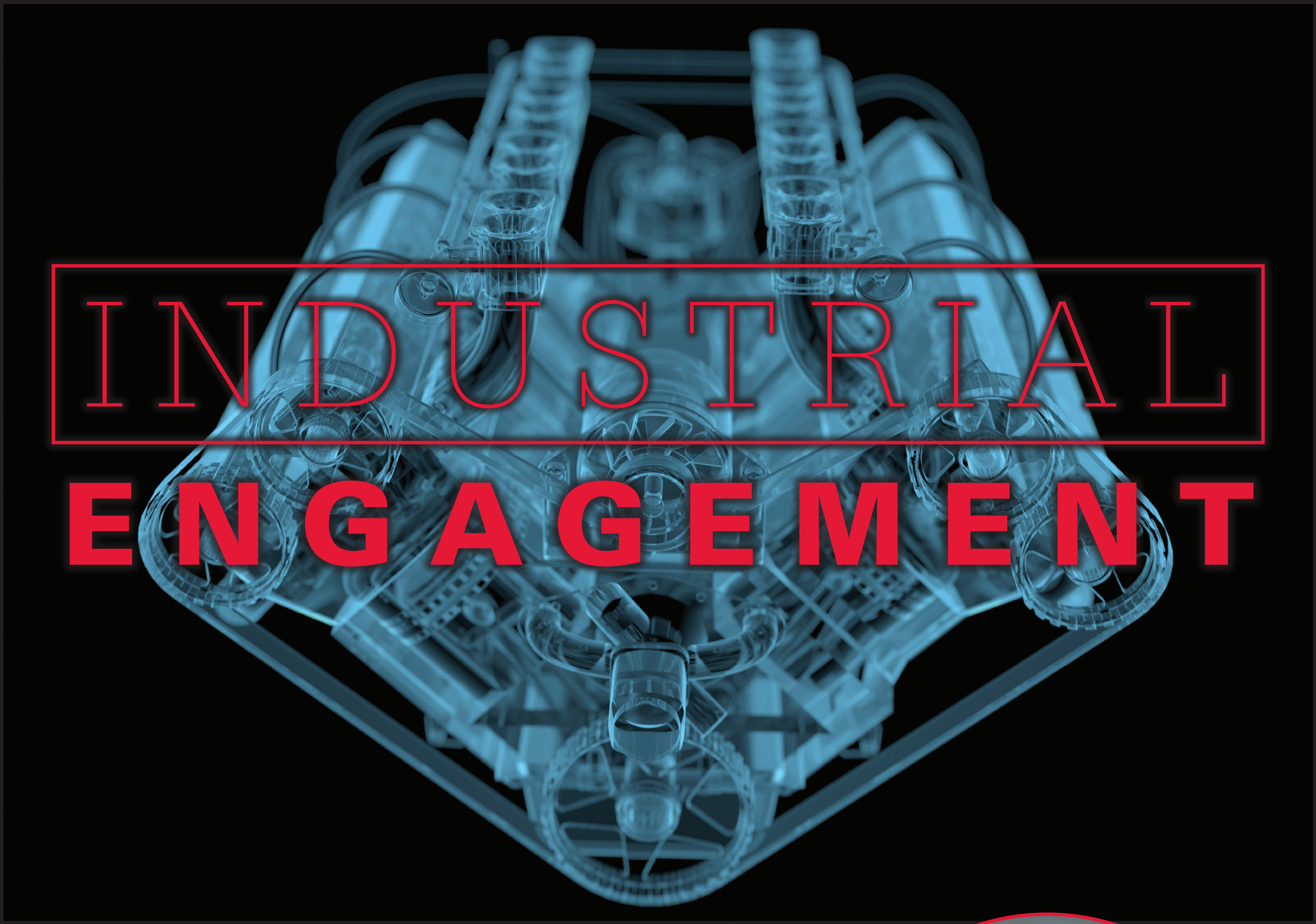




Illustrations: The charts illustrate Wang's team applying a mask (c) and d) to a noisy scenario (b) to produce speech reception (e) nearly identical to that of the original speech (a).

Project Lead: DeLiang Wang, Ph.D., The Ohio State University
Research Title: Large-scale computing for classification-based speech separation
Funding Source: Air Force Office of Scientific Research, Kuzer
Website: https://cse.osu.edu/people/wang.77

The Ohio Supercomputer Center has a legacy of supporting industrial research, reaching back to the Center's founding in 1987. Manufacturers have leveraged the Center's computational and storage resources to virtually test ceramic airplane components, simulate welding processes, and analyze volumes of enzyme sequencing data. This research, highlighted on the following pages, illustrates a sampling of OSC's partnerships with industry.



INDUSTRIAL ENGAGEMENT

"AltaSim is working with the Ohio Supercomputer Center to develop an online "manufacturing app" version of our modeling and simulation tool for designing ceramic-matrix composites. CMC components will boost next-generation aircraft engine performance, as well as benefit other industry sectors."

— **Jeff Crompton, Ph.D.**
Principal, AltaSim Technologies Inc.

CERAMIC COMPONENTS

Firm adapts tool for designing ceramic parts to manufacturing app

Aviation industry manufacturers have traditionally relied upon conventional metals and alloys for constructing internal engine parts. During operation, these engines can generate sufficient heat to raise temperatures to within 50 degrees of the melting point of the nickel-based superalloys, titanium, aluminum and steel used in engine construction.

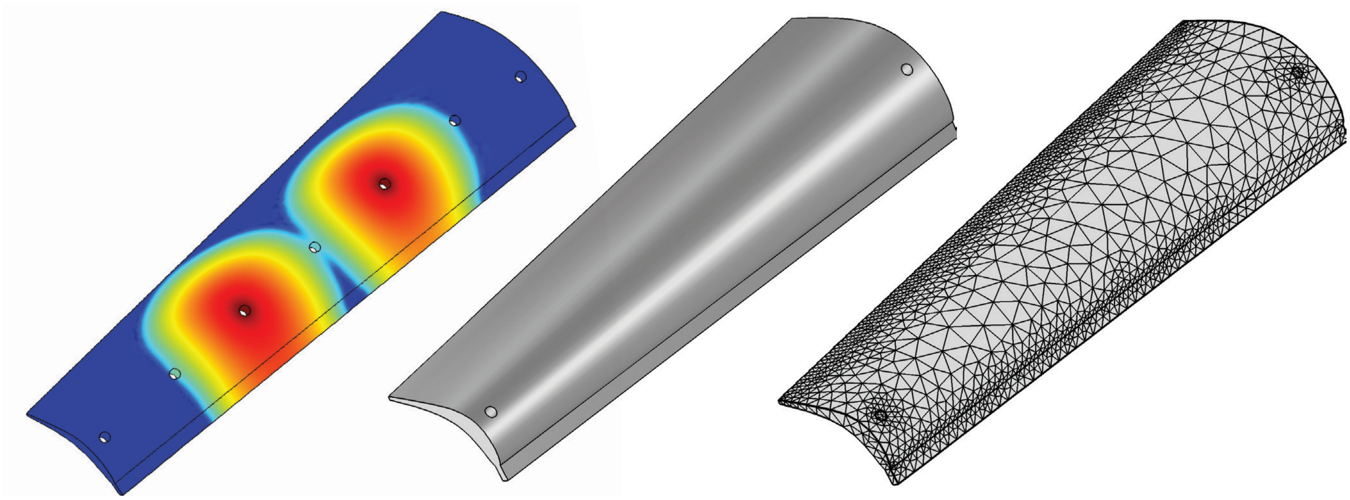
Next generation engines are being designed with increased power density to offer improved thrust and fuel efficiency, as well as reduced emissions. Operating temperatures approaching 2000° F are forecast for these design, thus requiring the use of new ceramic components that can withstand the severe environment.

When compared to metals, however, ceramics exhibit a relatively low resistance to fracture, a property that has restricted their extensive use in high-stress structural elements, such as turbines. To address this challenge, significant research has focused on the development of ceramic-matrix composites (CMCs), which fuse together a ceramic matrix and ceramic fibers to increase structural durability without losing high-temperature capabilities. Yet, the complexity of the manufacturing process for CMCs has precluded the routine, cost-effective manufacture of different components, shapes and materials.

"These barriers can be significantly reduced by using predictive computational design tools," said Jeffrey Crompton of AltaSim Technologies, a design and engineering firm that has developed a predictive computational modeling and simulation design tool for the CMC manufacturing process. "The range of physical phenomena that must be incorporated is large and the interactions that occur between them is complex; consequently no routine commercial simulation tool is currently available."

The design tool requires advanced computer software and HPC-based hardware, thus making it difficult for many practicing manufacturing engineers to use on a routine basis. Therefore, AltaSim engineers now are developing an online "manufacturing app" version of the tool in collaboration with the AweSim industrial outreach initiative at the Ohio Supercomputer Center. AltaSim also is expanding its existing CMC manufacturing design tool to reach applications in the automotive and chemical processing industries.

"To extend the commercial benefits of using CMCs to other industry sectors means that the design tool must be made readily available to the broader base of small and medium-sized businesses who routinely service the automotive and chemical processing industries," said Crompton. "This requires optimization of the design tool to meet the specific challenges of these industries and the development of intelligent interfaces around a common framework to allow non-expert users access to turn-key HPC based application solutions."



Above: Visualizations of an aircraft rotor made of ceramic-matrix composites. The CMCs will replace parts within next-generation engines to provide improved thrust and fuel efficiency.

Project Lead: Jeff Crompton, Ph.D., AltaSim Technologies
Research Title: Ceramic-matrix composite manufacturing technology
Funding Source: Department of Energy
Website: http://www.altasimtechnologies.com/advanced-materials/ceramic-matrix-composites/

WELDING SIMULATION

Engineering firm converts welding simulator to manufacturing app

The use of virtual design in the fabrication of large structures has enjoyed significant success in the heavy materials industry for almost two decades. Industries that have used virtual design and analysis tools have reduced material parts size, developed environmentally friendly fabrication processes, improved product quality and performance and reduced manufacturing costs.

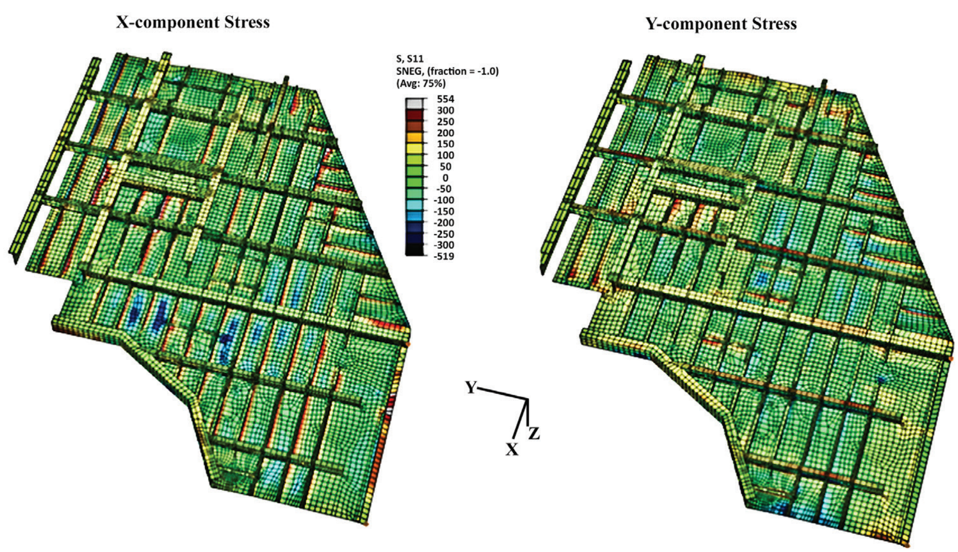
To boost this early success to a new level, the Engineering Mechanics Corporation of Columbus (Emc2) and its partners earlier this year secured a $1 million grant from the U.S. Department of Energy to develop a cloud-based tool that will simulate welding processes employed in the manufacture of metallic products. The funding was awarded through the federal agency's Small Business Innovation Research (SBIR) program, which encourages small businesses to develop and commercialize new technologies.

"Small and mid-sized manufacturing firms (SMMs) need improved weld-fabrication processes to ensure improved quality at lower costs to remain globally competitive," said Frederick "Bud" Brust, Ph.D., senior research leader at Emc2. "We are developing a sophisticated high performance computing based tool and making it accessible to SMM firms from a supercomputer center to easily permit use of these tools at affordable prices."

Emc2 seeks to adapt a welding design software package known as Virtual Fabrication Technology, or VFT, to a more accessible, open-source "manufacturing app" format through the Ohio Supercomputer Center's AweSim industrial engagement program. The project involves leveraging the existing code to address a broader range of applications and products for widespread use by SMMs.

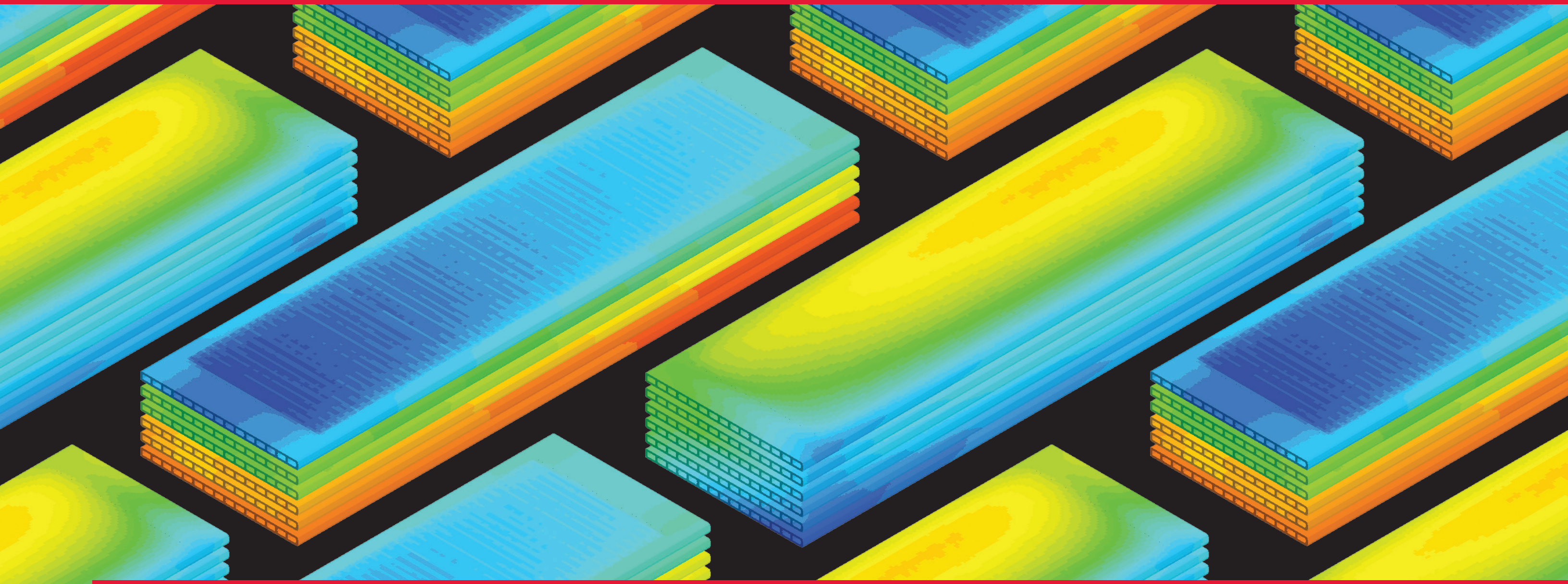
VFT is a mathematics-based computational tool that allows manufacturing designers to better control distortion, minimize residual stresses, and pre-determine welding parameters, such as weld-sequencing, pre-bending and thermal-tensioning, using various inputs, such as material properties and consumable properties. The code was developed in conjunction with Caterpillar in the late 1990s and currently is used by equipment manufacturers to design and model large welded structures prior to fabrication. Emc2 has licensed VFT for use across a broad range of fields, such as nuclear energy, shipbuilding and national laboratories.

Emc2 has made numerous improvements to VFT over the years to permit SMMs to take greater advantage of the benefits of high performance computing. Now, with the development and promotion of this simplified, affordable app version, SMMs will be able to access resources that could significantly reduce or eliminate undesirable outcomes prior to fabrication and avoid costly design changes after fabrication.



Above: Engineers at Emc2 use the welding design software package known as Virtual Fabrication Technology, or VFT, to visualize residual stresses in an oil rig panel. Control of these stresses can improve fatigue and corrosion life in deep sea drilling platforms.

Project Lead: Frederick "Bud" Brust, Ph.D., Engineering Mechanics Corporation of Columbus
Research Title: Adoption of high performance computational (HPC) modeling software for widespread use in the manufacture of welded structures
Funding Source: Department of Energy
Website: http://www.emc-sq.com/fea_code_devel.html



FUEL CELL MODELING

Manufacturer refines software to simulate heat, chemical, flow traits

High-temperature, solid-oxide fuel cells (SOFCs) are efficient electrochemical devices that produce electrical power from hydrocarbon fuels. SOFCs have received increasing attention in recent years as a clean and efficient power source for use in distributed power-generation applications. LG Fuel Cell Systems Inc. (LGFCS) is developing a megawatt-scale hybrid SOFC stationary power-generation system based upon its patented design.

To support product design and development activities, LGFCS has developed a SOFC multi-physics code (MPC) for performance calculations of its fuel cell structure. The MPC is based upon a computational fluid dynamics (CFD) software package, which has been enhanced with new models that allow for coupled simulations of the fluid flow, porous flow, heat transfer, chemical, electrochemical and current flow processes that occur in SOFCs. Simulations of single-cell, five-cell, substrate and multi-cell models have been validated successfully against LGFCS' experimental data. The MPC provides invaluable performance information, which drives design improvements, as well as enhancement in the fuel cell components, substrates, multi-cells and peripheral stack components.

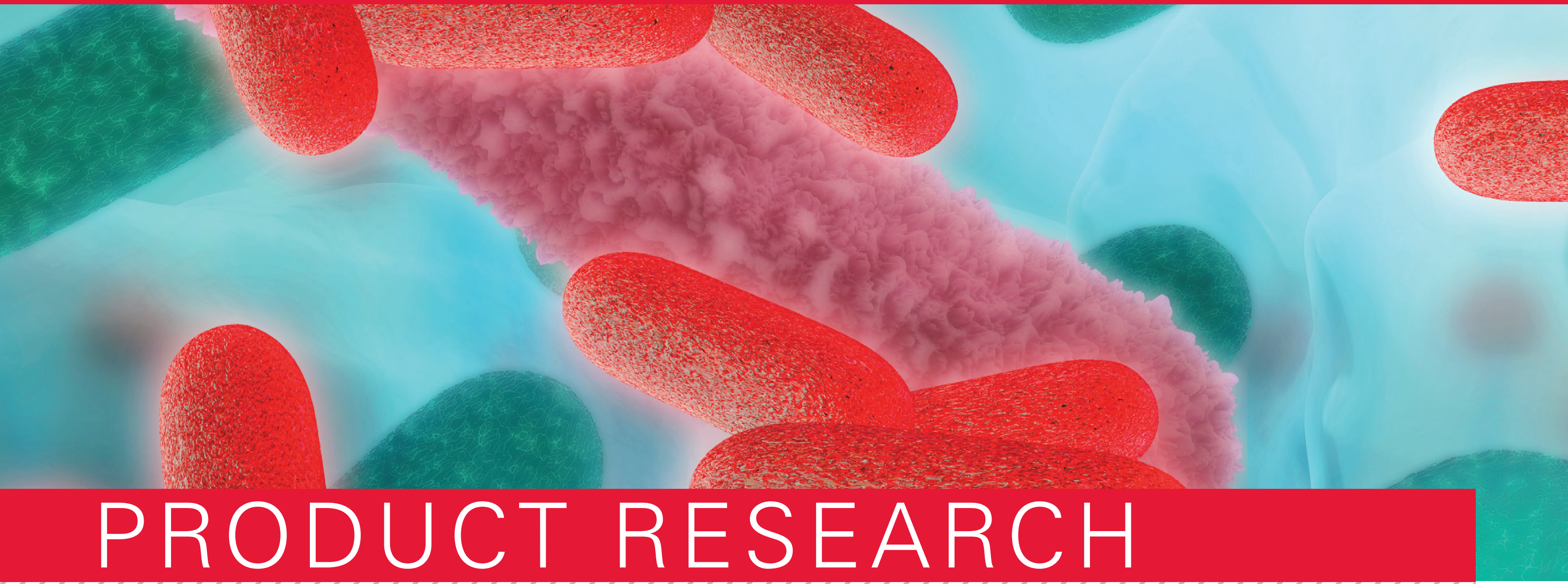
"LGFCS has been running the larger MPC models on Ohio Supercomputer Center systems. Typically, these MPC models are between one- and ten-million grid cells in size and are run in parallel using between 12 and 96 cores," said Carlos Martinez Baca, Ph.D., a CFD engineer with LGFCS. "A wide range of simulations have been run, from highly detailed models of electrochemistry and SOFC design to models of the peripheral components inside the LGFCS system."

To date, one of the most involved models is of a multi-cell simulation, which consists of a collection of six ceramic substrates with a printed cell pattern that includes hundreds of interconnected cells. Each of these interconnected cells comprises two porous electrodes (an anode on the fuel side and a cathode on the air side) that are separated by a gas-tight solid-oxide electrolyte layer. This multi-cell simulation also contains two main flow streams, a fuel-gas mixture rich in hydrogen flowing inside the substrates and a separate air stream flowing over the outside. The fuel-gas mixture diffuses through the porous substrate from the internal flows, and oxygen is supplied from the outside air stream. Electrochemical and chemical reactions occur in each cell and generate electrical power and heat.

Multi-cell simulations run at OSC have been used for a variety of purposes, including verifying on-design operation, analyzing off-design transients and performing analysis of new designs and operating modes.

Above: LG Fuel Cell Systems Inc. has developed a multi-physics code for performance calculations of its solid-oxide fuel cell structures. The code is based upon an enhanced computational fluid dynamics software package that allows for coupled simulations of the fluid flow, porous flow, heat transfer, chemical, electrochemical and current flow processes that occur in solid-oxide fuel cells.

Project Lead: Carlos Martinez Baca and Ben Haberman LG Fuel Cell Systems Inc.
Research Title: High temperature solid oxide fuel cell development in Ohio
Funding Source: Department of Energy
Website: http://www.rolls-royce.com/energy/energy_products/fuel_cells/



PRODUCT RESEARCH

Manufacturer analyzes how merchandise impacts biological systems

The Procter & Gamble Company, also known as P&G, is an Ohio-based multinational consumer goods company with manufacturing operations in approximately 70 countries worldwide. P&G markets a wide range of products, including cleaning agents and personal care products. With more than $80 billion in annual sales, P&G credits much of its success to its proven track record of innovation leadership, which includes consumer research, basic research, formulation science and an open innovation approach to collaboration.

"All the reasons that advanced modeling and simulation are used in the fields of aircraft, military, defense, electronics, automotive – all high-tech industries – are the same reasons we use it in our company ... to virtually test products and systems," asserted Tom Lange, director of modeling and simulation corporate R&D. "We use this rocket-science supercomputing for everyday products: to see whether formulations separate, that diapers fit on babies, how shampoos dispense, whether a razor breaks when you drop it, how tanks of toothpaste mix, how machines run and how they're scheduled."

As part of its basic research initiative, P&G scientists and engineers have pursued the identification and sequencing of genes, enzyme expression, molecular modeling simulation and use of X-ray crystallography to identify enzyme structure.

As an example, P&G researchers are actively applying various systems biology approaches to develop a more comprehensive understanding of how the company's products affect our consumers and the microbial communities that surround them. New sequencing technology has allowed the interrogation of various aspects of biological systems of interest, ranging from sequencing microbial genomes and analyzing microbial communities to generating transcriptome profiles. These trials produce data on the order of hundreds of megabytes to terabytes in size.

In collaboration with OSC, the P&G bioinformatics team has been able to process a high volume of sequencing data with the ability to customize software and to transfer data in and out of the cluster. Working together, P&G and OSC have effectively overcome the computational challenges to process and gain insight from these big biological data.

Additionally, P&G partnered with OSC and others in 2013 to form AweSim, a $6.4 million public/private initiative designed to promote the benefits of modeling and simulation to small and mid-sized manufacturers. The initiative was funded by the Ohio Third Frontier economic development initiative and program partners P&G, Intel, AltaSim Technologies, TotalSim USA, Kinetic Vision, Nimbis Services and OSC.

Above: P&G researchers are investigating microbes to develop a more comprehensive understanding of how the company's products affect their consumers and the microbial communities that surround them.

Project Lead: Tom Lange, Procter & Gamble
Research Title: M&S assistance for one of Ohio's largest manufacturers
Funding Source: Procter & Gamble
Website: http://www.pgscience.com/

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OSC extends its gratitude to all the researchers featured in the preceding pages for sharing their precious time, collaborative spirit and, most of all, fascinating scientific achievements.

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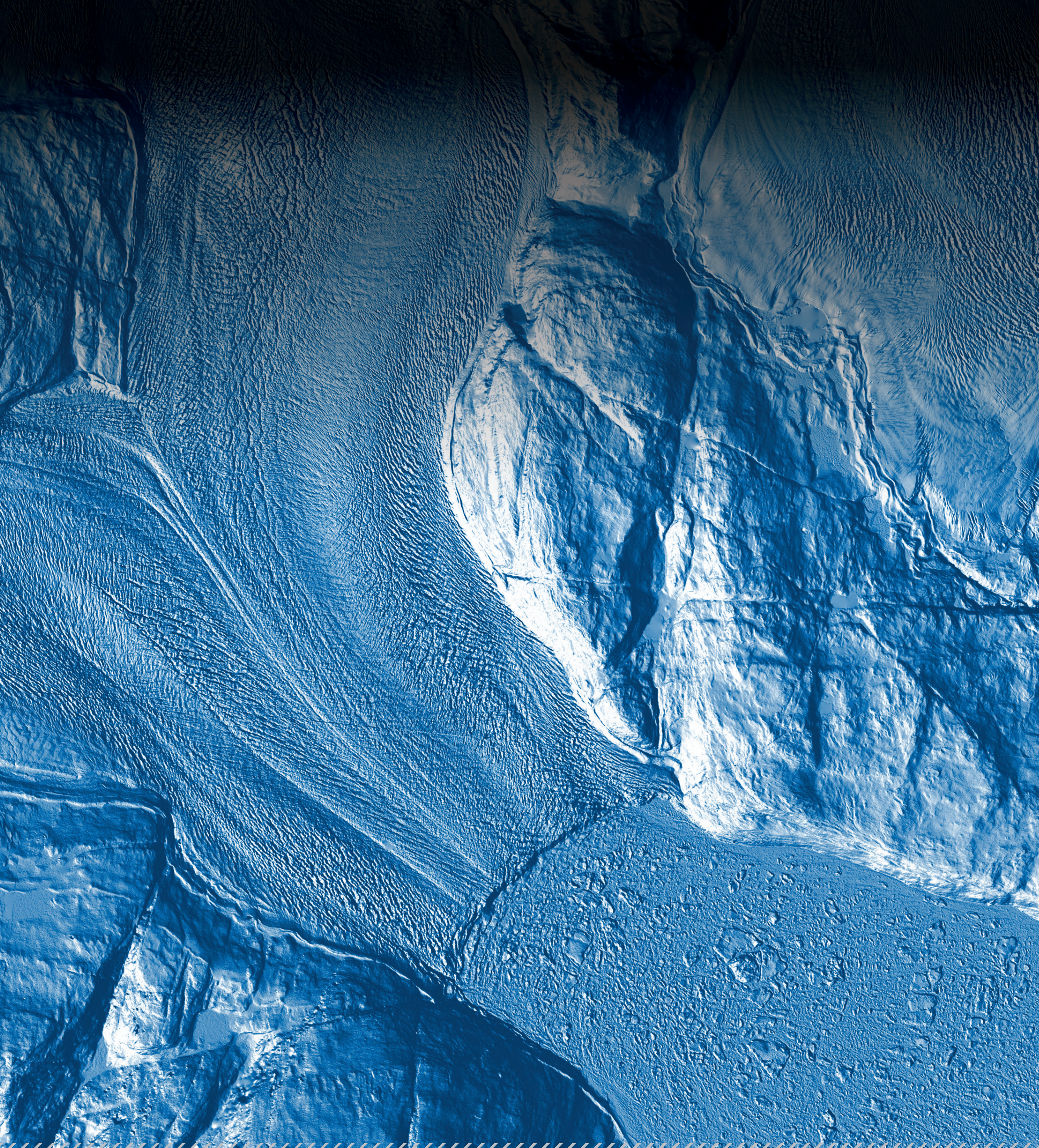

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