Ohio Supercomputer Center
An OH·TECH Consortium Member

2016 2017 RESEARCH REPORT

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osc.edu

"For more than 30 years, OSC has been a valuable tool for the state, helping to push Ohio to the forefront of the knowledge economy. Its clients across the state produce insights, discoveries and innovations that keep us healthier, safer, more productive and simply better informed."

— *John Carey, Chancellor, Ohio Department of Higher Education*

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

INTRODUCTION

With the passage of the state operating-budget bill in 1987, the Ohio Supercomputer Center was established "as a statewide resource available to Ohio research universities both public and private. It is also intended that the center be made accessible to private industry as appropriate."

For the past 30 years, the staff of the Center has been focused on fulfilling that mission. We have been providing core computational, storage, software, training and consulting services to each of these vital communities, helping to enhance Ohio's competitive position relative to other leading states. This Research Report is full of remarkable stories of our clients' many achievements across an extremely broad range of fields of study. It reflects just a small slice of the impact the members of the OSC staff have been able to make in supporting clients across those three decades.

Advancing Discovery

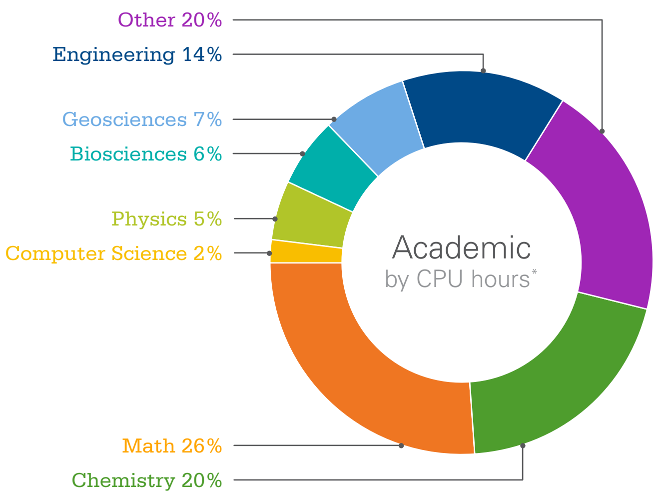
The establishment of a supercomputer center within Ohio was driven by the computational needs of faculty members at Ohio's research universities. Meeting those needs remains a pillar of our multi-faceted mission to this day; OSC provided services to more than 1,350 clients from 26 Ohio-based colleges and universities and 41 companies in 2016.

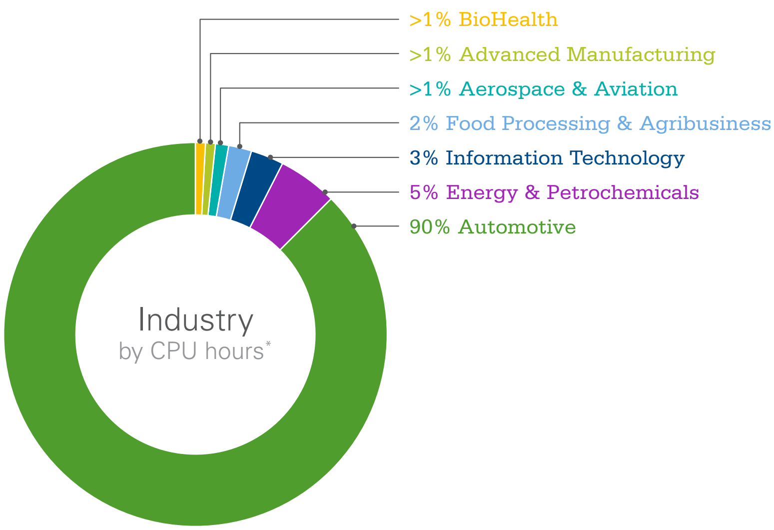
In March, OSC staff unveiled the most powerful supercomputer in the history of the Center, designed to serve the high performance compute (HPC) and storage needs of researchers at Ohio's colleges and universities. The Owens Cluster—named for iconic Olympic athlete Jesse Owens—offers our clients the computational power of more than 23,000 cores. We also recently upgraded our entire data storage environment and renovated our data center suite.

Additionally, some groups and organizations have invested in condo arrangements that provide them with priority usage on a small, but significant, number of nodes on our supercomputers. Beyond the hardware, the OSC staff also provides training, in the form of either workshops or consultations, to help research teams achieve the most efficient use of our multiple systems. In fact, more than 200 individuals attended workshops offered by the Center in 2016.

Enhancing Education

Another of our pillars is our role in supporting the academic enterprise of Ohio's colleges and universities. Many primary investigators employ





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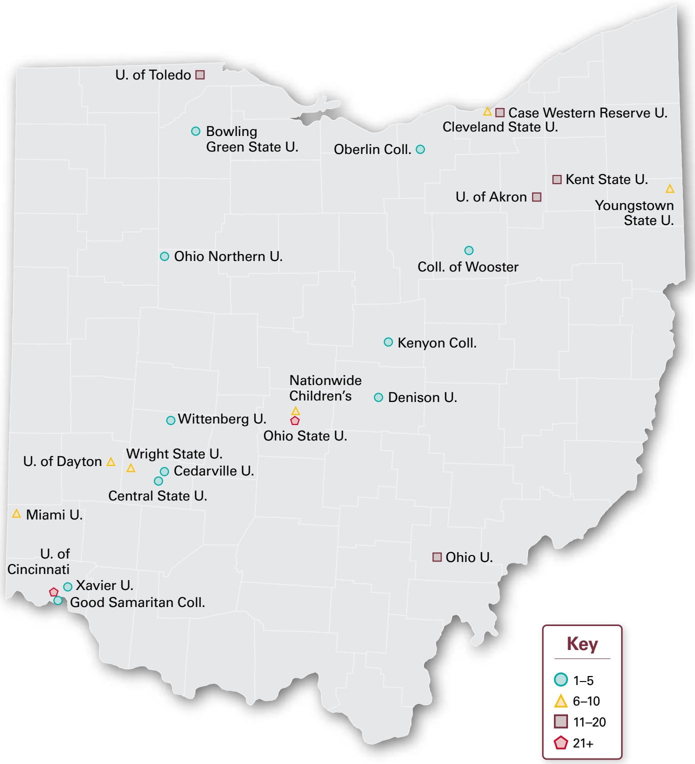
{TOP} David Hudak, Ph.D., Interim Executive Director, Ohio Supercomputer Center

ACTIVE PROJECTS*



NEW PROJECTS*

*All data CY2016

graduate and, sometimes, undergraduate students on their research teams. Access to OSC's systems often speeds the pace of their academic research projects, which would have taken far longer or might have been entirely impossible to complete on desktop units.

OSC also offers professors access to classroom accounts so that students can be given quality hands-on experience working on one of our clusters. Last year, OSC supported more than 31 academic courses with allocations of time on our systems, software provisioning and consultation. Additionally, we provide provosts and department heads with detailed information on OSC services to help recruit faculty members who see these services as a competitive advantage for locating in Ohio.

Driving Innovation

Supporting the research initiatives of Ohio business and industry is a third pillar of our mission at OSC. Charged with this goal from the beginning, OSC has become an international leader in the area of HPC industrial engagement. Just this spring, a business client leveraged 16,800 cores of the Owens Cluster to run the single-largest scale calculation in the Center's history to test its massive database software.

Whether a firm—from a start-up to a large, established manufacturer—needs to purchase cycles on our supercomputer systems to run projects, wants to purchase access only for times when its in-house systems are at maximum capacity or prefers to address computational issues easily through our web-based AweSim portals, we have a solution to fit almost any computational challenge.

Making access to supercomputing simpler and more intuitive has always been a goal of OSC, whether the client comes from industry, universities, government labs or elsewhere. This year, we launched Open OnDemand 1.0, an open-source version of OSC OnDemand—our "one-stop shop" for access to our high performance computing resources. Open OnDemand is available to HPC centers worldwide. To date, about a half-dozen HPC centers have installed and deployed the package, and another half-dozen have installed the portal for testing and evaluation.

OSC advances knowledge of

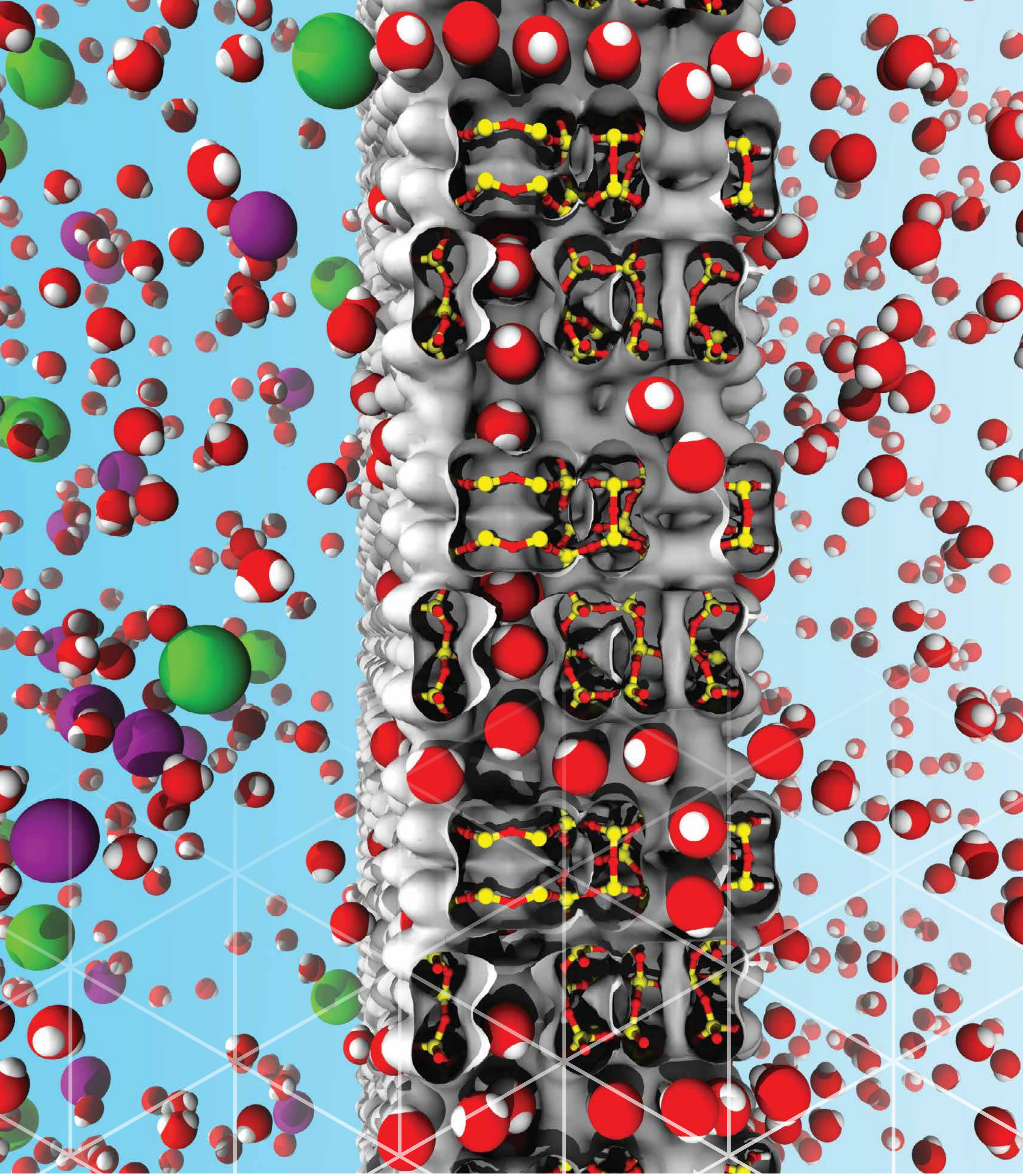
Advanced Materials

Scientists researching advanced materials rely heavily upon microscopy, data analytics and high performance computing. These next-generation technologies boost studies in areas, such as polymer design, hydrogen storage and atomic-scale semiconductors.

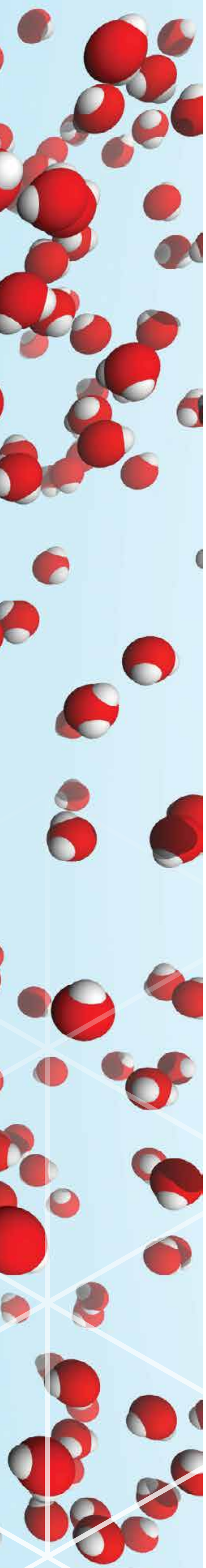
The computational and storage services offered by the Ohio Supercomputer Center enable engineers to synthesize data in less time and model complex nanostructures, accelerating their research and the emergence of new materials into the marketplace.

"There's no way to do my work without HPC; I'd just quit and do something else. I do research in such a way that I can visualize things experimenters can never see. If we don't have a visual representation, it's very hard to go forward and invent things."

— *Alexey T. Zayak, Ph.D., Department of Physics & Astronomy, Bowling Green State University*



Lin's group uses OSC to simulate molecules for water desalination such as aluminosilicate nanotubes that can transport water while limiting the amount of salts that pass through.



WATER DESALINATION

Lin's group tests nanomaterials for optimal filtration properties

Over 96 percent of the water on Earth is undrinkable and unusable for most human purposes. While removing salt from ocean water is possible, desalinated water costs up to 10 times more than typical groundwater. Li-Chiang Lin, Ph.D., and his team at The Ohio State University's Chemical and Biomolecular Engineering Department, with additional collaborators, are working to bring these costs down by identifying ideal water desalination materials. They have narrowed down candidates by using molecular simulations through the Ohio Supercomputer Center and identified promising ultrathin-film membrane candidates that provide maximum water fluxes while blocking any salts from coming through.

"The role of the supercomputer over here is it allows us to study a number of materials efficiently to explore promising ones," Lin said. "We perform molecular simulations, which also allows us see exactly how water molecules can permeate through a membrane and how salt ions are going to interact with the membrane."

Lin's group has identified two promising groups of materials as favorites for efficient water desalination. One is single-walled aluminosilicate nanotubes. These materials easily transport water due to their hydrophilic properties, as well as straight and uniform channels. The group runs tests on nanotubes of varying pore sizes to find the right structure that will most efficiently trap salts while allowing a high degree of water flow through the membranes.

The other group involves man-made, three-dimensional crystalline structures called zeolite materials. These structures can be made into an ultrathin film, down to a nano-scale thickness (so-called zeolite nanosheets), an excellent property for separations. Molecular simulations were carried out to model varying pore sizes, channel sizes and structure of different zeolite materials to identify their potential in water desalination.

"There are in fact millions of zeolite materials that may possibly exist, so this is why we first studied 27, trying to create a guideline for the rational design of novel materials," Lin said. "One million structures is a little bit too many to study."

Lin's studies have taken him around the country to places, such as UC Berkeley and the Massachusetts Institute of Technology, where he used internationally regarded, state-of-the-art supercomputing clusters. He remains impressed by what OSC can offer researchers in Ohio.

"It has been an amazing experience to use OSC for research projects," Lin said. "OSC offers excellent support, and OSC's supercomputers, in particular the newest machine Owens, are very fast. Additionally, the typical waiting time for jobs is relatively short. All of these have largely helped facilitate the progress of our projects, and we really appreciate all the resources provided from OSC." ◀

PROJECT LEAD // LI-CHIANG LIN, PH.D., THE OHIO STATE UNIVERSITY RESEARCH TITLE // COMPUTATIONAL DISCOVERY OF NANOPOROUS MATERIALS FOR WATER DESALINATION FUNDING SOURCE // THE OHIO STATE UNIVERSITY WEBSITE // LIN-GROUP.ENGINEERING.OSU.EDU/PEOPLE/LIN.2645

COMPUTATIONAL CHEMISTRY

Del Bene marvels at OSC's growth, continues theoretical breakthroughs

Janet Del Bene, Ph.D., has dedicated five decades of her career to research in theoretical chemistry. And she's done it with, and without, the help of the Ohio Supercomputer Center. Of course, the only time she didn't use the Center's high performance computing capabilities was when they didn't exist.

As a professor and computational chemist at Youngstown State University, Del Bene participated in many of the early efforts that led to the establishment of OSC in 1987. In the late 1980s, she was the third chairperson of the OSC Statewide Users Group.

"That was a really exciting time," she said. "I was on sabbatical in 1988–89 working with Professor Isaiah Shavitt at The Ohio State University. This was when the first Cray was being installed. The machine was in the shape of a 'C' and on the outside was the cooling system, which had cushioned seating. That was the most expensive seat I have ever had.

"I was fortunate to have been involved in the early stages of computing. When I first began using computers, it was necessary to write code, since there were no canned chemistry programs available. Because most chemistry students today do not write code, I think they are missing out on appreciating the intricacies of computers, and how computers work to carry out instructions."

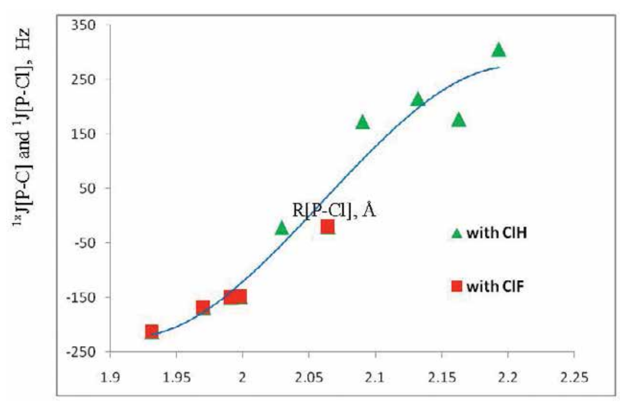
Del Bene has been on a "continuous sabbatical" for 19 years, during which time she has continued to be a leader in theoretical studies of intermolecular interactions, publishing 285 papers to date. These are interactions between two molecules when they come together to form some type of complex.

Since 2002, Del Bene has been collaborating with Ibon Alkorta, Ph.D., and José Elguero, Ph.D., from the Spanish National Research Council. Together, they compute and analyze the structures and binding energies of complexes, and many other properties.

Del Bene uses an ACES II code on OSC's Oakley Cluster to calculate Nuclear Magnetic Resonance spin-spin coupling constants for complexes.

"These computations are very demanding even for today's machines," Del Bene said. "I continue to marvel that I can run a job for days and get a lot of numbers, and then make chemical sense out of them. Doing this allows me and all of us to better understand the wonderful physical world in which we live. All of this work has been made possible through the support of OSC." ◀

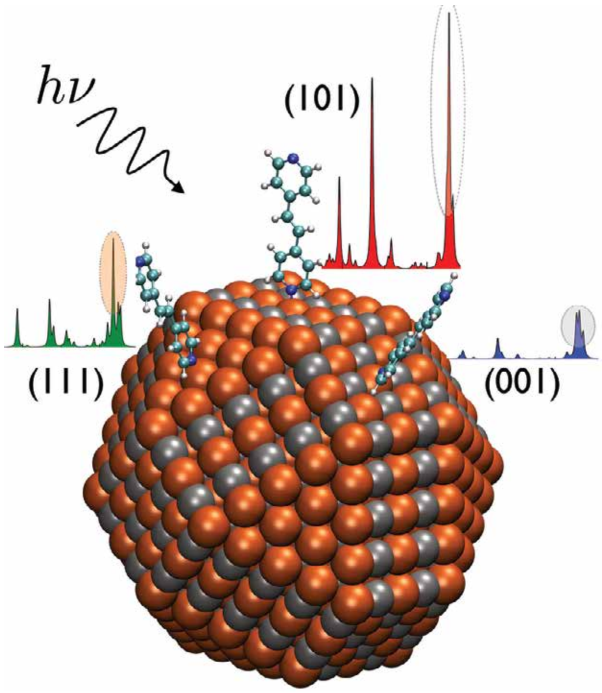
{LEFT} Janet Del Bene, Ph.D. {RIGHT} Del Bene sitting on the OSC Cray in 1988. {GRAPH} Nuclear Magnetic Resonance spin-spin coupling constants are calculated using ACES II code on OSC's Oakley Cluster.



PROJECT LEAD // JANET DEL BENE, PH.D., YOUNGSTOWN STATE UNIVERSITY RESEARCH TITLE // EOM-CCSD STUDIES OF MOLECULAR PROPERTIES IN ELECTRONIC EXCITED STATES FUNDING SOURCE // YOUNGSTOWN STATE UNIVERSITY WEBSITE // RESEARCHGATE.NET/SCIENTIFIC-CONTRIBUTIONS/39799772_JANET_E_DEL_BENE

RAMAN SPECTRA

OSC helping BGSU's Zayak give scientists valuable insight



A schematic representation of face-dependent Raman spectra.

From solar cells to electronic tools, new devices are created every day by combining two or more different materials to create a heterogenous interface. Those interfaces play a major role in how those devices function.

But while developers and experimentalists know the properties of individual materials—whether it's graphene, metal, gold or any number of materials—they don't know enough about what is happening between those materials at the point of contact.

"You need some spectroscopic way to extract that information," said Alexey Zayak, Ph.D., assistant professor of physics and astronomy at Bowling Green State University.

A longtime client of the Ohio Supercomputer Center, Zayak uses the Oakley Cluster to establish a computational approach for a quantitative spectroscopic analysis of the vibrational dynamics within heterogenous interfaces.

"You can't go inside the interface and extract data yet," Zayak said. "A lot of the knowledge is empirical. Empirical knowledge is varied and slow. It's hard to expect big discoveries in this case. But if you have a predictive model, you can get a deep understanding of what is happening and design systems to optimize certain parameters of the interaction."

Zayak's goal is to develop a new type of spectroscopy to find out exactly what is happening at those interfaces. He is using electronic structure calculations of Raman spectroscopy at interfaces to compare the Raman spectra of isolated systems with the Raman spectra of the same systems after they have been merged together. Raman spectroscopy is capable of observing the interfacial interactions on the scale of a single chemical bond.

"I can then explain where the differences in the spectra of the combined systems come from and what they mean," he said. "By looking at those differences, I can tell what is happening with the molecule on that surface, which helps people interpret experimental data. Now, the data is available but no one can read it."

Using Raman spectroscopy and computational "experiments," Zayak can show how electrons at heterogeneous interfaces are responding to the vibrations of molecules and substrates. That is valuable information for scientists to gain a conceptual understanding of what is happening at the interface.

And what Zayak is doing would be impossible without high performance computing.

"I would quit and do something else," he said. "OSC is such a great resource. There's no way to do my work without HPC." ◂

PROJECT LEAD // ALEXEY ZAYAK, PH.D., BOWLING GREEN STATE UNIVERSITY RESEARCH TITLE // VIBRATIONAL SPECTROSCOPY OF HETEROGENOUS CHEMICAL INTERFACES FUNDING SOURCE // BOWLING GREEN STATE UNIVERSITY WEBSITE // PHYSICS.BGSU.EDU/~AZAYAK

PHARMACEUTICAL DESIGN

Paluch infuses supercomputing into undergraduate chemistry classrooms

In his classroom, Andrew Paluch, Ph.D., is not only teaching classical theories but also training a new generation of supercomputer-savvy scientists. The Miami University Department of Chemical, Paper and Biomedical Engineering professor is helping undergraduates design molecules, such as pharmaceuticals, at the atomic level and predict their physical properties using molecular simulation and electron structure calculations performed with the help of the high performance computing systems and software packages at the Ohio Supercomputer Center.

"Everything I do is focused with undergraduates in mind, so I try to have some educational aspect to everything," Paluch said. "Our goal is to try and link state-of-the-art computational technologies to traditional physical-modeling approaches. The novelty in what we do is trying to link these two worlds, which are often disconnected."

One particular application is the design of pharmaceuticals. New drug candidates can be designed at the molecular level to bind to a particular protein target. Paluch's group then goes further and applies electronic structure calculations and molecular simulation to predict properties, such as toxicity and water solubility.

"Imagine you have proposed a new drug candidate or a new molecule has been synthesized. Early in the design process experimental data is often lacking and sufficient material does not exist for measurements," Paluch said. "We're trying to estimate these properties to see if this would be a realistic product to pursue further."

Paluch's undergraduate students see a direct connection to their coursework through the projects they are pursuing with the help of OSC's computational power. Many of their active classroom research projects have been published, and they have also presented at OSC's annual Statewide Users Group conference. The flash talks and poster competitions allow students to present their research at an off-campus location, an opportunity most would not be able to pursue until at least graduate school.

"OSC is pretty invaluable to me. I'm in a non-Ph.D.-granting department so my financial pockets are much shallower than (other researchers)," Paluch said. "Without OSC I would never have been able to do anything that I've done with these undergrads, and they wouldn't have had the experiences that they've had." ◄

Paluch takes advantages of opportunities, such as OSC's Statewide Users Group Conference, to expose undergraduates to research early in their academic careers.

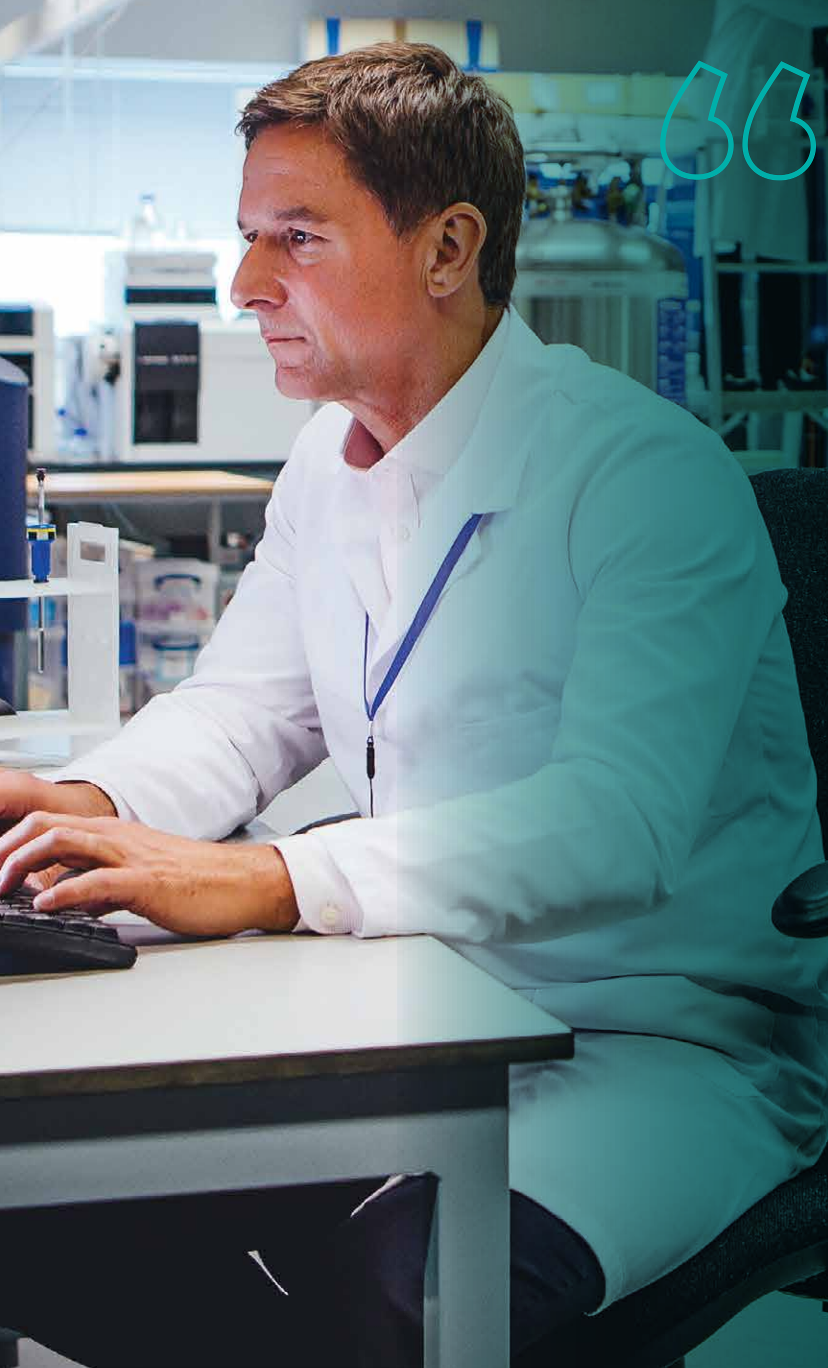
PROJECT LEAD // ANDREW PALUCH, PH.D., MIAMI UNIVERSITY RESEARCH TITLE // MOLECULAR DESIGN OF NOVEL IONIC LIQUID-BASED SOLVENTS FOR PHARMACEUTICAL APPLICATIONS FUNDING SOURCE // MIAMI UNIVERSITY WEBSITE // MIAMIOH.EDU/CEC/ACADEMICS/DEPARTMENTS/CPB/ABOUT/FACULTY-STAFF/PALUCH

OSC helps untangle the

Biological Sciences

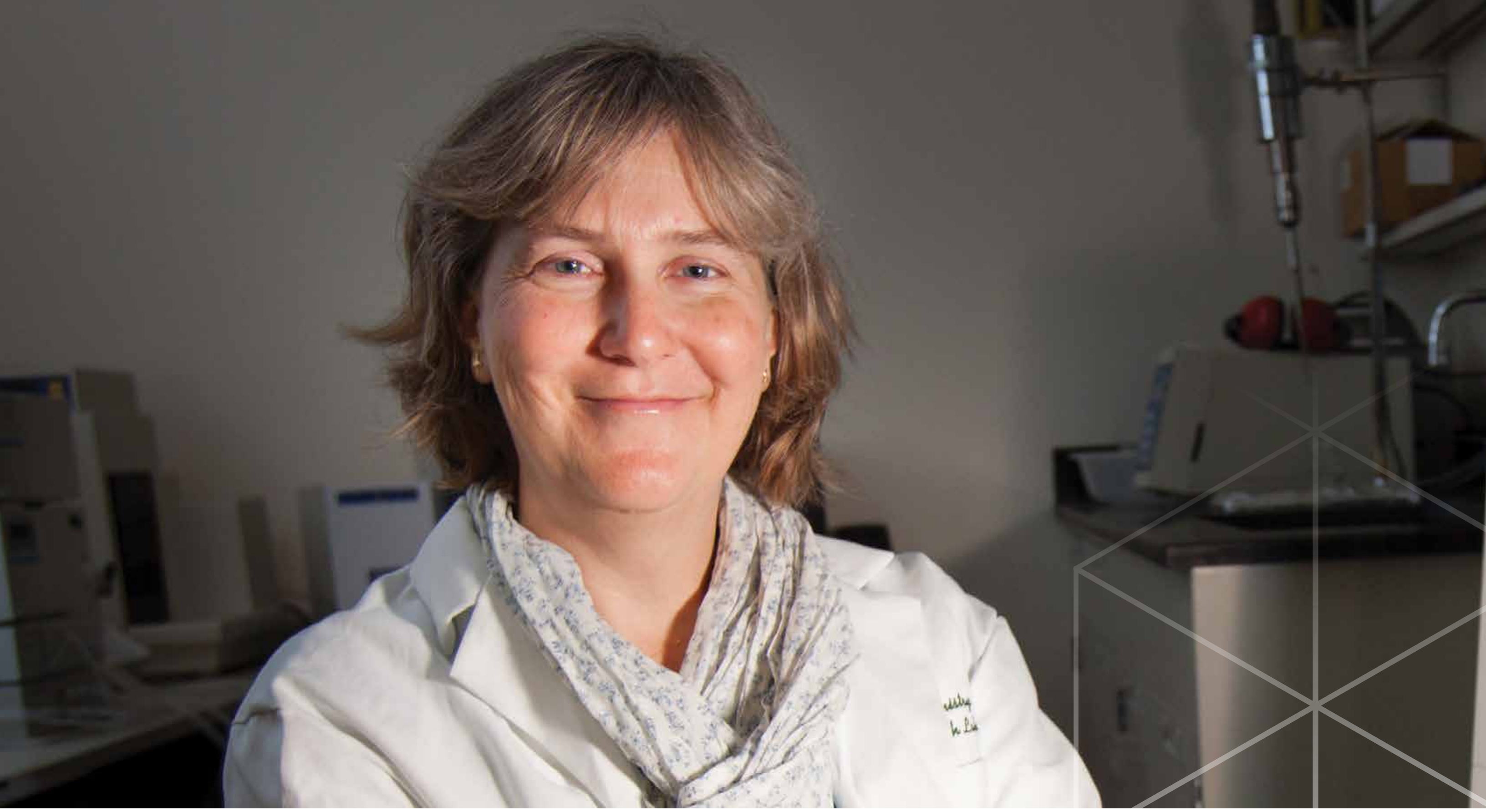
Researchers in the biosciences leverage modeling and simulation to improve quality of life. These technologies play a crucial role, enabling researchers to track disease outbreaks, sequence the genomes of entire species and even model new pharmaceuticals.

The Ohio Supercomputer Center staff recently deployed the powerful Owens Cluster and an upgraded data center infrastructure to provide the computing, networking and storage solutions required to support this crucial, sophisticated research.



"In the field of biomechanics, computational methods and simulations are becoming more prevalent and more essential. Whether it's to study the basic science, physiology, mechanobiology or it is in the productive development, the future is in simulation."

— *Rouzbeh Amini, Ph.D., Department of Biomedical Engineering, The University of Akron*



RNA SIGNALING

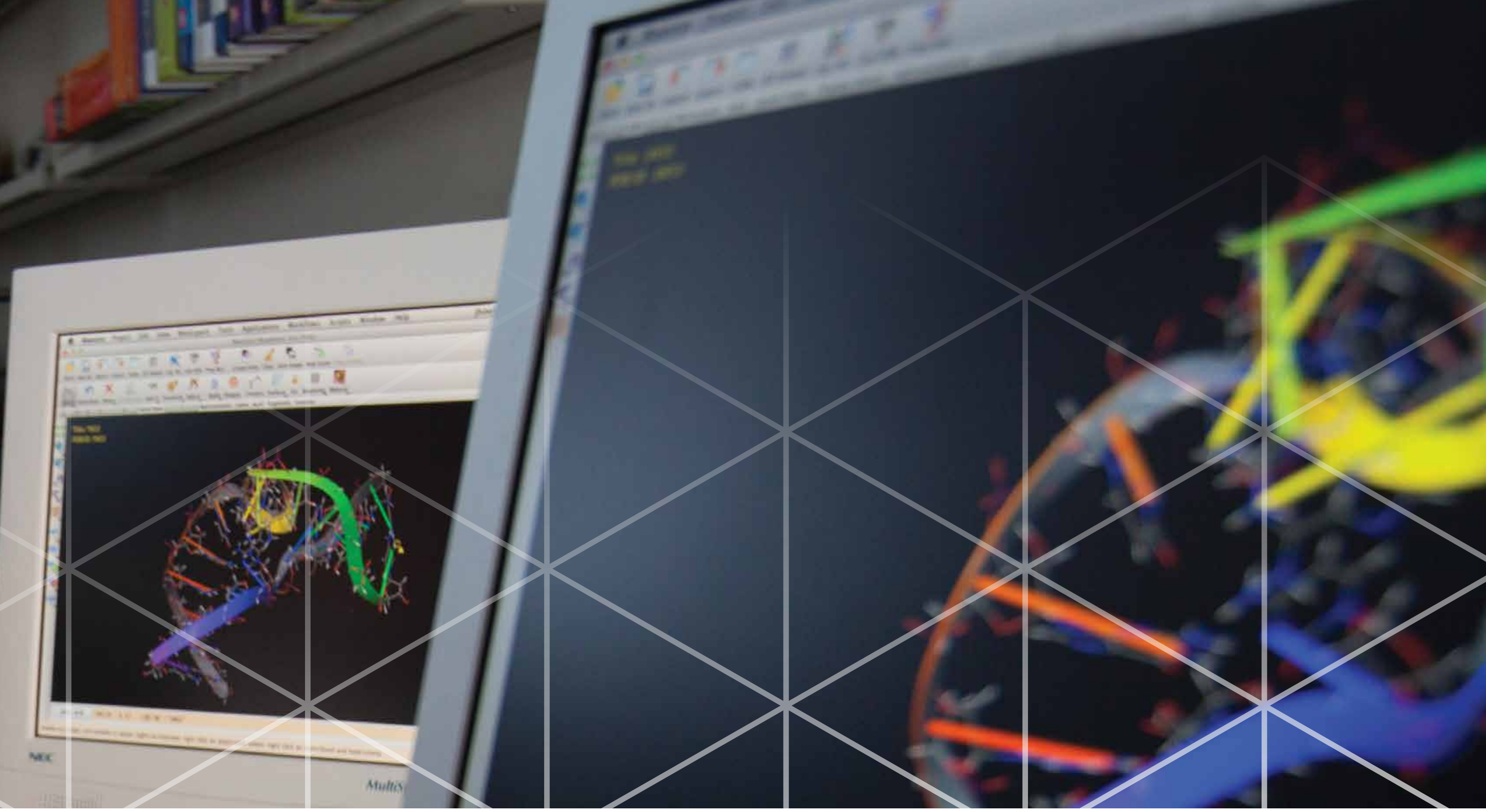
Hines revolutionizes drug discovery with RNA in the spotlight

The rise of antibiotic resistance among common infectious bacteria is a worrisome health threat that has many scientists looking for a solution. Jennifer Hines, Ph.D., professor of chemistry and biochemistry at Ohio University, is one of the few looking to ribonucleic acid (RNA) structures for new drug discovery. Her research group is studying a key regulator for bacterial gene expression made up of RNA, called a riboswitch, that could be crucial in designing new drugs to kill bacteria.

"Just like a light switch you flick with your finger and turn on or off the light, the global fold of the RNA changes in response to interactions with the signaling molecule," Hines said. "My research group is working toward designing small molecules that can disrupt that key RNA signaling molecule interaction in order to permanently turn off the switch and kill the bacteria specifically."

To determine the structure of these potential new antibiotics, Hines' group tests how different small molecules interact with the RNA riboswitch. Since Hines has to test the docking of entire libraries of small

{ABOVE} Jennifer Hines, Ph.D., is studying RNA riboswitches as a possible new approach to killing harmful bacteria. [Photo courtesy of Ohio University]



molecules on the riboswitch, she uses the power of the Ohio Supercomputer Center's Oakley Cluster to speed up the calculation process. This allows her to test multiple RNA sites against many different small molecules to identify the best pairing.

While performing a single calculation with one molecule may take Hines two minutes on her lab computer, the same calculation on the Oakley Cluster is done almost as soon as she enters it in the system. She also realizes cost savings through using MacroModel and Glide shared software licenses through OSC.

"Bottom line, I cannot afford more than one computer in my lab to be working on it," Hines said. "If I have multiple students with different projects, they have to line up after one another, whereas with the Ohio Supercomputer Center, they can all be working on it at the same time. It allows more people to investigate simultaneously, and the calculations just run a lot faster."

Antibiotics are not the only pharmaceutical area where RNA holds promise.

Traditionally, significant advances in drug discovery have occurred through targeting specific proteins or DNA. RNA also is present in every living cell, but in the past was overlooked as a potential therapeutic target. Because it is involved in nearly every biological chemical process, yet has a relatively simple structure, RNA makes for an enticing target in the world of drug discovery. Hines said it is only within recent years that RNA has become a major player for structural and molecular biologists who are looking for novel therapies.

"It is just mind-blowing what RNA does in bacteria, in humans and in viruses," Hines said. "We're just at the dawn of targeting RNA for drug discovery purposes, and so with RNA being so elegantly involved in all sorts of regulatory processes, if you get more information about the best ways to target RNA with small molecules, you could potentially open up new areas for anticancer research and antiviral research, in addition to the antibacterial research that I'm doing." ◄

PROJECT LEAD // JENNIFER HINES, PH.D., OHIO UNIVERSITY RESEARCH TITLE // MODELING LIGAND BINDING TO NONCODING, REGULATORY RNA FUNDING // OHIO UNIVERSITY WEBSITE // OHIO.EDU/CAS/CHEMISTRY/CONTACT/PROFILES.CFM?PROFILE=HINESJ

CANCER RESEARCH

LaFramboise analyzes inherited genetic mutations linked to leukemia

In the Department of Genetics at Case Western Reserve University, Thomas LaFramboise, Ph.D., and his research team are discovering which genetic mutations determine a person's susceptibility to developing leukemia.

Whether or not someone develops cancer depends on where certain mutations are located within your genetic material. LaFramboise, an associate professor, and his team leverage the processing power of the Ohio Supercomputer Center's Owens Cluster to find exactly where these potentially cancerous mutations occur.

"There are certain inherited mutations that probably give people a slightly elevated risk of acquiring a specific disease. In our case, we're looking at things that are related to leukemia," LaFramboise said.

In most cases, no one knows exactly in which genes the mutations reside. To find them, LaFramboise and his team use software packages, such as Bowtie, SAMtools and GATK, which are available via OSC. These tools allow the team to view and compare healthy individuals' genes to genes in patients with leukemia. The team can then identify the location where the mutations occur.

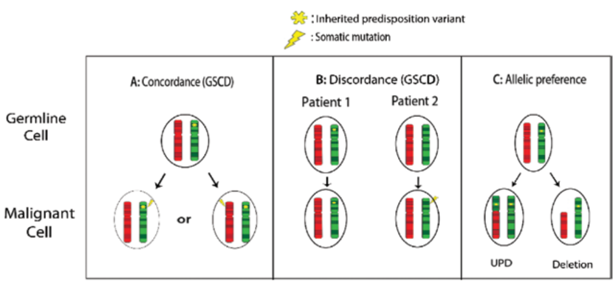
While there is already extensive research on non-inherited (sporadically occurring) mutations, there is less information about inherited mutations in leukemia.

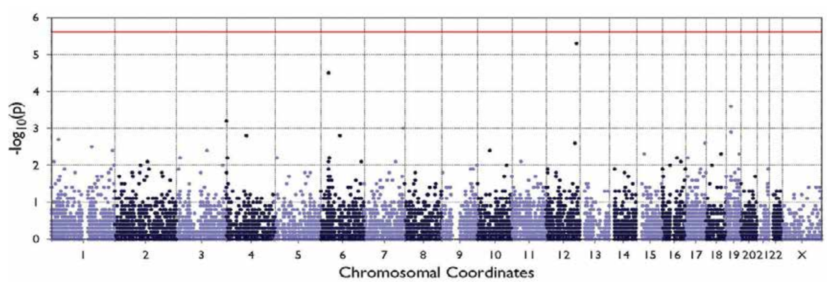
"The project I'm using OSC for is about mutations that are inherited from the patient's father or mother," LaFramboise said.

LaFramboise's research involves studying thousands of people with leukemia and thousands without, giving the team a large amount of raw DNA sequences—composed of four nucleotide bases of a DNA strand, represented as various combinations of As, Cs, Gs and Ts—to comb through.

"We have six-and-a-half billion of these letters in each of our cells, so there is a lot of data analysis that goes on, which is why OSC is such a valuable resource," LaFramboise said. "Because we have to store all that data and analyze all that data, we lean heavily on the Cluster."

There are several outcomes possible from LaFramboise's research. The first is a genetic test that could tell people their risk level of developing leukemia. Another is advancements in genetic counseling, so parents can learn the likelihood of their child developing leukemia. A third possibility is that if researchers, LaFramboise and his team, can identify why a certain mutation plays a role in the onset of cancer, drugs might be developed to prevent or treat it. ◂





{LEFT} Thomas LaFramboise, Ph.D., associate professor at Case Western Reserve University, is working toward a way to discover which genetic mutations determine a person's susceptibility to developing leukemia. This image shows the biological rationale for statistical tests. In each case, an inherited susceptibility allele is present in the gene. {RIGHT} Here each point represents a gene, and is plotted according to its chromosomal location (horizontal axis) and statistical significance for carrying inherited mutations that contribute to leukemia susceptibility (vertical axis).

PROJECT LEAD // THOMAS LAFRAMBOISE, PH.D., CASE WESTERN RESERVE UNIVERSITY RESEARCH TITLE // GERMLINE CONTRIBUTORS TO MDS SUCEPTIBILITY: INTEGRATING CLUES FROM THE MALIGNANT GENOME FUNDING SOURCE // CASE WESTERN RESERVE UNIVERSITY WEBSITE // MENDEL.GENE.CWRU.EDU/LAFRAMBOISELAB

LUNG MICROBIOME

Keller sequences lung genetic data for improved transplant outcomes

For patients facing chronic lung disease, the third leading cause of death in the U.S., the ultimate end-stage treatment is a lung transplant. Unfortunately, the survival rate for lung transplant patients is lower than that of other organ transplants due to infections and tissue rejection.

Brian Keller, M.D., Ph.D., a pulmonologist at The Ohio State University's Wexner Medical Center, is working to improve patients' lung transplant outcomes by studying lung microbes and viruses that could affect them. Keller is using the Ohio Supercomputer Center to store massive amounts of genetic sequencing data.

"The lung field is a little bit behind some of the other fields, particularly the skin and the gut," Keller said. "Part of the reason was, it was actually left out of the human microbiome project because at the time it was thought that the lung was a sterile environment. I think the data now is pretty convincing that there is a lung microbiome."

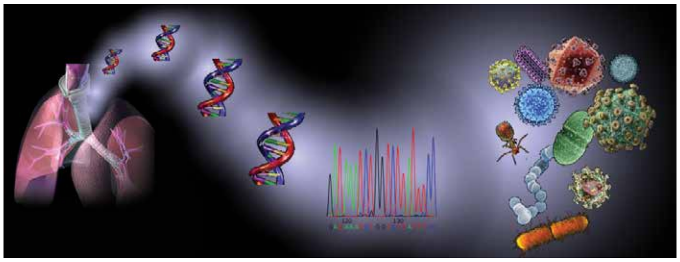
The viruses Keller is studying target microbes, not necessarily humans themselves. However, if viruses adversely affect key microbial processes in the lung, it could lead to problems, especially for those in need of a lung transplant—usually patients with cystic fibrosis or chronic obstructive pulmonary disease (COPD). To identify microbial viruses in the lungs, Keller and his team take a sample from the lung and sequence all the genetic material in it to find the part that contains viruses—which is only one percent of total genetic sequences.

Once they sort through millions of sequencing reads and eliminate human and bacteria information, Keller's team can then identify the sequences that reflect the viruses present in the lung using reference databases.

"All of those processes require higher-level computing than what can be done on your desktop machine, and I think that's the biggest benefit that we receive from (OSC)," Keller said.

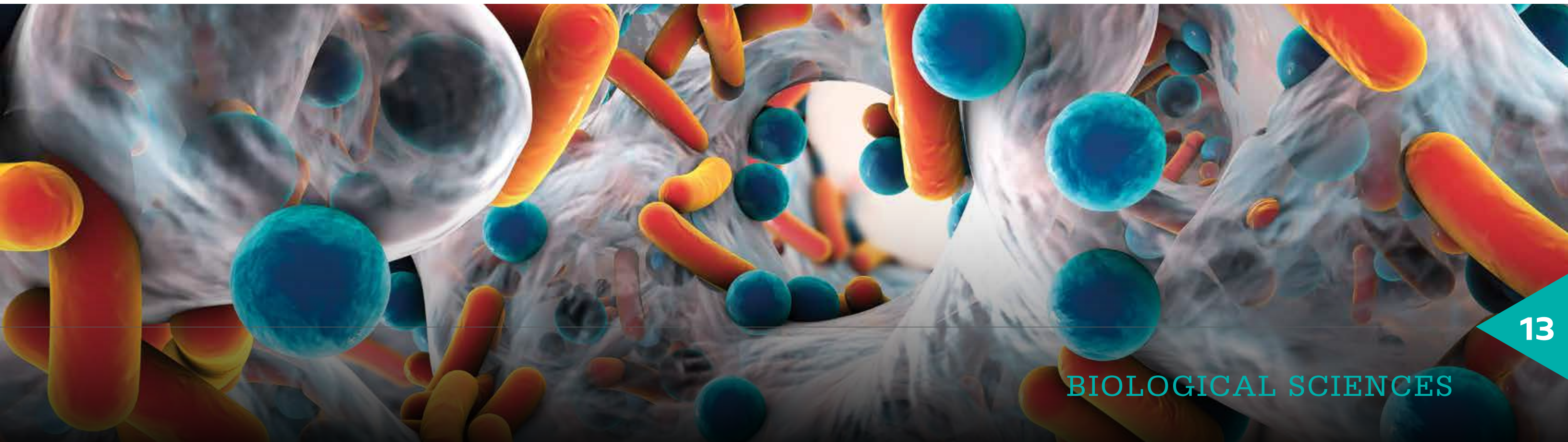
Though Keller's work on developing a more robust understanding of the lung microbiome and virome is in its early stages, it could quickly have an impact on lung transplant outcomes. The next phase of Keller's work will incorporate modeling of changes that occur in the lung microbiome after a transplant.

"What we'd like to do is look at the virome in the donor before transplant, the virome in the recipient and then model the dynamics that occur as you take the lung from a donor and put it in a new person, and how do those microbes change. Do they persist? Are they replaced by microbes from the recipient upper airway?" Keller said. "None of that is known." ◄



Keller's goal is to characterize the components of the lung virome and to evaluate the ecology of the population in relation to clinical outcomes. He is developing a lung transplant specimen biorepository and comprehensive clinical database.

PROJECT LEAD // BRIAN KELLER, M.D., PH.D, THE OHIO STATE UNIVERSITY WEXNER MEDICAL CENTER RESEARCH TITLE // VIRUS-MICROBE ECOLOGY AND EFFECTS ON LUNG TRANSPLANT OUTCOMES FUNDING SOURCE // THE OHIO STATE UNIVERSITY WEBSITE // WEXNERMEDICAL.OSU.EDU/TRANSPLANT/CONTENT/RESEARCH/BRIAN-KELLER-MD-PHD

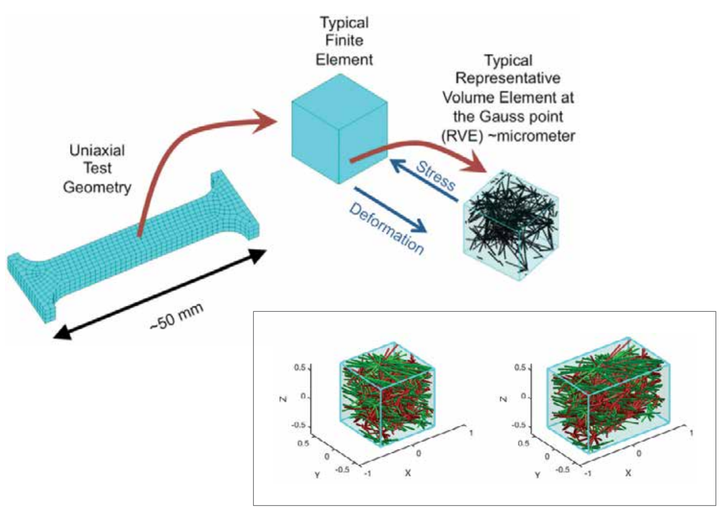


TRICUSPID VALVES

Amini using finite element analysis to improve long-term surgery resilience

Tricuspid valve surgery is a common heart-valve procedure in the United States, but it is one with poor long-term outcomes. In fact, studies show that up to 45 percent of those who receive tricuspid-valve surgery suffer a recurrence of problems, in some cases as early seven years after surgery. In one-third of the cases, a second operation is required.

But little is understood about the process by which repaired tricuspid valves change following surgery. Rouzbeh Amini, Ph.D., is trying to shed light on those changes.



Overview of the multi-scale model. Displacements are passed from the macro level to the micro level, and the calculated stress at the micro level is passed to the macro level as a domain volume average. {INSET} The multi-scale model is capable of predicting the responses of fibrous (i.e. collagen (red) and elastic (green) and non-fibrous (cyan) constituent component of the valve.

The University of Akron's assistant professor in the Department of Biomedical Engineering is using the Ohio Supercomputer Center's Oakley Cluster to develop a finite element model that can discover why tricuspid valves aren't holding up long-term.

The tricuspid valve—which prevents backflow of blood into the right atrium of the heart—is the most understudied of the four valves in the heart, mostly because the left side of the heart is where most problems occur. Tricuspid valves often need repair surgeries when the valve doesn't close completely, thus not guaranteeing one-way flow, or when the valve doesn't open fully to allow enough blood flow.

After years of focusing on the left side, clinicians and surgeons started to notice tricuspid valve surgery wasn't as successful as they had once hoped it would be.

Discovering why that is requires a detailed mathematical framework that can quantify how the fibers of the proteins elastin and collagen, which mainly make up the leaflets of the valve, react to the stretching and stresses needed for the valve to work.

"Imagine each one of these protein fibers as a single spring," Amini said. "You stretch it, it resists. You can model a network of springs. The problem is it requires a great deal of computational resources.

"If you apply a certain amount of load to the valve, mechanical load, you want to know how the leaflets perform."

Because Amini is dealing with a gargantuan amount of protein fibers, and the structure in the tissue is complex, the computational aspect is intense. Amini and his team use codes composed in the program "C" to run finite element analysis through Oakley on the mathematical framework they've developed.

"Because of OSC, we don't have to maintain the hardware and software; we can just focus on what we're good at, which is writing codes and translating biological problems into computational models," Amini said. ◀

PROJECT LEAD // ROUZBEH AMINI, PH.D., THE UNIVERSITY OF AKRON RESEARCH TITLE // A DETERMINISTIC MULTI-SCALE FINITE ELEMENT MODEL OF TRICUSPID VALVE LEAFLETS FUNDING SOURCE // AMERICAN HEART ASSOCIATION WEBSITE // AMINI.UAKRON.EDU

OSC generates insights into

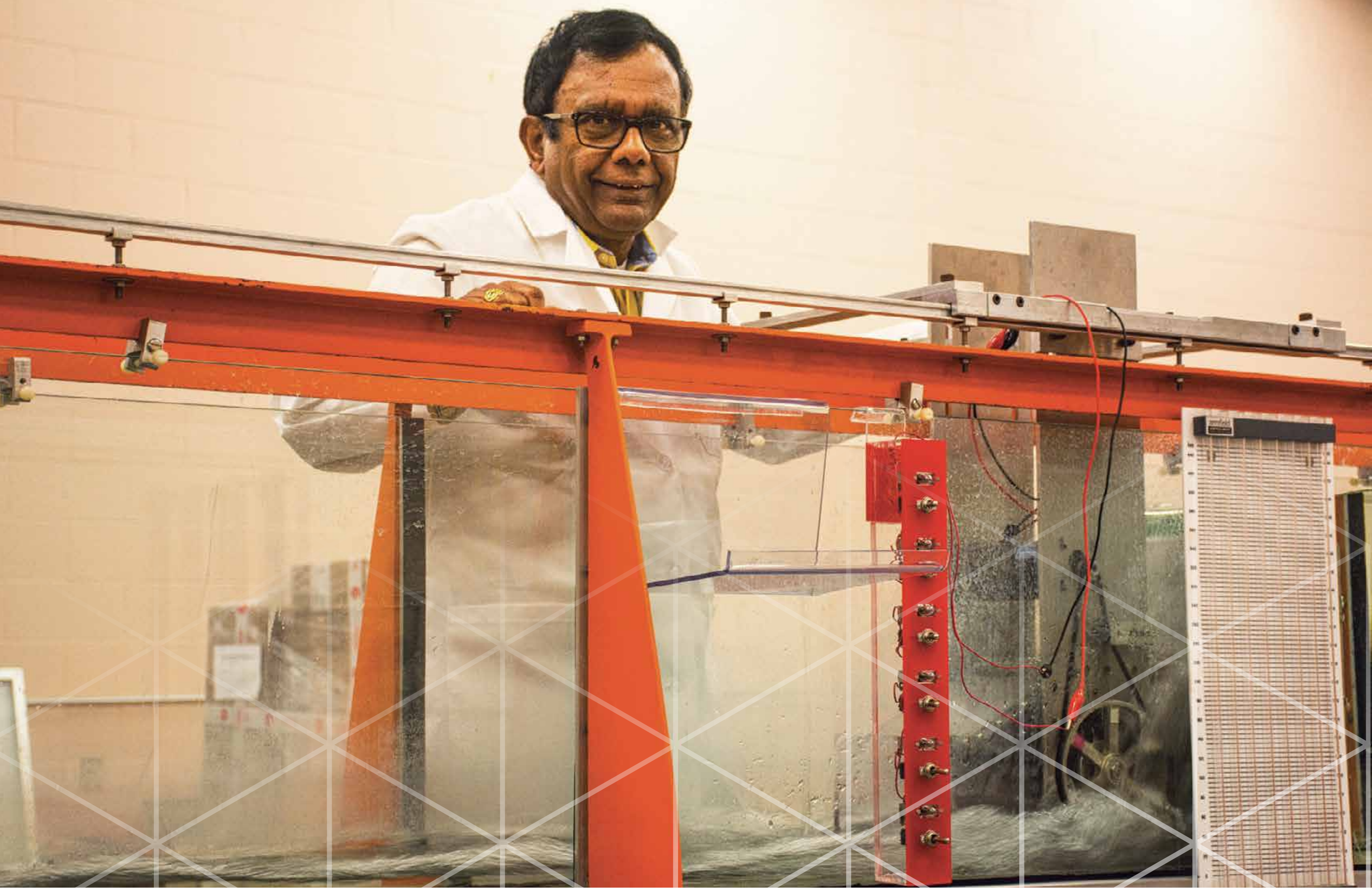
Energy Systems

Modeling and simulation powered by high performance computing is used across almost all facets of research into current and future sources of energy, such as wind turbine design, carbon-fueled combustion systems and fission/fusion studies.

Engineers and scientists access systems at the Ohio Supercomputer Center to examine the potential of various energy sources. Large-memory nodes and graphic processing units found on the center's Owens Cluster boost their ability to chart our energy future.

"It is essential to have access to a supercomputer. The CPU speed is important because some of these simulations run for days or weeks on the supercomputer, and it wouldn't be feasible to do the same research on the desktop or even a work station."

— *Amir Farajian, Ph.D., Department of Mechanical and Materials Engineering, Wright State University*



{TOP} Central State University's Subramania Sritharan, Ph.D., is using CFD analysis on the Ohio Supercomputer Center's Oakley Cluster to develop a cross flow turbine that can be used in non-powered dams across the U.S. These turbines could result in clean renewable energy, new jobs and better boating and swimming safety on the nation's rivers. [Photo courtesy of Central State University]

RENEWABLE ENERGY

Simulation helps Central State's Sritharan develop hydropower turbines

Central State University's Subramania Sritharan, Ph.D., is fine-tuning a product that could result in clean renewable energy, new jobs and better boating and swimming safety on many of the nation's rivers.

The project centers on using a computer-modeling software package on the Ohio Supercomputer Center's Oakley Cluster to research using cross-flow turbines within non-powered dams. The FLUENT software, a product of ANSYS, uses computational fluid dynamics to model flows of substances such as water or air.

"The technology we are trying to develop can result in a lot of power generation," said Sritharan, associate director of research for CSU Land Grant programs. "It's a great renewable-energy option and, of course, can result in a lot of employment and manufacturing within the United States."

There are more than 80,000 non-powered dams in the U.S., and Ohio has a considerable number of these dams, especially on the Ohio River.

A recent study conducted by Oak Ridge National Laboratory found that the potential turbine hydropower within in these NPDs is estimated at 12 gigawatts, which would complement solar, wind and other clean-energy sources. In the 100 existing NPDs along the Ohio, Mississippi, Alabama and Arkansas rivers alone, the National Hydropower Association estimated that converting them into power-generating facilities would serve more than 250,000 households in those regions, while avoiding two-million metric tons of carbon-dioxide emissions per year.

Sritharan's objective is to determine the optimal parameters for the Williams Crossflow Turbine, which takes advantage of downward water flow in small dams to generate power. The WIliams Crossflow Turbine is named after Fred Williams, owner of Dayton Hydroelectric Ltd., which has worked with CSU on the project.

"We are working on the details to develop a prototype and test it," Sritharan said. "We use crossflow turbine technology to tap into hydropower generation, but it also prevents boating accidents and swimming accidents in smaller dams because people can get trapped in the hydraulic broil on the toe of the dam."

Sritharan's history with OSC goes back many years but ramped up when he discovered the Center offered FLUENT's CFD software. "That's something we took advantage of," he said. "We had to generate our own algorithms, work out our own codes. When we found this was available, we were able to ratchet up our use of OSC and benefit greatly."

FLUENT testing has helped develop the optimal parameters of the turbine, including information about the velocity vectors, torque, power and overall efficiency of the system. The results are being used to develop a physical model that will be tested in the hydraulic laboratory at CSU.

The final objective of the project is to install and monitor for a year a prototype of the Williams Crossflow Turbine in a dam across the Miami River near the university in Hamilton, Ohio.

"We have brought a team together to test and develop this turbine into a full-scale model and test it," Sritharan said. "This has the potential to not only be of good use across the United States, but internationally, with a lot of job creation in Ohio. And the help we've gotten from OSC is fantastic." ◄

PROJECT LEAD // SUBRAMANIA SRITHARAN, PH.D., CENTRAL STATE UNIVERSITY RESEARCH TITLE // CFD ANALYSIS OF CROSS FLOW TURBINES FOR HYDROPOWER FUNDING SOURCE // CENTRAL STATE UNIVERSITY WEBSITE // CENTRALSTATE.EDU/ACADEMICS/CSE/PAGES01.PHP?NUM=17

ENERGY STORAGE

Buldum using HPC capabilities for graphene research

With the rise of energy-storage applications for such things as rechargeable Lithium ion batteries and solar cells, graphene and graphene-based nanocomposites have attracted a lot of interest.

Graphene is incredibly strong, more than 100 times stronger than steel, but is very thin and flexible. It is also highly conductive and seems to be impermeable to most gasses and liquids.

The University of Akron's Alper Buldum, Ph.D., is using the Ohio Supercomputer Center's high performance computing capabilities to perform experiments to further understand the physical properties and capabilities of graphene. This understanding will assist nanotechnologists and engineers in developing the material for use in areas, such as energy storage, friction reduction and mechanical properties.

"It's very promising," said Buldum, a professor within the University of Akron's Department of Mechanical Engineering, Integrated Biosciences Program. "Graphene is a very popular material. The idea for this project started with the interest in packing molecules together like pancakes on top of each other, creating larger molecular structures, eventually using them for technology—solar cells and other areas of molecular electronics."

Using the Quantum Espresso and cp2k softwares on the Oakley Cluster, Buldum performs computer modeling and simulations, such as quantum modeling, atomic scale modeling and simulation, quantum mechanics, quantum chemistry and classical molecular dynamics.

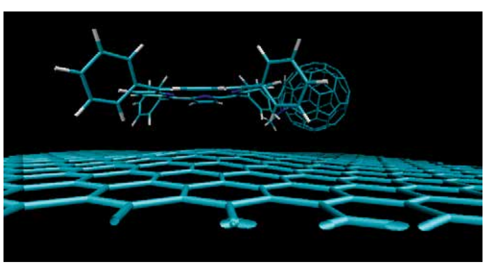
Buldum is also performing investigations on n-conjugated molecules and their supramolecular structures for photovoltaics; and using computational design of novel molecular nanowires for organic solar cells.

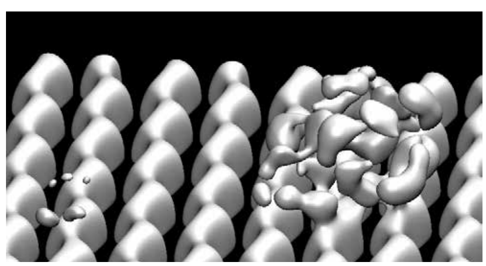
"We guide and give ideas to the chemists, physicists and material scientists so they can synthesize," Buldum said. "And if the materials have novel properties, they can use them.

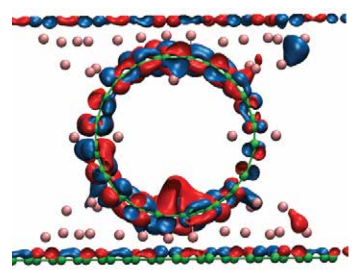
"Material research is quite colorful and dynamic. Computer modeling is very good in that before we conduct expensive physical experiments, we can quickly use these models to check if the material has the desired properties, and we can optimize it."

When it comes to developing advanced materials, Buldum and OSC together are part of a bigger chain that ends in better, more efficient products.

"We're an important part of this chain," he said. "We have an interesting design of these materials, and it can be synthesized and used in solar cells. If we don't have OSC, maybe somebody in five years can do it, but maybe not. OSC is crucial."







{LEFT} This illustrates the frontier electronic states of the combined structure. {CENTER} A geometrically optimized fullerene-porphyrin dyad-graphene structure from Buldum's quantum chemistry calculations. {RIGHT} Buldum's group has studied potential cathode materials for lithium ion batteries. One promising structure is a graphene-carbon nanotube nanocomposite. Buldum has researched lithium intercalation of such nanocomposites with different lithium ion densities by performing ab initial electronic structure calculations. This structure is in an electronic state. The pink balls represent lithium Iona and the green balls represent carbon atoms.

PROJECT LEAD // ALPER BULDUM, PH.D., THE UNIVERSITY OF AKRON RESEARCH TITLE // MODELING AND SIMULATIONS OF ADVANCED MATERIALS FOR ENERGY APPLICATIONS FUNDING SOURCE // NATIONAL SCIENCE FOUNDATION WEBSITE // UAKRON.EDU/PHYSICS/FACULTY-STAFF/BIO-DETAIL.DOT?U=BULDUM

NOVEL NANOSTRUCTURES

Farajian models nanomaterials for improved thermal management

For most energy applications, heat is a byproduct of a reaction, cast off as unusable energy. But as the world moves toward energy efficiency, scientists are looking at ways to effectively channel heat back into electricity so that less energy is wasted. Better thermal management could even change the future for our favorite electronic devices, such as smart phones and vehicle entertainment systems. At Wright State University, Amir Farajian, Ph.D., is testing the thermal energy transport properties of nanomaterials to make this a reality.

Farajian's group in the Department of Mechanical and Materials Engineering works with nanoribbons: tiny strings of atoms 10 by negative 9-meters wide, arranged in the form of ribbons. The group is testing the elements carbon, boron, nitrogen and silicon to see which element or combination of elements holds the most promising thermal transport abilities. They use the Ohio Supercomputer Center's Oakley and Owens Clusters to simulate these nanoribbons, the changes in their structures and the effect on thermal conductivity.

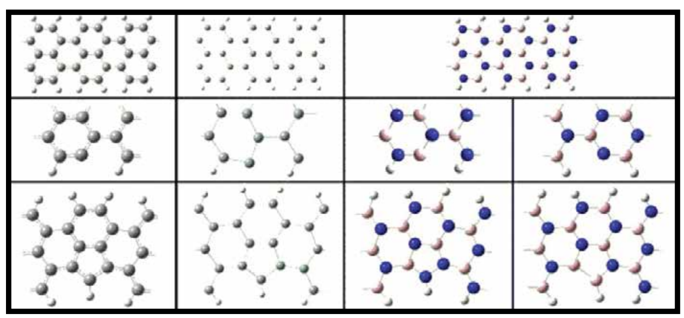
Sometimes this involves intentionally creating defects in the materials to find the effects on the nanoribbons that will best carry heat.

"The novel aspect of this work, because similar work has been done before, was to consider some realistic changes in the structures," Farajian said. "The simulation should take care of all electrons in the system…so when you put these all together for a real system on the nanometer scale, this is a huge burden computationally. It is absolutely essential to have access to a high performing computer system.

"We are really grateful for this access to the Ohio Supercomputer Center."

What does this mean for the everyday consumer? Farajian said his department's newest program involves research into renewable and clean energy, an area where materials science can play a significant role. Any electronics we use daily, including cell phones, laptops and cars, can use new, more efficient materials to improve performance and save energy.

"If these materials are used, they can dissipate or manage the heat which is a big obstacle in the performance of a device," Farajian said. "In fact, if there is not a reliable thermal management system installed, it can be catastrophic for the device. But with these new materials and the thermal management system that we simulated, it is possible to have… better performance for various smart devices." ◀



Nanoribbons based on carbon, boron, nitrogen and silicon, with realistic structural defects, were investigated by Farajian for their thermal transport properties [Source: Appl. Phys. Lett. 109, 173102 (2016)]

PRINCIPAL INVESTIGATOR // AMIR FARAJIAN, PHD, WRIGHT STATE UNIVERSITY RESEARCH TITLE // COMPUTATIONAL MODELING OF NOVEL NANOSTRUCTURES FOR SENSOR AND ENERGY APPLICATIONS FUNDING SOURCE // NATIONAL SCIENCE FOUNDATION WEBSITE // WRIGHT.EDU/~AMIR.FARAJIAN

FUEL EFFICIENCY

Selamet uses CFD modeling, physical testing to eliminate engine 'knock'

More than 140 years ago, when the first four-stroke cycle, internal combustion engine was invented, it became the prototype for the modern automobile powertrains. As long as those engines have existed, however, “knock” has been a limiting factor to the performance of engines.

With the help of the Ohio Supercomputer Center, Ahmet Selamet, Ph.D., is tackling that problem head on.

“The ultimate goal is improving fuel efficiency,” said Selamet, a professor in the Mechanical and Aerospace Engineering Department at The Ohio State University. “OSC is a tremendous enabler to develop realistic models for the very complex physics we are dealing with. If it weren’t that complex, we would have had the answer in 140 years.”

Selamet simulates the chemical kinetics and unsteady fluid motion and heat transfer within an engine’s combustion chamber to learn ways to suppress engine knock, which could lead to much improved fuel efficiency.

The term “knock” refers to the sound you hear—literally, a knock or a ping—from inside your engine. This is due to an abnormal combustion process in which “end gas” ahead of propagating flame within the combustion chamber gets auto-ignited. The resulting high amplitude pressure fluctuations cause stress on the engine.

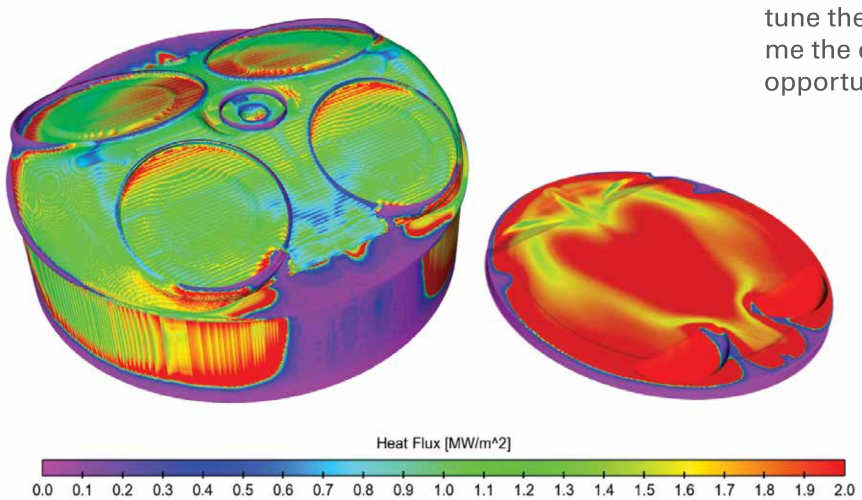
“We try to predict conditions that will lead to knock,” Selamet said. “We hear it as a noise because the engine is subject to tremendous oscillating pressure forces. It’s highly undesirable for the structural integrity and longevity of the engine and deteriorates performance.”

Understanding time-resolved heat transfer—which dictates the temperature of end gas and its susceptibility to auto-ignition through reaction rates within the combustion chamber—is critical. Therefore, Selamet is developing a detailed heat-transfer model based on physics and computational fluid dynamics to help fine-tune a simplified model. That model can be used by manufacturers to design more efficient engines.

In North America each year, close to 20 million engines are produced just for passenger cars and trucks.

Selamet combines three-dimensional CFD using CONVERGE software on OSC’s Oakley Cluster with physical experiments at Ohio State’s Center for Automotive Research.

“OSC gives us superior ability to run CFD in a meaningful fashion,” Selamet said. “While CFD is a powerful tool, you still need experiments to fine-tune the modeling. Having both capabilities gives me the entire picture and presents a tremendous opportunity to make a true impact.” ◀



This computational fluid dynamics model shows the predicted spatial variation of instantaneous heat flux on (left) the combustion chamber walls (cylinder head and liner) and (right) the piston surface.

PROJECT LEAD // AHMET SELAMET, PH.D., THE OHIO STATE UNIVERSITY RESEARCH TITLE // SIMULATION OF IN-CYLINDER CHEMICAL KINETICS AND UNSTEADY HEAT TRANSFER FOR SUPPRESSION OF ENGINE KNOCK AND IMPROVED FUEL EFFICIENCY FUNDING SOURCE // CHRYSLER, THE OHIO STATE UNIVERSITY WEBSITE // ENGINE.OSU.EDU

OSC boosts understanding of

Earth's Environment

Whether examining Northwest Passage ice floes, endangered species or agricultural runoff, scientists use high performance computing to model life systems using vast data sets compiled from satellites, mobile devices, cameras and microphones.

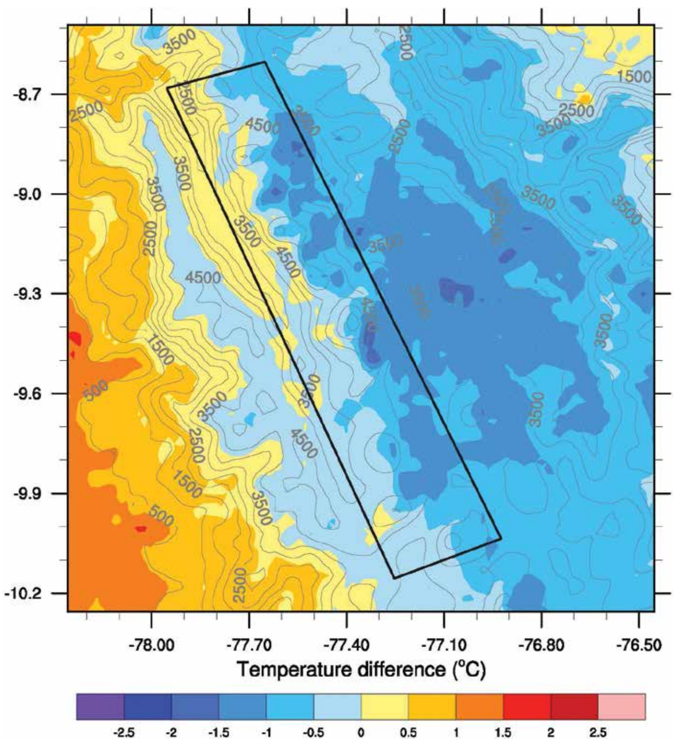
The computational power of Ohio Supercomputer Center systems helps researchers produce critical simulations of our planet's organic formations, models of impassable terrain and intense data calculations to help answer today's earth-science questions.

"OSC helps us significantly. If we don't have this high-speed simulation capability, students have to physically simulate the research. They all have limited time to finish their Ph.D. study, and a physical simulation could take them as much as a year."

— *Lingying Zhao, Ph.D.,*
Department of Food, Agricultural and Biological Engineering,
The Ohio State University

TROPICAL GLACIERS

Mark's high-resolution simulations gauge impact of Andean climate change



This figure shows the spatial distribution of the difference between two simulations performed at OSC: one simulation (CRTL) represented the climate of August 2005 as it is in the real (modeled) world, while the other (LCC) corresponded to the same month and year, but the land cover in the Amazon has been modified in the WRF model. The variable represented is air temperature and the rectangle encloses the region in the Cordillera Blanca (Peru) where most tropical glaciers are found.

Going back to the 1990s, a significant amount of research has been dedicated to the rates of deforestation in the Amazon and what this could mean for climate change throughout the world. Additional studies have focused on climate change impacts to Andean mountain glaciers that lie downwind of the Amazon.

This research has quantified both the land-cover change by deforestation in the Amazon basin, and the extent of Andean glacier retreat and drought in this region of the world. But while these studies illustrate diverse outcomes tied to the global climate, there has been less focus on how they interconnect locally.

For instance: Is there a link between deforestation, globally rising temperatures and melting glaciers in the Andes Mountains? How might these large-scale dynamics impact the local populations?

Bryan Mark, Ph.D., professor in the Department of Geography and Byrd Polar and Climate Research Center at The Ohio State University, and his team are part of a program called AMAZONIAN-LINCAGES (Amazonian Land-cover-INduced Climate And Glacier Enhanced System). This program is mechanistically trying to understand the influence of observed and simulated Amazonian land-use and land-cover change on glacier-mass balance across the tropical Andes.

"The regional climate of the area is characterized, for the most part, by land-ocean interactions, the atmospheric convection in the Amazon and the effect of the Andes on circulation patterns," Mark said. "So, it follows that changes occurring on one of those regions may affect the other. Research that looks into the climatic interaction between the Amazon Basin and the Andes is uncommon, being parceled through specific, and often unconnected, disciplinary pathways."

One of the areas for which his team has turned to the high performance computing capabilities of the Ohio

Bryan Mark, Ph.D., (far left), and his team, which includes computation specialist Alfonso Fernandez, Ph.D. (second from right), are using Ohio Supercomputer Center resources to understand what climate changes in South America mean for local residents.

Supercomputer Center is to investigate what these climate changes mean for Peru, Bolivia and Columbia.

"The changes in the Amazon on glaciers is extremely important because it's a key source of water for people in this region," said Alfonso Fernandez, Ph.D., who leads the computational modeling efforts for Mark's group.

During the May-to-September dry season, people in the region rely on glacier meltwater and groundwater resources. Glaciers provide important reservoirs of water storage that buffer stream flow and recharge groundwater.

"We want to know if there's a signal from the Amazon deforestation that might increase the effect of the global climate change or might otherwise decrease the effect of global climate change," Fernandez said.

Using a Weather Research and Forecasting (WRF) model on OSC's Oakley Cluster, Fernandez performs high-resolution simulations to determine possible outcomes of climate change on the Andes Mountains.

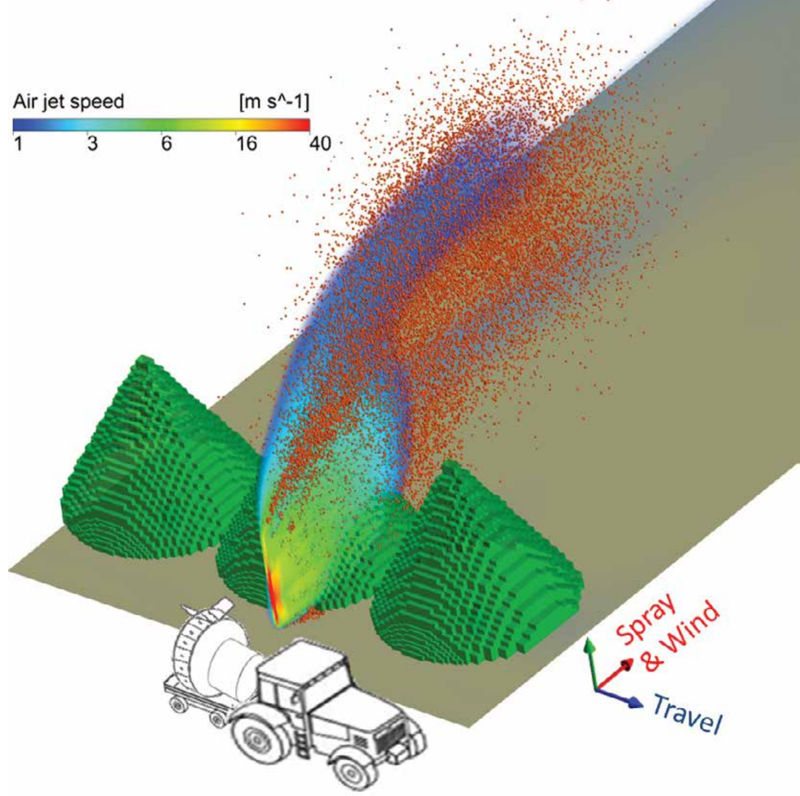
Typically, WRF is used to research large areas of hundreds of kilometers, in which local features, such as glacier-covered valleys (typically 1 to 5 kilometer in width), are poorly represented. The high-resolution simulations performed at OSC, however, allow Fernandez to study down to a smaller area for a more focused picture, in some cases an area of 2-by-2 kilometers.

"We want a bigger picture of the tropical Andes compared to the Amazon," Fernandez said. "The first goal is to get an idea of the mechanisms driving these changes and if there's a signal on a smaller scale. Then we can do field work to see if the signal is better or worse for the impact on the global climate change of these glaciers in the tropical Andes." ◄

PROJECT LEAD // BRYAN MARK, PH.D., THE OHIO STATE UNIVERSITY RESEARCH TITLE // AMAZONIAN LAND-COVER-INDUCED CLIMATE AND GLACIER ENHANCED SYSTEM FUNDING SOURCE // THE OHIO STATE UNIVERSITY WEBSITE // RESEARCH.BPCRC.OSU.EDU/GLACIERCHANGE/PEOPLE

AGRICULTURE EFFICIENCY

Through CFD, Zhao's group visualizes more efficient farming



Zhao's research group produced this CFD simulation of pesticide droplet drifts discharged from an air-assisted orchard sprayer.

The agricultural industry strives to maintain a balance between keeping up with consumer demand and maintaining a safe, clean and sustainable environment for humans and animals. Lingying Zhao, Ph.D., and her research group at The Ohio State University, conduct research to find solutions that help the industry strike this balance. Zhao's research group in the Department of Food, Agriculture and Biological Engineering has been using computational fluid dynamics to model everything from air flow in chicken coops to pesticide spray application on orchards.

"We want to understand the environment to help farmers first assess the problem, if any, and second, help them improve their management, environmental quality and production efficiency, with the ultimate goal for sustainable food production," Zhao said.

Much of the research done in Zhao's group is funded by Agriculture and Food Research Initiative grants from the U.S. Department of Agriculture. Since it's not feasible to collect data from every farm, Dr. Zhao's group extrapolates from the collected data, using intensive mathematic modeling to simulate and understand different environmental conditions of large-scale commercial farm facilities.

Ryan Knight, a graduate student in Zhao's group, is building an electrostatic precipitator, a device that captures particles from gas, for mitigation of dust on farms. The precipitator consists of two grounded metal plates with high-voltage wires that run between them, creating an electrical and magnetic field. When dusty air from the field flows between the plates, the dust particles become ionized and can be collected on the plates. This gives Knight an idea of how much dust is in the air. However, testing and building a prototype is time-consuming and expensive. Knight uses OSC's COMSOL license to model the electrostatic precipitator.

"Using the Ohio Supercomputer Center and COMSOL allows me to simulate a wide range of scenarios with different values for these parameters," Knight said. "I'm able to figure out what the optimal configuration of these parameters might be, and so once we have the optimized parameters then we can move forward with building a prototype and testing that in the lab.

"Instead of me spending months and months in the lab…having to do that manually, I can just tell COMSOL 'try all these cases at once,' so it definitely saves me a lot of time."

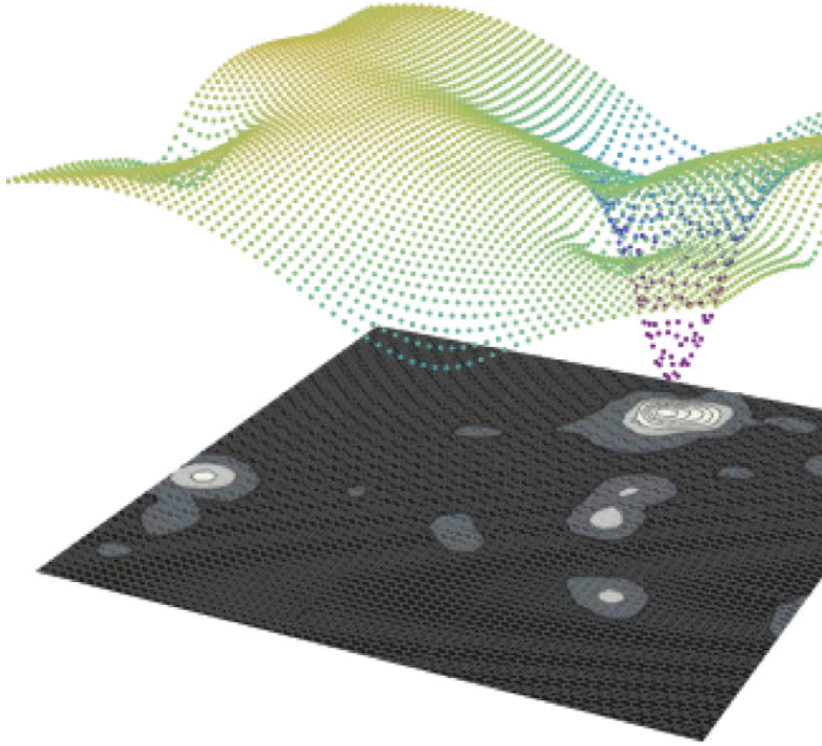
As Zhao pointed out, students pursuing graduate and doctoral degrees have a limited time to conduct research, with an average of about three to four years. To physically simulate environmental conditions or model equipment could take students upward of a year. Access to OSC's high performance computing resources, as well as COMSOL and ANSYS FLUENT software licenses, saves students valuable time and money.

"We appreciate this nice facility and capacity," Zhao said. "(OSC) enables us to do a lot of research work we could not do before without this resource." ◂

PROJECT LEAD // LINGYING ZHAO, PH.D., THE OHIO STATE UNIVERSITY RESEARCH TITLE // COMPUTATIONAL FLUID DYNAMICS APPROACH FOR AIR QUALITY AND BIOENVIRONMENTAL ENGINEERING RESEARCH FUNDING SOURCE // U.S. DEPARTMENT OF AGRICULTURE WEBSITE // FABE.OSU.EDU/OUR-PEOPLE/LINGYING-ZHAO

PARTICLE PHYSICS

Kenyon's Giblin understands fundamental science through cosmic inflation research



Tom Giblin, Ph.D., is developing models to better understand the different phases of the universe's development. This image is a visualization of the spatial density (greyscale on bottom) of a region of the universe after inflation and the corresponding gravitational reaction (color dots and height). [Image courtesy of Christian Solorio, Kenyon College]

Understanding particle physics gives us answers to the fundamentals of science.

To better understand particle physics, Tom Giblin, Ph.D., looks to cosmology, the study of the evolution of the early universe.

The associate professor of physics at Kenyon College is using Ohio Supercomputer Center resources to tackle unanswered questions about cosmic inflation: The theory that following the Big Bang, the early universe expanded exponentially.

"It's not well understood how the universe just stopped growing very quickly and entered the thermal history we know it had to have in order to develop planets and people and galaxies," Giblin said. "There's a period after inflation, called 're-heating,' to a state full of particles that are a very high temperature."

Giblin is trying to develop models to better understand the different phases of the universe's development. Cosmology and particle physics go hand-in-hand, because there's a limit to how much energy we can give a particles in colliders on Earth.

To go to higher-energy scales, one has to look to the early universe because "that's the laboratory in which those temperatures actually existed, and that's the place we can probe particle physics at higher energy," Giblin said. "Generally, these physics help us understand how energy in matter exists."

Creating a model of particle physics that accurately describes the early universe could result in an understanding of the fundamental interactions of matter and energy.

"In fundamental physics, it's easy to write down a guess as to what particles look like at high energies. But it's hard to test and disprove those models," Giblin said. "We test and explore a lot of models and help put constraints on some of those guesses. Our greatest service is that we test and explore a lot of models, and OSC is critically important to that."

Giblin develops these models locally on his clusters before turning to OSC for large-scale simulations. Giblin and his team use a software they developed, called GABE (Grid And Bubble Evolver), a C++ program that can run a variety of particle-physics scenarios.

Another important aspect in which OSC helps Giblin is his work with undergrad students, who have been able to finish their senior thesis by performing many of the computational runs that need completed. ◄

PROJECT LEAD // TOM GIBLIN, PH.D., KENYON COLLEGE RESEARCH TITLE // NON-LINEAR DYNAMICS IN THE EARLY UNIVERSE FUNDING SOURCE // NATIONAL SCIENCE FOUNDATION WEBSITE // KENYON.EDU/DIRECTORIES/CAMPUS-DIRECTORY/BIOGRAPHY/JOHN-GIBLIN

STRESS TOLERANCE

OSC data processing helps Benoit's group survey tick populations

While most of us try to distance ourselves from biting, blood-sucking creatures, Josh Benoit, Ph.D., and his research group at the University of Cincinnati spend their days getting to know them very well—down to the genes and genomics. The idea is the more we understand ticks and other blood-feeding arthropods, the better we can avoid and eliminate them. Through the power of the Ohio Supercomputer Center's high-speed computing services, Benoit's group is learning about the biology of pests, such as ticks, through next-generation sequencing.

The group is taking a deep look into how ticks survive stressful conditions, such as the cold winter months or heat and dehydration during the summer. The group has found one reason might be their ability to control genes involved in detoxification and those regulating the accumulation of specific metabolites that decrease stress-induced damage.

"When we see them under stress, we see them upregulating a lot of genes involved in detoxification," Benoit said. "So maybe it's not the best time to try to spray pesticides on a dry day or a hot day, because ticks already have these genes upregulated to detoxify pesticides and prevent damage from stress."

Through some of the group's initial sweeps of tick populations in Ohio, they estimate the 2017 population more than doubled from 2016. More ticks means a rise in tick-related diseases in humans and livestock. To better understand underlying aspects of tick behavior and physiology, the group used RNA sequencing to analyze gene expression differences. While ticks don't have fewer actual genes than larger species like humans, there are fewer resources and fewer cells to draw from each individual.

"A human is big. You can get a lot of the same cells from one organism," Benoit said. "Versus (ticks), you have to process multiple ticks to get enough RNA or DNA. So you have to make sure they're inbred in order to get enough material from what is equivalently the same genetic background."

OSC's resources provide the group with fast data processing and ease of access through OSC OnDemand, so Benoit's students can view at home the same data they see in the lab.

"Everybody has a laptop, but the heavy processing is done on the cluster, so we would have needed to have five or six more local servers built if we didn't have access to OSC resources," Benoit said. "Not only does it give us access to a lot more processing power and space, it saves us probably $20,000 to $30,000 by not having to build our own." ◀

Benoit's group collects tick samples in the field to be studied in the lab for stress regulation.

PROJECT LEAD // JOSHUA BENOIT, PH.D., UNIVERSITY OF CINCINNATI RESEARCH TITLE // RESEARCH TITLE: RNA-SEQ ANALYSIS OF TICK FUNDING SOURCE // UNIVERSITY OF CINCINNATI WEBSITE // INSECTPHYSIOLOGY.UC.EDU

OSC excels at supporting

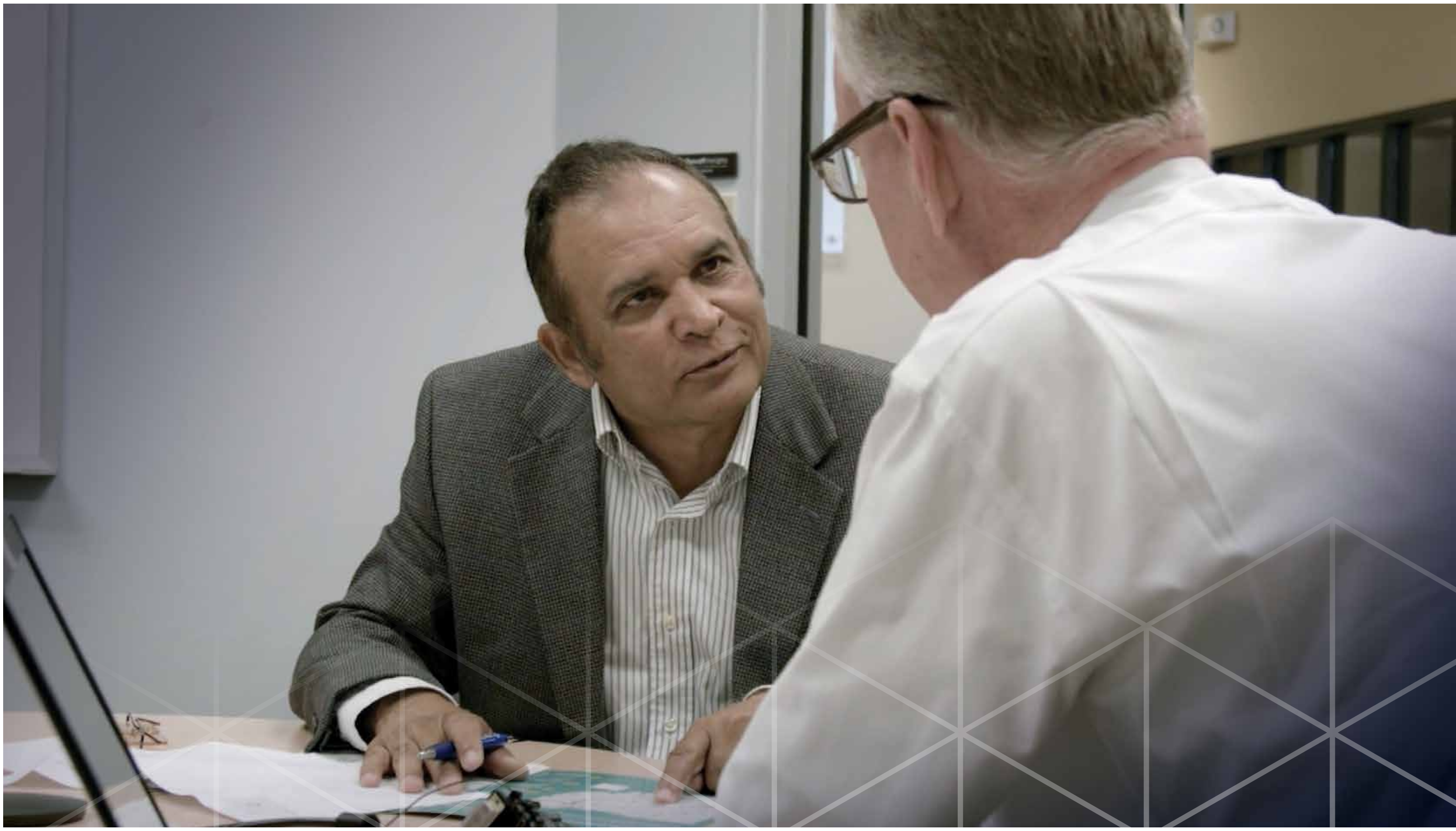
Industrial Innovation

Today, industry is leveraging high performance computing to analyze troves of collected data. As a result, innovation is exploding in such fields as consumer behavior, aerodynamics, financial services and data-intensive modeling and simulation.

The Ohio Supercomputer Center's powerful computing and storage systems help small and large businesses solve these multi-faceted Big Data challenges. Our clients, consequently, are able save both time and money while reaping game-changing insights.

> **"At Scientel, we are concentrating on the awesome power that HPC systems such as OSC's Owens Cluster can provide in making a difference dealing with Big Data. The support and enthusiasm of the OSC staff for projects of this nature are outstanding."**

— *Norman T. Kutemperor, CEO, Scientel Information Technology Corporation, Inc.*



BIG DATA

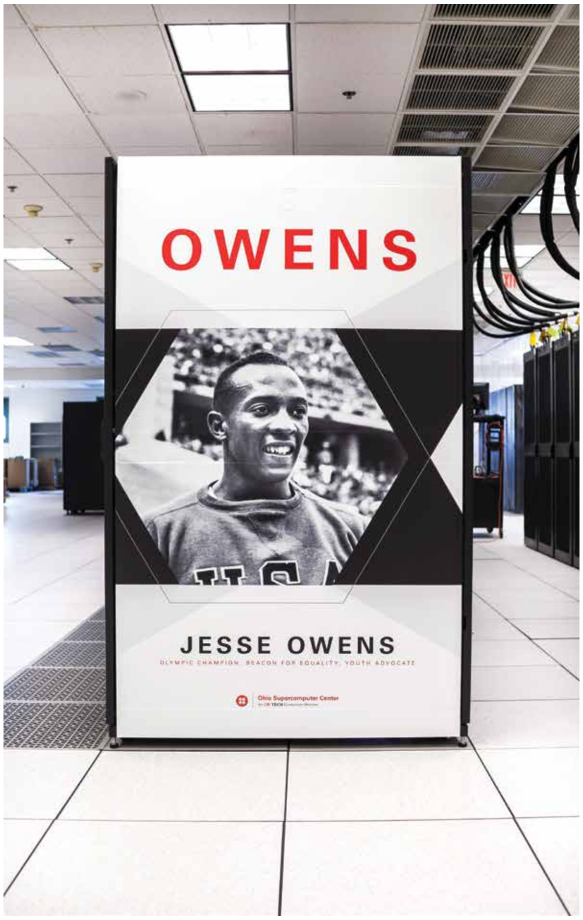
Scientel IT Corp software showcases power of OSC's Owens Cluster

In 2017, the Ohio Supercomputer Center partnered with Scientel Information Technology Corporation to demonstrate the power of the Owens Cluster by running the single-largest scale calculation in its history.

Scientel, a Big Data specialist company, used 16,800 cores of the Owens Cluster to test a new database software optimized to run on supercomputer systems. The seamless run created 1.25 Terabytes of synthetic data.

Scientel developed Gensonix Super DB, a software designed for Big Data environments that can use thousands of data-processing nodes compared to other database software that use considerably fewer nodes at a time. Scientel CEO Norman Kutemperor said Gensonix Super DB is the only product designed and optimized for supercomputers to take full advantage of high performance computing architecture that helps support Big Data processing.

PROJECT LEAD // NORMAN KUTEMPEROR, SCIENTEL INFORMATION TECHNOLOGY CORPORATION, INC. RESEARCH TITLE // SCIENTEL IT CORP GENSONIX DB SOFTWARE SHOWCASES POWER OF OSC OWENS CLUSTER FUNDING SOURCE // SCIENTEL IT CORP WEBSITE // SCIENTEL.COM



"This is a wonderful testimonial of the capabilities of Gensonix Super DB for Big Data," Kutemperor said. "The robust nature of the OSC Owens Cluster provided the reliability for this large parallel job."

To demonstrate the power of Gensonix Super DB, the Scientel team created a sample weather database application to run using OSC's Owens Cluster. For this rare large run, Scientel used 600 of the system's available 648 compute nodes. During the run, the Owens Cluster reached a processing speed of over 86 million data transactions per minute with no errors.

"As the largest-scale run ever completed on OSC's systems, Scientel helped us demonstrate the power of the Owens Cluster," said David Hudak, Ph.D., OSC interim executive director. "Owens regularly delivers a high volume of smaller-scale runs, providing outstanding price performance for OSC's clients. The ability to scale calculations to this size demonstrates another unique capability of Owens not found elsewhere in the state and unmatched by our previous systems."

With satisfactory test results on the software, Scientel will push Gensonix Super DB to the forefront of technology to process large varieties of data and compute intense problems in areas such as cancer research, drug development, traffic analysis and space exploration. A single application written for Gensonix Super DB can use more than 100,000 cores to handle multiple petabytes of data in real time.

"(The OSC staff members) are extremely knowledgeable and very capable of understanding customer requirements, even when jobs are super scaled," Kutemperor said. "Their support and enthusiasm for projects of this nature are outstanding." ◂

{FAR LEFT} Norman Kutemperor, Scientel CEO, speaks with the OSC team about future data processing projects. Earlier this year, his company conducted the largest-scale run ever on an OSC system.

INNOVATIVE ANSWERS

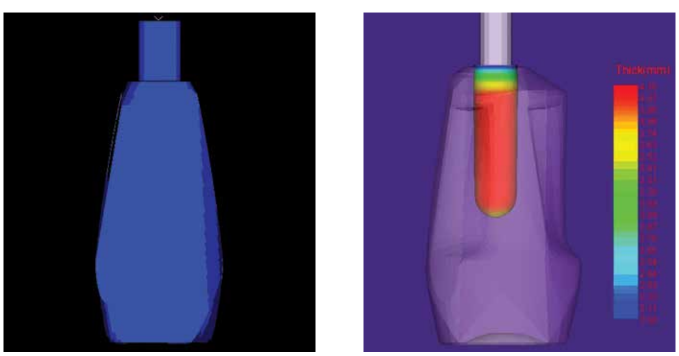
P&G gains competitive edge through modeling and simulation

"Innovation" is not merely a buzzword thrown around at Procter & Gamble. It's at the heart of everything the Ohio-based, multinational consumer goods company does, and high performance computational modeling and simulation is a major enabler.

"We compete on our ability to bring new and meaningful innovations to our consumers," said Don Bretl, associate director for modeling and simulation at Procter & Gamble. "Modeling and simulation gives us an edge. Some experiments you run on your computer you can't run in the physical world. If it's worth building, should you build it? That's one of the questions we ask a lot."

Modeling and simulation in consumer-goods products, such as understanding how a laundry detergent works or the performance of a diaper, often isn't as straightforward as in other industries for which the methods and tools were originally designed to serve.

"We have unusual characteristics we model, and there have been big challenges," Bretl said, "but in the fast-moving consumer goods, we've tried to be a leader in this area."



Modeling and simulation of consumer goods helps P&G save money and time by using computational experiments rather than physical testing. Those experiments lead to better products.

P&G was also a leader in collaborating with the Ohio Supercomputer Center in 2013 to get the AweSim program rolling in order to promote the benefits of modeling and simulation to small and mid-sized manufacturers.

"(In the past) it's been large-scale manufacturers like ourselves who can understand how best to use simulation to drive value to the product design, which is why AweSim is important, bringing that capability to smaller manufacturers," Bretl said.

One important AweSim aspect is making engineering service providers available to small- and medium-sized manufacturers as mentors to help fine-tune how software can be optimized to individual organizations, such as supply-chain businesses and large manufacturers like P&G.

"You really need to develop simulations specific to a group's need. You need a platform, a way to deliver those efficiently," Bretl said. "AweSim put all the pieces together to support somebody at a small enterprise to use sophisticated HPC software for getting better, cheaper, faster results in one stop."

While P&G has its own HPC resources, OSC has helped in P&G's biotech area with regard to workflows and open-source software. In the 2016 fiscal year, P&G turned to OSC for nearly 300,000 core hours of run time. ◀

PROJECT LEAD // DON BRETL, PROCTER & GAMBLE RESEARCH TITLE // M&S ASSISTANCE FOR ONE OF OHIO'S LARGEST MANUFACTURERS
FUNDING SOURCE // PROCTER & GAMBLE WEBSITE // PGSCIENCE.COM

APP ECO-STRUCTURE

TotalSim US developing tools to help companies fine-tune products

TotalSim US has taken great advantage of the Ohio Supercomputer Center's mandate to support commercial research as an economic driver. And it's paying off.

"We've had a long relationship with OSC," said Ray Leto, president of TotalSim US. "It's one of the reasons we've stayed in central Ohio and grown our business here."

TotalSim was a founding partner of AweSim—OSC's program to promote the benefits of modeling and simulation to small- and mid-sized manufacturers. The combination of developing web applications and using engineering service providers, such as TotalSim, is what has made AweSim a powerful program.

"The idea with this AweSim app eco-structure is to get modeling and simulation in the hands of people who couldn't afford it or didn't have the time to become an expert," Leto said. "That's part of the reason we got involved in AweSim, it's where we see things going."

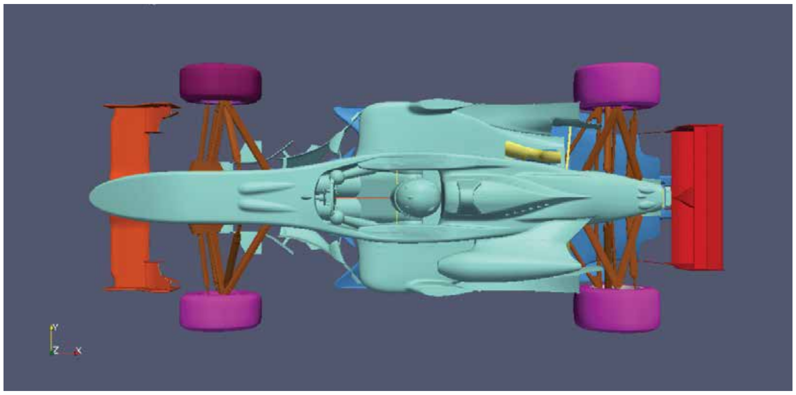
The eco-structure has allowed TotalSim to develop applications that companies are able to use to fine-tune products. Some of those companies include:

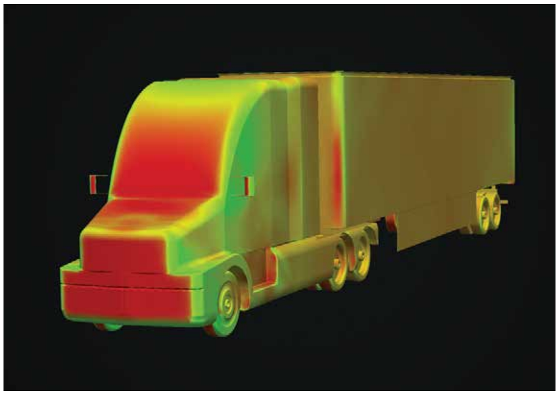
iRacing is the world's premier motorsports racing simulation. iRacing's portal puts members in the driver's seat to experience today's newest form of competitive motorsport: virtual racing. To make its simulation portal as realistic as possible, iRacing uses TotalSim's Automotive Aero App. The Automotive Aero App allows iRacing to perform aerodynamics simulations at OSC and get wind tunnel-like data to better characterize how race cars are run in their virtual environment.

Swift Engineering is a product development company that designs and builds high performance vehicles, specializing in unmanned systems, autonomy, robotics and advanced composites. Swift uses TotalSim's Aero App for preliminary design studies on UAV-type aircraft. The engineers can run the aircraft at various speeds to assess performance and obtain surface pressure and force data that can be used in their details design work.

Rocketail, LLC is a trailer and trailer equipment business within the transportation sector. The company uses the Truck Add-On App for CFD modeling and simulation to test its range of tractor-trailer drag reduction devices. Through the app, the small firm can do virtual testing of its concepts and design prior to any expensive prototype builds or on-road testing.

"Through AweSim and the apps, we hope to lower the barriers for the smaller companies that, up to now, have done everything with physical testing or traditional design methods," Leto said. ◄





TotalSim US and AweSim have developed modeling and simulation web applications that help companies, such as those in the auto racing and tractor-trailer industries, perform aerodynamics tests using computational fluid dynamics software.

PROJECT LEAD // RAY LETO, TOTALSIM US RESEARCH TITLE // APP ECOSYSTEM ALLOWS COMPANIES MODELING AND SIMULATION RESOURCES
FUNDING SOURCE // TOTALSIM US WEBSITE // TOTALSIM.US

DATA CLASSIFICATION

Super-H helps companies get ahead of competition with boost from OSC

When Richard Hughes, Ph.D., set off to found his own data-analytics company, The Ohio State University physics professor stuck with what he knew: proprietary algorithms, machine learning and use of the Ohio Supercomputer Center's high performance computational resources. Super-H, founded in 2015, is a data-analytics firm that helps companies strike a competitive advantage in their industry by providing Big Data solutions and fast, accurate answers to strategic questions.

"Our product is a website that basically organizes data related to research that's being done in different areas," said Hareesh Menon, software developer at Super-H. "We organize it and provide it to clients in a way that they can use to understand the areas they can focus on or what their competitors are doing.

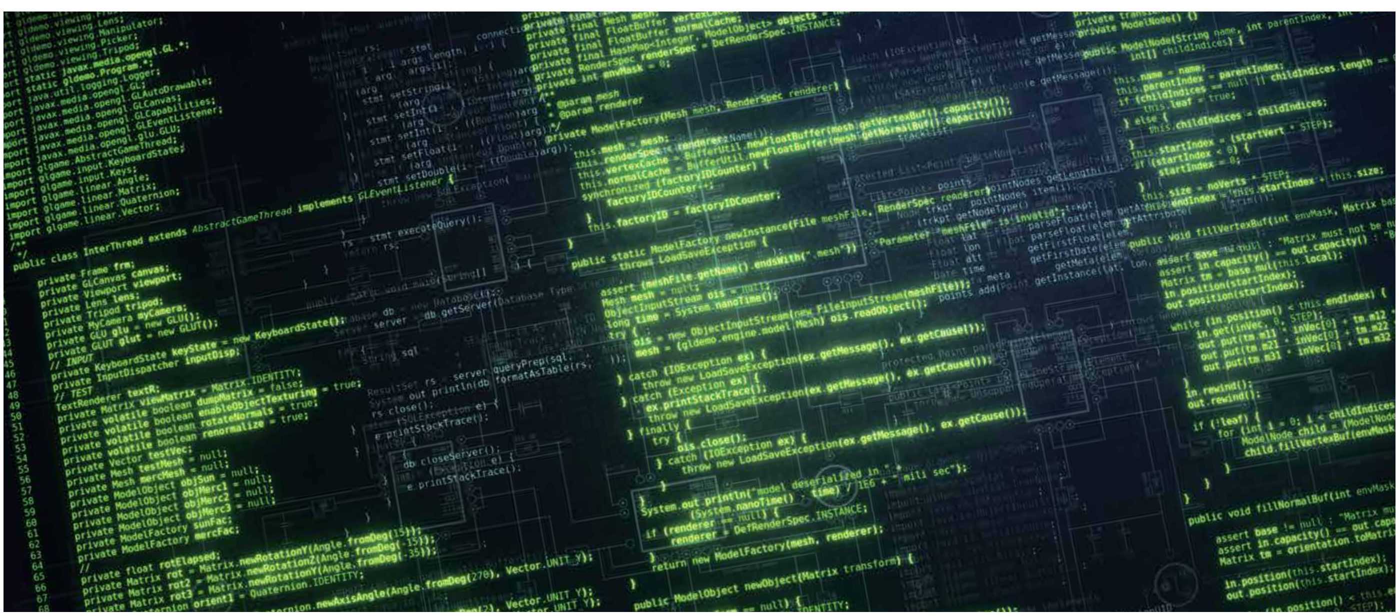
"We use OSC for a lot of data processing and analytics of our data."

The company also has used OSC's Oakley Cluster for processes, such as MySQL hosting, raw data processing and data classification. For example, one of the specific projects involves institution disambiguation. Super-H collects research institution data from PubMed. The institution names could be entered into the database in multiple ways, so one of Menon's jobs is to run the names to find every iteration of each institution and group them together as one.

"Because we're processing so much data, it takes a lot of time, and so using the supercomputer helps decrease the time," Menon said. "It's been a great resource for us, and I don't know if we'd be at the point where we are now in the same time period if we hadn't had the Ohio Supercomputer Center."

Currently, Super-H has a prototype of its web-based customized research platform and soon will create a minimal viable product to gain more clients, with plans to expand the product and features in the near future.

"Super-H is a great example of what OSC can do for small, up-and-coming businesses that need extra computing power," said OSC Director of Strategic Programs Alan Chalker, Ph.D. "We look forward to seeing them grow and helping provide whatever high performance computing resources they may need in the future." ◀



PROJECT LEAD // RICHARD HUGHES, PH.D., SUPER-H RESEARCH TITLE // INFORMATION PROCESSING AND ORGANIZATION THROUGH BIG DATA AT SUPER-H FUNDING SOURCE // SUPER-H WEBSITE // SUPERHINDEX.COM

OSC unlocks secrets across the

Research Landscape

The research landscape includes fields of science not normally associated with high performance computing, as well as many humanities-related sciences. Researchers are analyzing Big Data to track human behavior, create works of art, forecast economic trends and translate hundreds of languages.

The Ohio Supercomputer Center supports the use of its services by researchers in all fields, providing allocations on our HPC systems and offering training via workshops and one-on-one consultations.

"We're answering fundamental questions about what it means to be human and have language and be the animal that talks to each other. But accomplishing this requires the type of HPC infrastructure OSC gives us. It's tremendous, really a game-changer."

— *William Schuler, Ph.D., Department of Linguistics, The Ohio State University*

DISASTER RELIEF

Schuler's team discovering grammar rules of lesser-known languages

It is estimated there are more than 7,000 languages worldwide. For those involved in disaster relief efforts, that breadth and variety can be overwhelming, especially when addressing areas with meager resources.

William Schuler, Ph.D., linguistics professor at The Ohio State University, is part of a project called Low Resource Languages for Emergent Incidents (LORELEI), an initiative through the Defense Advanced Research Projects Agency (DARPA). LORELEI's goal is to develop technology for languages about which translators and linguists know nothing.

Schuler and his team use the Ohio Supercomputer Center's Owens Cluster to develop a grammar-acquisition algorithm to discover the rules of lesser-known languages so disaster relief teams can react quickly.

"We need to get resources to direct disaster relief and part of that is translating news text, knowing names of cities, what's happening in those areas," Schuler said. "It's figuring out what has happened rapidly, and that can involve automatically processing incident language."

Schuler's team is working to build a Bayseian sequence model based on statistical analysis to discover a given language's grammar rules. It is hypothesized this parsing model can learn a language and make it syntactically useful.

"The computational requirements for learning grammar from statistics are tremendous, which is why we need a supercomputer," Schuler said.

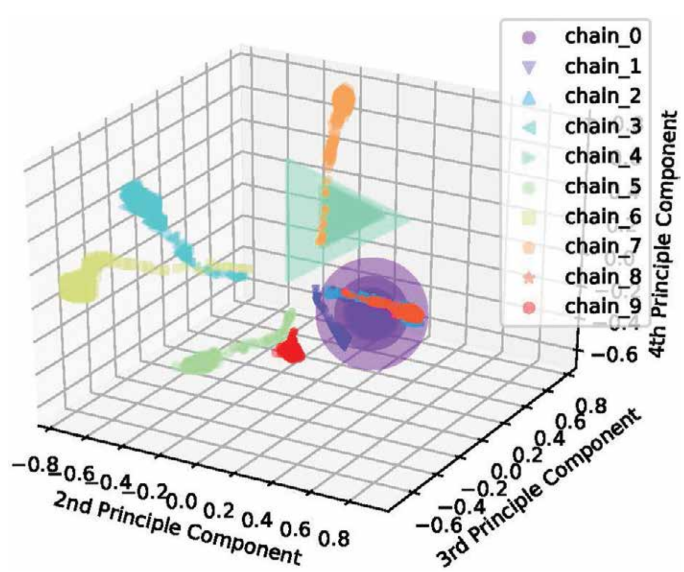
On a powerful single server, Schuler's team can analyze 10 to 15 categories of grammar, according to Lifeng Jin—a Ph.D. student who oversees the computational aspects of the project. GPUs on the Owens Cluster allow Jin to increase the number of categories greatly.

GPUs–graphics processing units—are a complementary processing unit to CPUs—central processing units, composed of hundreds of cores that can handle thousands of threads simultaneously.

"We can increase the complexity of the model exponentially," Jin said. "It's a more realistic scenario of imitating what humans are doing."

In August, DARPA organized a trial run to simulate two disasters in Africa. Schuler's group used 60 GPUs on Owens for seven days for four grammars of two languages, illustrating the importance of OSC's resources to the project.

"We're answering fundamental questions about what it means to be the animal that talks to each other," Schuler said. "The ability to ask these questions and get answers is a relatively recent innovation that requires the high performance computing infrastructure OSC gives us. It's a game-changer." ◀



This graph displays an algorithm that explores the space of possible probabilistic grammars and maps out the regions of this space that have the highest probability of generating understandable sentences.

PROJECT LEAD // WILLIAM SCHULER, PH.D., THE OHIO STATE UNIVERSITY RESEARCH TITLE // COGNITIVELY BASED UNSUPERVISED GRAMMAR INDUCTION FOR LOW-RESOURCE LANGUAGES FUNDING SOURCE // DARPA WEBSITE // LING.OHIO-STATE.EDU/~SCHULER.77

POPULATION IMPACT

Data processing helps Dunn uncover impact of loan forgiveness programs

In 2017, 44.2 million Americans held student loan debt, totaling more than $1.4 trillion, according to the U.S. Federal Reserve. With the cost of tuition rising at most higher-education institutions and enrollment increasing, these numbers are expected to keep climbing.

To evaluate the wide-reaching effects student loan policy change could have on borrowers' lives, researchers from the Department of Economics at The Ohio State University ran thousands of situational simulations using the Ohio Supercomputer Center.

To reduce the weight of student loan debt on borrowers, Congress passed the College Cost Reduction and Access Act in 2007. This major change in loan-repayment plans can relieve debt for many Americans sooner than expected. This legislation created two programs: one that would forgive student loans after 10 years of service in the public sector, and another that would allow borrowers at a certain income to make reduced payments and, after 20 years, have the outstanding loan balance forgiven.

Working under the guidance of Lucia Dunn, Ph.D., professor of economics at Ohio State, Graduate Assistant Hongyu Chen used data from the National Longitudinal Survey of Youth to model individuals' education, career, borrowing and spending decisions based on whether or not they were part of a loan-forgiveness program. Chen wrote a program that ran simulations of over 151 parameters on a population of approximately 2,500 individuals between the ages of 18 to 65 during different periods of their lives.

"The estimation takes around 10 years if I'm running just one single computer," Chen said. "That's why I have to use the cluster of computers, like the supercomputer, that use multiple cores at the same time, so that saves me a lot of time."

Still, the model took Chen around six months to complete on OSC's Oakley Cluster, using a program he wrote specifically for this project.

Chen found that the population affected by the change in student loan repayment plans increased the average total years of postsecondary education by 9 percent. Individuals were also more likely to take on more debt, holding 12 percent more before age 30 under the new plan, when knowing their loans would be forgiven. Chen said this data could be useful in informing federal government policies.

"(Student loans) are very expensive for the government. So, this directly provides the evidence (for determining) the best policies for the government to improve college enrollment or social welfare," Chen said. "It has very important direct policy implications." ◂

PROJECT LEAD // LUCIA DUNN, PH.D., THE OHIO STATE UNIVERSITY RESEARCH TITLE // THE IMPACT OF STUDENT LOAN REPAYMENT REFORM ON SCHOOLING, WORK, AND BORROWING DECISIONS FUNDING SOURCE // THE OHIO STATE UNIVERSITY WEBSITE // ECONOMICS.OSU.EDU/PEOPLE/DUNN.4

MECHANICAL SYSTEMS

Murray, Myszka developing algorithms for more efficient manufacturing

The lifeblood of manufacturing development hinges on increasing production, lowering costs and deftly overcoming any engineering problems that may arise. The backbone of any industrial facility is the mechanisms by which products are produced.

Andrew Murray, Ph.D., a professor in the University of Dayton's Mechanical & Aerospace Engineering Department, and David Myszka, an associate professor, are using the Ohio Supercomputer Center's high performance computing resources to investigate techniques for designing better machines to help manufacturers continue to become more efficient.

"The goal is improved algorithms for the synthesis of mechanical systems, like what we see in scissor jacks, dump trucks and folding lawn chairs, for example. These mechanisms are incredibly common," Murray said. "And in many cases, you don't need a fancy design process to solve the problem; engineers do it every day. But to push into new areas and try to design their new machines, we need to develop the corresponding mechanism design algorithms."

Murray and his research team are working toward creating a novel approach to designing three-dimensional spatial linkages and analyzing their kinematic output—the kinematics is essentially the motion you want a system to have. To do that, they have to tackle the intense mathematics associated with the design analysis.

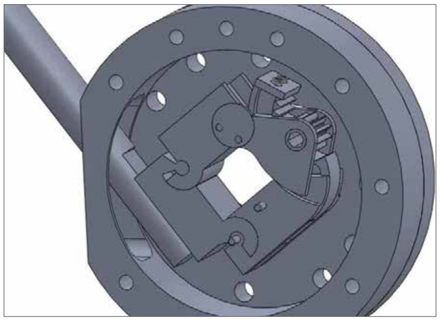
Many of the designs within the machines manufactured are described by a collection of three components: Revolute Joints (hinge or pin joints), Prismatic Joints (sliders or pistons), and Rigid Bodies (links or connectors).

"The kinematics are typically described by algebraic equations," Murray said. "As we write these equations for increasingly complicated systems, the mathematics explode. It's beyond our capacity. But we're using supercomputers to help do the problems that are building to that."

Murray's method is first to construct a mathematical model for spatial linkages. He then uses OSC's Oakley Cluster for a software package called Bertini, which requires parallel computation. Matlab analyzes the results. The results are then validated through physical models.

"Bertini is beautiful because it starts with a simple version of your problem and grows from that," Murray said. "Because it grows, it tracks every solution possible to that system of equations.

"We don't just get to look at what we have via optimization, we get to look at everything. And because these systems have so many solutions, there can be a solution sitting right next to the one you optimized that may be better." ◀



{LEFT} The design algorithms help synthesize the mechanism inside a variable geometry extrusion die. The die extrudes plastic parts with varying cross-section, a novel capacity in extrusion. {CENTER} Model of the design in the above figure. {RIGHT} The mechanism is inside the die shown. The variation in the extrusion as it exits the die is seen here.

PROJECT LEAD // ANDREW MURRAY, PH.D., THE UNIVERSITY OF DAYTON RESEARCH TITLE // DEVELOPING METHODS TO DESIGN AND ANALYZE SPATIAL MECHANISMS FUNDING SOURCE // UNIVERSITY OF DAYTON WEBSITE // SITES.GOOGLE.COM/A/UDAYTON.EDU/DIMLAB

STATEWIDE USERS GROUP

Research using Ohio Supercomputer Center resources continues to break new ground, and OSC clients continue to gain more high performance computing power and a better experience.

Statewide Users Group conferences in October of 2016 and April of 2017 brought OSC representatives face-to-face with clients and the research being done on their supercomputer clusters.

SUG is a volunteer group composed of the scientists and engineers who provide OSC leadership with program and policy advice and direction to ensure a productive environment for research.

At these past two SUG conferences, keynote speakers included NVIDIA's Jonathan Bentz, Honda R&D Americas Inc.'s Duane Detwiler and Bowling Green State University's Alexey T. Zayak, Ph.D.

Both conferences also featured breakout sessions on a variety of topics and poster and flash talk competitions. Nearly 40 participants in each conference competed, with winners receiving 5,000 resource units of time on OSC systems and runners-up receiving 2,500 RUs.

OCTOBER 2016

Flash Talk Winners

Ohio University's Tomas Rojas won the chemistry flash talk competition, and Aaron Wilson, from The Ohio State University, won the non-chemistry portion of the flash talks.

In the flash talk competition, Wilson won for the second straight meeting. His flash talk discussed "Pushing the Next-Generation Arctic System Reanalysis to the Human Scale," while Solorazano's chemistry flash talk was on "Strain Fields and Electronic Structure of CrN."

Poster Winners

Ohio State's Stephanie Kim and Sean Marguet tied for first place in the poster competition

Kim's poster was titled "Novel Binding Site of Cyclin A2 and Potential Inhibitors." Marguet's poster was titled "Computationally Guided Resonance Raman Spectroscopy of Nickel-Substituted Rubredoxin, A Model Hydrogenase Enzyme."

APRIL 2017

Flash Talk Winner

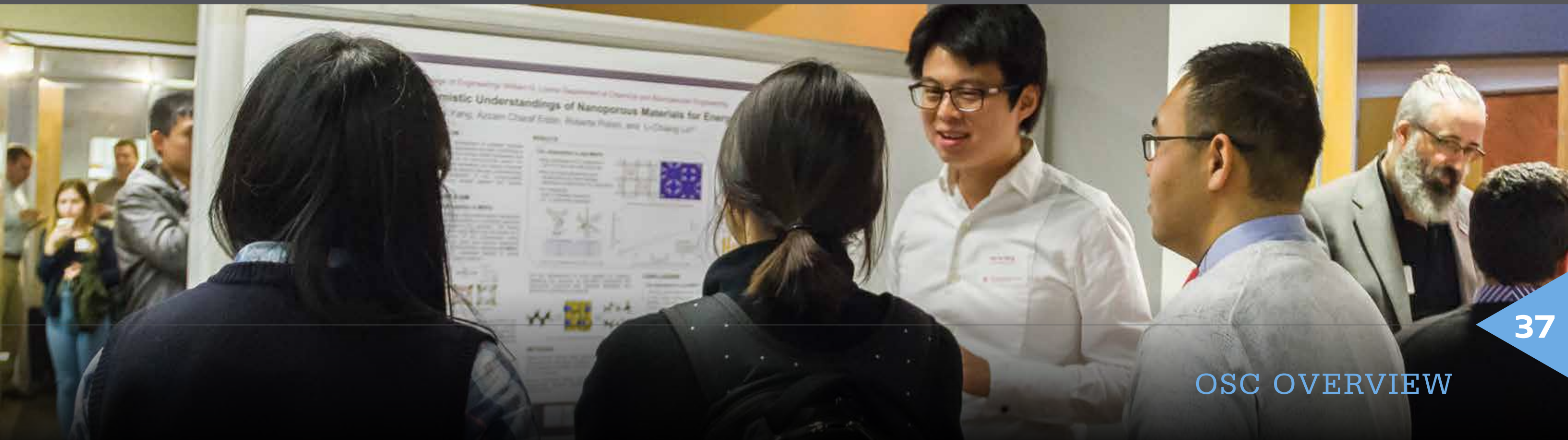
Sandip Mazumder, from Ohio State, took first place for his flash talk titled "Phonon Boltzman Transport Equation-Based Modeling of Time Domain Thermo-Reflectance Experiments." In Mazumder's study, the experiments are simulated using large-scale parallel computations of the phonon BTE in a two-dimensional computational domain, according to his abstract.

Ohio State's Gregory Wheeler was the runner-up for his flash talk, titled "Identification of Carnivory in Plants via Genomic Functional Annotation."

Poster Winner

Ohio State's Ryan Lundgreen won the poster competition for his presentation, titled "Heat Transfer and Deposition in Gas Turbine Engines."

Ohio State's Melanie Aprahamian claimed runner-up for her poster, titled "Incorporation of Mass Spectrometry Covalent Labeling Data into Rosetta Protein Structure Prediction."



TRAINING & EDUCATION

More than 200 clients attended OSC training sessions this past year, most at their home institution. OSC training and education experts visit campuses all around the state to provide personalized instruction, facilitate classroom projects, train students on the basics of supercomputing and demonstrate OSC's broad service offerings. This takes an instructional load off faculty members so their time is maximized to focus on content and solving problems.

Workshops

New groups, departments and disciplines just starting to use high performance computing (HPC) face the challenge of users who don't have seasoned colleagues to turn to within their own department or college who have used OSC previously.

OSC is addressing this learning gap through its workshops, held at a different location in Ohio each month. Though OSC has held these workshops throughout the years, this year we've been working to coordinate more stops throughout the state to help introduce academic clients to HPC and to address roadblocks they may have.

Our goal is to get to each of the different regions of Ohio at least once per year, if not once per semester.

OSC's workshop for new users includes:

- An introduction to OSC
- The basics of HPC, and why a client would use HPC
- Examples of projects that have been done on our systems
- What a supercomputer is
- What types of hardware we have and how a client can use them
- How to get an account
- How to create and submit a job to the batch system
- An introduction to the OnDemand web portal, so clients can access those systems.

OSC also offers more specialized workshops such as HPC for Big Data analysis, which incorporates Hadoop and Spark.

For future workshops, OSC is creating classes on profiling and debugging, optimizing code, an R workshop for HPC to accompany OnDemand and potentially, a course for using our new NVIDIA Tesla P100 GPUs.

OSC also can offer an introduction workshop for a department or a research group level to meet a group's specific needs.

Our goal with these workshops is to help more researchers quickly discover amazing breakthroughs that benefit the entire scientific community.

Brian Guilfoos, OSC HPC client services manager, leads an Introduction to OSC workshop for those new to supercomputing. These are held around the state throughout the year, along with other training and education opportunities.

CLIENT SERVICES

OSC employs subject-matter experts to assist with individual client requests. For any issues that arise, OSC's 24/7 support desk, which includes Level-2 engineering support, is available to provide clients with technical expertise and consulting services at any hour of any day.

Cluster Computing

OSC's cluster computing capabilities make it a fully scalable center with mid-range machines to match those found at National Science Foundation centers and other national labs.

The new Owens Cluster, with its 23,000-plus cores and single-core scheduling, allows clients to run large parallel jobs, or large numbers of small independent calculations, in the same environment. Collectively, OSC supercomputers provide a peak computing performance of nearly 1,900 teraflops. The center also offers more than 5 petabytes of disk storage capacity distributed over several file systems, plus 5.5 petabytes of backup tape storage.

Visualization and virtual environments

OSC's award-winning Interface Lab translates technology into effective training and assessment tools for use by various sectors, such as the health care, automotive and manufacturing industries. With recent upgrades, the lab soon will work toward shared virtual environments where individuals can move around freely without tethered devices.

Software development

Researchers can access a wide variety of software packages as well as run software for which they provide the license, open-source packages or in-house developed applications.

Through Open OnDemand, an open-source software based on the proven OSC OnDemand platform, HPC centers around the U.S. and world can allow researchers and students to install and deploy advanced web and graphical interfaces.

For industrial clients, OSC's AweSim app developers can share apps through the AweSim dashboard, a mobile app store featuring client-developed resources. This makes modeling and simulation more affordable and accessible to even small businesses, allowing them to compete in a world driven by cutting-edge technology and lightning-fast production.

26 Ohio-based universities

41 companies

1,358 clients

218 trainees

8 training opportunities

218 awards made

533 projects served

31 academic courses used OSC's supercomputers

SYSTEMS & SOFTWARE

In March 2017, the Ohio Supercomputer Center unveiled the most powerful system in the history of the Center, the Dell/Intel Xeon Owens Cluster. The name pays tribute to renowned Olympic sprinter, beacon for racial equality and youth advocate James C. "Jesse" Owens.

The Owens Cluster, which increased the center's total computing capacity by a factor of five, provides clients with a peak performance of 1.9 petaflops, tech-speak for the ability to perform 1.9 quadrillion calculations per second. The system is powered by Dell PowerEdge servers featuring the latest family of Intel Xeon processors, includes storage components manufactured by DDN, provides Pascal P100 GPU accelerators made by NVIDIA and utilizes interconnects provided by Mellanox.

In 2016, OSC staff members also tackled the installation of an entirely new storage infrastructure and a renovation of the data center suite. The Center now offers clients nearly 5.5 petabytes of disk storage, as well as new NetApp software and hardware for home directory storage. Engineers also installed Plexiglas containment walls around two of the clusters to improve cooling efficiency, laid new raised-floor tiles and built a viewing gallery, among a host of improvements. At the same time, OSC migrated infrastructure services to new hardware, and updated software versions. These components, not directly accessible to OSC's users, are fundamental to the operation of the HPC systems.

Additionally, the center provides researchers with more than 115 different software packages, with about 15 of them being licensed packages. Researchers can bring their own licensed software, open-source packages or in-house developed applications. Among the most-used software codes this past year were VASP for atomic scale materials modeling, OpenFOAM for computational fluid dynamics, LAMMPS for molecular dynamics simulation and Python for scientific programming, scripting and data analytics.

HIGH PERFORMANCE COMPUTING & STORAGE

In 2016, more than 1,350 researchers across Ohio depended upon several key OSC systems:

Dell/Intel Xeon Owens Cluster
23,392 compute cores and 160 GPU accelerators provide a total peak performance of 1,600 teraflops

HP/Intel Xeon Ruby Cluster
4,800 compute cores and 20 GPU accelerators provide a total peak performance of 144 teraflops

HP/Intel Xeon Oakley Cluster
8,304 compute cores and 128 GPU accelerators provide a total peak performance of 154 teraflops

DDN/IBM Spectrum Scale and NetApp Clustered Data ONTAP Storage
Contains more than 5 petabytes of disk storage

3.4 M+
computational jobs

115 M+
core hours consumed

97.9%
up-time (target: 96%)

1,101 TB
data stored

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Ohio Supercomputer Center
An OH·TECH Consortium Member

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

Ohio Technology Consortium: Governed by the Chancellor of the Department of Higher Education, OH-TECH serves as the technology and information division of the Ohio Department of Higher Education. The consortium comprises a suite of widely respected member organizations unsurpassed in any other state: OSC, OARnet and OhioLINK.

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