OAK RIDGE NATIONAL LABORATORY

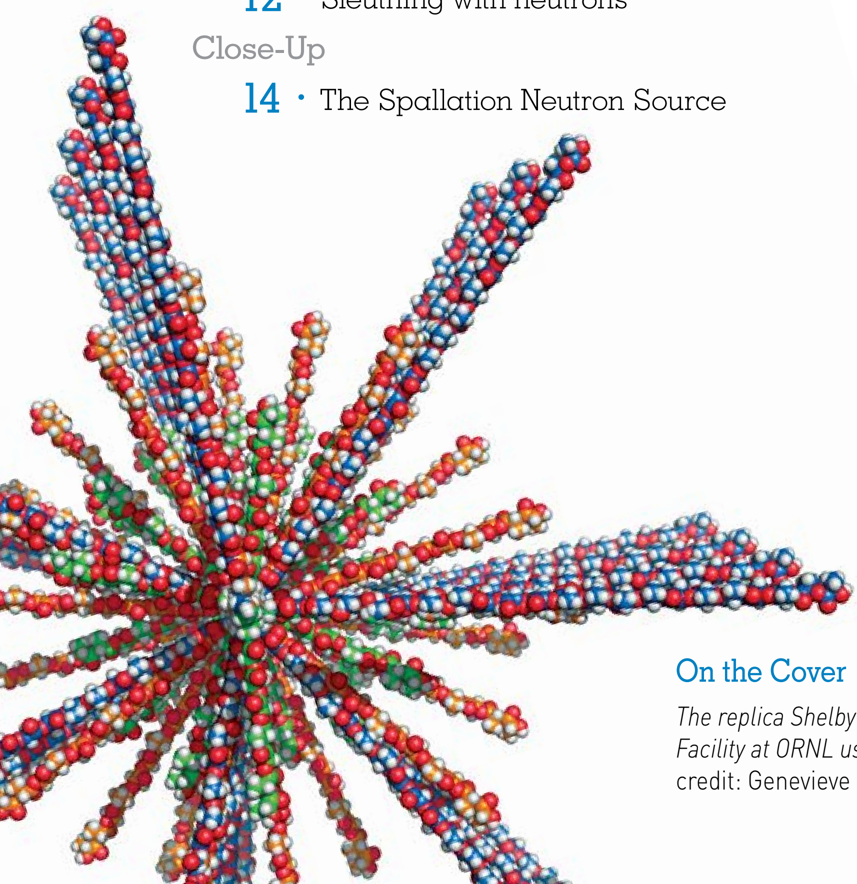
Review

OAK RIDGE National Laboratory

Vol. 48 | No. 1 | 2015
www.ornl.gov/ornlreview

OAK RIDGE NATIONAL LABORATORY
Review
Vol. 48 | No. 1 | 2015

Contents



On the Cover

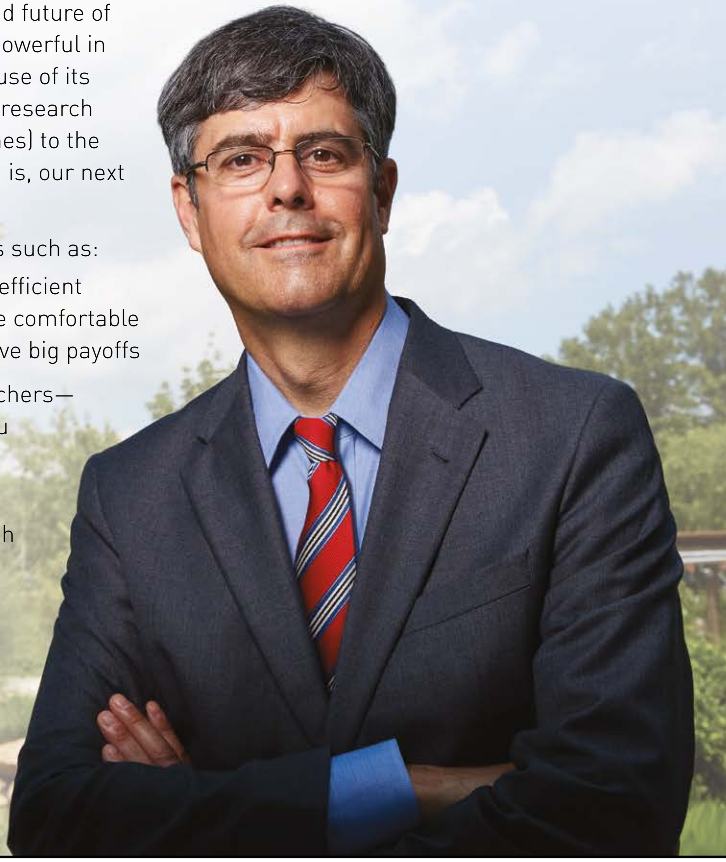
The replica Shelby Cobra was printed at DOE's Manufacturing Demonstration Facility at ORNL using the Big Area Additive Manufacturing machine. Image credit: Genevieve Martin, ORNL

Growing with ORNL's science and technology

Welcome to the new *ORNL Review*. With this issue, we begin taking a different approach to our presentation of the lab's latest research. Instead of focusing almost entirely on work in a specific field—with a single issue dedicated to neutron research, supercomputing, advanced materials, national security, clean energy and other leadership areas—we will provide a regular look at the breadth of our science and engineering.

The change is necessary because ORNL's research portfolio continues to mature and expand. The *Review* will still focus on the big news of the moment, such as the CORAL supercomputing announcement highlighted in this issue, but we also will make room for regular updates about work across the lab.

Our new look and feel aims to make this information easily accessible. Many stories are shorter, with links to more information online. We rely on informational graphics where they tell our story more effectively. We also want to introduce you to more of our talented researchers—the people behind science that's being recognized around the world.



This edition brings you an important update on the present and future of supercomputing at ORNL. Our Titan system is the second-most powerful in the world (behind China's Tianhe-2), and we're making excellent use of its abilities for the advancement of science. Go to page 6 to discover research from the practical (making the most of internal combustion engines) to the existential (the evolution of the Milky Way). As impressive as Titan is, our next system, Summit, will be five to 10 times more powerful.

I hope you'll also check out our updates on important projects such as:

- Research that will make transportation safer and more efficient
- Technologies that will make buildings smarter and more comfortable
- Advances at the atomic and molecular scale that will have big payoffs

On pages 26 and 27, you'll meet some of our youngest researchers—graduate students and post-doctoral researchers who will tell you about their work and their choice of science as a career.

Finally, we spotlight the High Flux Isotope Reactor, which recently turned 50 and continues to do yeoman's work for research and isotope production alike. It's evidence of our rich history in nuclear science that HFIR continues to offer unique and world-leading capabilities entering its sixth decade of operation.

Our lab is filled with bright people doing extraordinary work. I hope you find each edition of the new *ORNL Review* to be an entertaining and informative reminder of the power of applying diverse scientific expertise to some of the biggest challenges of our time.

Thomas Mason

Thomas Mason
Laboratory Director

ORNL, Chinese institute advance nuclear tech

ORNL is working with the Shanghai Institute of Applied Physics to develop advanced nuclear reactors that are cooled with salts rather than water.

The Chinese Academy of Sciences—parent agency to the Shanghai Institute—has launched a major program to develop reactors cooled with fluoride salts. Plans call for two reactors, both of which will use low-enrichment uranium fuel. The first will produce up to 10 megawatts of thermal power; the second, 100 megawatts. The agency is pushing the technology to supply industrial process heat and electricity to China's growing economy, especially in areas with limited water.

Chinese researchers are interested in working with colleagues from ORNL because of the lab's expertise in advanced reactor design. In addition, ORNL was home to the world's first and only salt-cooled reactor to date—the Molten Salt Reactor Experiment—which operated from 1965 to 1969.

The collaboration—specifically in the form of a Cooperative Research and Development Agreement—grows from cooperation between the Chinese Academy of Sciences and DOE, ORNL's parent agency. Insights generated by the collaboration will be available to companies in both countries.

The research and development agreement focuses on a Chinese design known as fluoride salt-cooled high-temperature reactors. The project will draw on ORNL's expertise in fuels, materials, instrumentation and controls, design concepts, and modeling and simulation for advanced reactors.

ORNL researchers join tropical forest study

More than a dozen researchers from ORNL's Climate Change Science Institute will join colleagues from other agencies and national labs to increase our understanding of tropical forests and the role they play in the Earth's climate.

The project—known as Next-Generation Ecosystem Experiments (NGEE)-Tropics—will shine a light not only on the influence tropical forests play in climate, but also on how that influence is likely to change as global temperatures rise, greenhouse gas levels rise, and precipitation patterns shift.

"Tropical forests cycle more carbon and water than any other biome, and as such they're a critical player in the planet's energy balance and in climate change. But there's a lot we don't know," said principal investigator and project director Jeff Chambers of Lawrence Berkeley National Laboratory.

Over the next decade, NGEE-Tropics scientists will work with other researchers to carry out experiments in tropical forests around the globe. This research will fuel a tropical forest ecosystem model that extends from the bedrock to the top of the forest canopy. The model will capture myriad soil and vegetation processes at a resolution better than 10 kilometers, which is the resolution that next-generation Earth system models will achieve during the project's lifetime.

ORNL's collaborators will lend their expertise in ecology, environmental science, biology, modeling and data management to the project.

"This modeling of the tropics is unprecedented in its scale, complexity and number of processes that are being incorporated," said ORNL's Scott Painter.

The project is being led by Berkeley Lab, with other collaborators from Brookhaven, Los Alamos and Pacific Northwest national laboratories, the Smithsonian Tropical Research Institute, the U.S. Forest Service, the National Center for Atmospheric Research, and NASA. Plans call for $100 million in funding from DOE's Office of Science, spread over 10 years.

For more information: http://go.usa.gov/3WjX4

ORNL researchers work to make cars cybersafe

Many drivers think of their car as a protected bubble, an isolated space during their commute. However, vehicles are only as isolated as the technologies connected to them, including phones, navigation systems, Bluetooth and Wi-Fi. Even familiar automated sensors, such as adaptive cruise and traction control, are connected to a central communications network in the vehicle.

Moreover, as auto manufacturers introduce autonomous and semi-autonomous vehicles into the market, the U.S. Department of Transportation has announced plans to enable vehicle-to-vehicle communication in lightweight vehicles and is researching vehicle-to-infrastructure communication.

While vehicle-to-vehicle and vehicle-to-infrastructure communications are

The future of tropical rainforests in the Amazon (pictured) and worldwide is the focus of a new research project that combines field experiments and predictive modeling.

expected to reduce highway accidents and fatalities, decrease traffic congestion, and curb transportation-related carbon emissions, vehicles with these capabilities also need adequate protection against cyberattacks that can spread malware or disrupt controls.

"When there's a cyberattack on your laptop, it's not a physical or life-threatening attack, but with cars, it's different," said Joseph Raetano, research scientist with ORNL's National Transportation Research Center.

Researchers like Raetano are concerned that if vehicle cybersecurity systems are not preventively strengthened and standardized, malevolent hackers could remotely disable or manipulate brakes, steering, and other controls, causing disasters.

"Until recently, vehicles didn't normally have external communications," Raetano said. "But now, the electronic attack surface has expanded, and the safety standards that make vehicles safe are critically impacted."

Over the next two years, the ORNL team is developing a Trustworthy Vehicle Computing System that likely will be a combination of hardware and software that can detect and counter cyberattacks in real time.

"As a national laboratory, it is our mission to defend our energy resources," Raetano said. "We're designing a system that is as impervious to attacks as possible."

The initial step to developing a cybersecurity system is identifying the vulnerabilities already present across vehicle communication systems and those soon to be introduced. As private manufacturers promote new autonomous features, Raetano said, national labs and universities can play a role in standardizing an assessment framework to determine defensive security measures so that vehicles are protected from attacks when they go on the market.

For the first year of the Laboratory Directed Research and Development TVCS project, the team will analyze common hardware and software vulnerabilities across a broad range of vehicle makes and models to create such an assessment framework.

"Automakers focus on their own vehicles," Raetano said. "We want to compare and contrast vulnerabilities over all vehicles to determine the safest vehicles, why they are so safe, and what automakers can do to improve security."

The team will use these assessments to build a library of possible methods of cyberattack by vulnerability and scope, which will lead to the development of the TVCS that can simulate and model attacks and evaluate safety responses.

The team is engaging other national labs and universities in building a reference database of vehicle characteristics to reduce duplication and upfront costs that go into this kind of baseline research, and ORNL researchers have already started collaborating with students and faculty at the University of Tennessee and Tennessee Technological University.

For more information: http://go.usa.gov/3WyEh

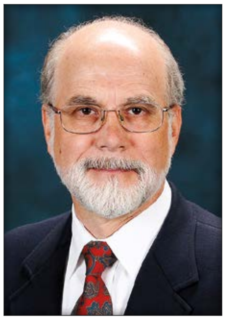
Two energy research centers led by ORNL

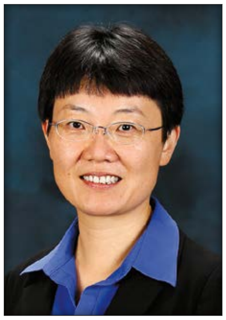
DOE has endorsed two ORNL-led research efforts—one looking into fluid interfaces, the other at the reaction of materials to high-stress environments—by naming them Energy Frontier Research Centers.

Energy Secretary Ernest Moniz made the announcement. In all, DOE will provide $100 million to 32 such research centers, with the goal of accelerating the pace of breakthroughs in energy research. In addition, ORNL scientists are participating in six centers led by other institutions.

"Today, we are mobilizing some of our most talented scientists to join forces and pursue the discoveries and breakthroughs that will lay the foundation for our nation's energy future," Moniz said. "The funding we're announcing today will help fuel scientific and technological innovation."

The two ORNL-led centers are the Fluid Interface Reactions, Structures and Transport Center and the Energy Dissipation to Defect Evolution Center.





David Wesolowski is director of the Fluid Interface Reactions, Structures and Transport Center. Yanwen Zhang leads the Energy Dissipation to Defect Evolution Center.

The former, led by David Wesolowski, is a renewal expected to receive $15.2 million over four years. The goal of the center is to develop a nanoscale-level understanding of fluid–solid interfaces—an effort that promises to bear fruit in research areas such as batteries, capacitors, solar panels, fuel cells and catalysts. Eventually, center collaborators want to predict and control the interaction of electrons, atoms, ions, and molecules for new energy technologies.

Participants come from ORNL and Argonne National Laboratory as well as universities across the country, including Vanderbilt, Drexel, Penn State, the University of Delaware, the University of Virginia, and University of California campuses at Davis and Riverside.

The Energy Dissipation to Defect Evolution Center, led by Yanwen Zhang, is a new award, with the center expected to receive $14.8 million over four years. The center will be working toward a fundamental understanding of energy dissipation in materials under irradiation. The project is intended to help in the effort to control the evolution of defects in structural alloys used in high-radiation environments such as nuclear reactors.

Collaborators come from ORNL and Los Alamos National Laboratory, as well as the University of California at Berkeley, the University of Wisconsin at Madison, and the universities of Michigan and Tennessee.

"The thing that defines these energy frontier research centers is the fact that it brings together people from different disciplines to work together to solve a big problem," noted Michelle Buchanan, ORNL's associate laboratory director for physical sciences. "The other thing that's happened is they have a really vibrant bunch of students and postdocs that work with them, and that's been a real plus in these EFRCs."

For more information: http://go.usa.gov/3jNVB

Report: national labs are great for postdocs

A recent report from the National Academies reinforces a point we've known all along: Postdoctoral positions at ORNL and other national laboratories are great opportunities for young researchers.

"The Postdoctoral Experience Revisited" is less enthusiastic about university postdocs, especially for all but the relatively few emerging Ph.D.s destined for academic positions. Writing on *Science* magazine's website, Beryl Lieff Benderly says the report "comes all the way up to, but does not actually state, some inconvenient realities: For all but a small percentage of aspiring researchers, doing a postdoc at a university is a lousy idea because it will neither result in an academic job nor otherwise advance one's career."

Postdocs at national labs and industry research facilities, on the other hand, fare better, according to the report.

"Testimony from current postdoctoral researchers and the experience of some committee members indicated that the experience of these postdoctoral researchers differs in significant ways from their academic counterparts: salaries are higher, the term of the appointment is usually shorter, their position in the institution is more clearly defined, and there is a reasonable chance that the postdoctoral researcher will eventually be hired for permanent employment."

ORNL Postdoctoral Program Manager Danny McKenna isn't surprised to hear that national laboratory positions are good for postdocs.

"When we brought the Postdoc Program in-house in 2012, it was largely in recognition of the strategic importance of postdocs to fulfilling the ORNL mission. However, we also recognized that we could make this a worthwhile experience for the postdocs regardless of what they do after their postdoc. Having an ORNL postdoc training experience is an enhancement to an academic resume that can open doors in academia, industry and other national labs."

The report is available at http://www.nap.edu/catalog/18982/the-postdoctoral-experience-revisited

This replica Shelby Cobra was printed at DOE's Manufacturing Demonstration Facility at ORNL using the Big Area Additive Manufacturing machine. BAAM can manufacture strong, lightweight composite parts larger than a cubic meter. This Cobra comes in at about 1,400 pounds and contains 500 pounds of printed parts made of 20 percent carbon fiber. Image credit: Genevieve Martin, ORNL. *For more information: http://go.usa.gov/3W9SA*

Doctoral students learn the wonders of neutrons

Thirteen Ph.D. students from the University of Missouri, Indiana University, and North Carolina State University gathered at ORNL in April for an intensive course applying neutron scattering to their studies of materials science and biological systems.

The hands-on workshop used instruments at ORNL's Spallation Neutron Source and High Flux Isotope Reactor to demonstrate how neutron probing of materials is useful in a variety of research endeavors.

The event was co-hosted by ORNL and the National Science Foundation's Integrative Graduate Education and Research Traineeship program as part of its five-year, $3 million project, "Neutron Scattering for the Science and Engineering of the 21st Century."

"Neutrons are a powerful and unique tool for understanding how our world works, but their application is still relatively new in many areas of science," said Greg Smith, ORNL lead for the workshop. "Through partnerships such as this effort with NSF, we improve the chances that scientists use all the options available to advance their research."

The workshop series—the first of which was held in 2013 at ORNL—was led by University of Missouri physicist Haskell Taub, director of the NSF program's neutron scattering project.

While at ORNL for five days, the 13 trainees listened to lectures from neutron science experts, shadowed instrument scientists, and explored the HFIR and SNS facilities to learn how the latest developments in neutron scattering techniques are advancing important new science.

For more information: http://go.usa.gov/3KjZ9

Environmental record found in fish ears

ORNL researchers supported the Tennessee Valley Authority's restoration efforts in the wake of the 2008 coal ash spill in Kingston, Tenn.

Using lasers and mass spectrometry to analyze a structure in the inner ear of fish, researchers assessed contaminant levels in different areas and across time. This hard structure, called an otolith, develops over time, allowing researchers to examine it much the way they would look at tree rings.

The spill at TVA's Kingston Fossil Plant released 5.4 million cubic yards of fly ash into the Emory River.

"TVA is really concerned about finding out how well their restoration is going because they put a lot of money, time and effort into it," said Brenda Pracheil of ORNL's Environmental Sciences Division.

The ORNL team plans to analyze otolith samples collected over the last five years. During the study, the researchers will pay close attention to selenium, mercury and arsenic levels, with selenium being of particular interest because of its tendency at high concentrations to disrupt a fish's reproductive system and early life stages.

For more information: http://go.usa.gov/3WTsS

Atom-thick graphene desalinates seawater

An ORNL-led team has demonstrated a technology that efficiently desalinates water using a porous membrane made of strong, slim graphene—a carbon honeycomb one atom thick.

Less than 1 percent of the Earth's water is drinkable, so removing salt and other minerals from our biggest available source of water—seawater—may help satisfy a growing global population thirsty for fresh water.

But desalination takes a lot of energy. Current methods include distillation—which requires you to heat the water—and reverse osmosis, in which smaller water molecules are pushed through a membrane while larger salt ions stay behind. The ORNL technology improves on reverse osmosis.

"Our work is a proof of principle that demonstrates how you can desalinate saltwater using freestanding, porous graphene," said Shannon Mark Mahurin, who co-led the study with ORNL colleague Ivan Vlassiouk.

"It's a huge advance," said Vlassiouk, pointing out that a wealth of water travels through the porous graphene membrane. "The flux through the current graphene membranes was at least an order of magnitude higher than [that through] state-of-the-art reverse osmosis polymeric membranes."

The team's results are published in the March 23 advance online issue of *Nature Nanotechnology.*

For more information: http://go.usa.gov/3KbfP

Researchers analyze fish otoliths using a laser to understand environmental changes related to the Kingston spill.

SUMMIT will take computing to new heights

by Leo Williams
williamsjl2@ornl.gov

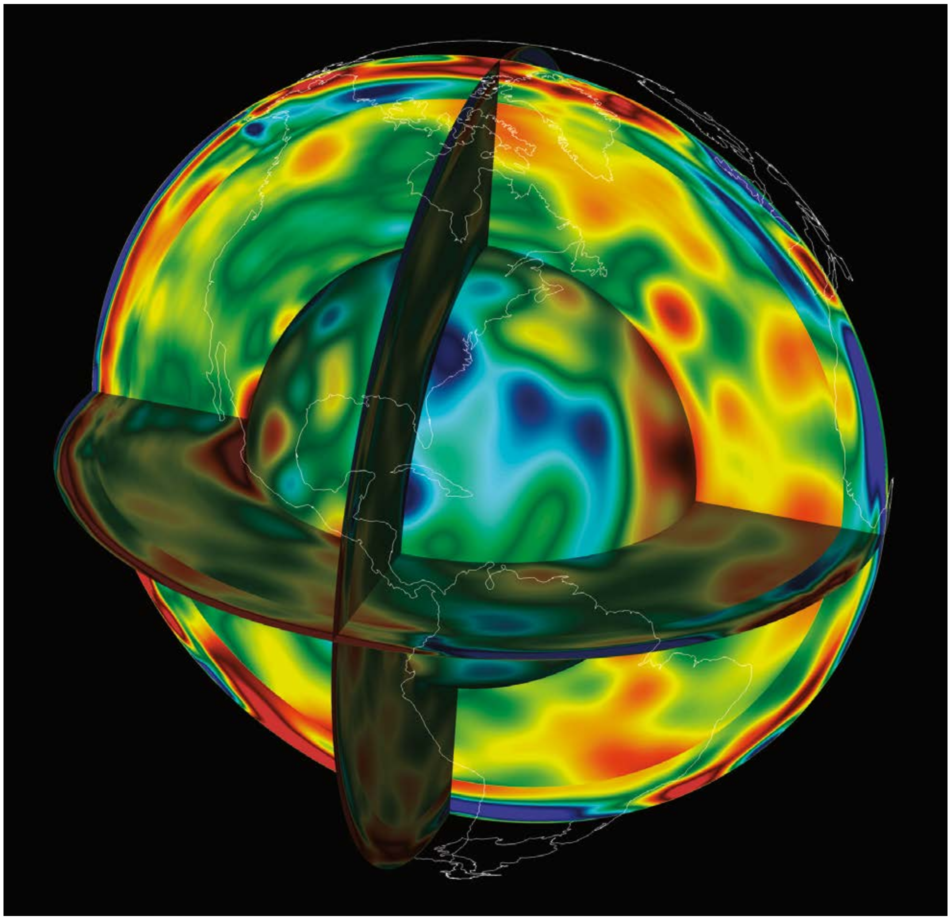
There's a good reason research institutions keep pushing for faster supercomputers: They allow the researchers to develop more realistic simulations than slower machines. This is indispensable for scientists and engineers striving to understand the workings of the universe or to create powerful new technologies.

ORNL's next step in this endeavor will be Summit, a system that will rely on traditional central processing units, which have been running computers for decades, combined with graphics processing units, which were created more recently to accelerate video processing.

Summit is being built by IBM and powered by two as-yet-unreleased processors: IBM's own Power9 CPUs and Volta GPUs from NVIDIA. It is part of a three-supercomputer acquisition coordinated by DOE among ORNL, Lawrence Livermore National Laboratory in California and Argonne National Laboratory in Illinois.

At a research institution such as ORNL, supercomputers are used to accurately simulate the physical world, but the physical world is a complicated place. To do their job well, these machines must process a lot of information on vastly different scales, from subatomic particles moving unbelievably fast to galaxies nearly as old as the universe. As a result, researchers need more powerful computers.

Progress has been impressive. The world's most powerful computer today is more than 400 times faster than the top machine a decade ago, and that system was more than 400 times faster than the top machine a decade before. ORNL is already home to the world's second fastest supercomputer, Titan (see "Titan has a very good year," page 7), which can chew through as many as 27 million billion calculations each second—or 27 petaflops—but there are many pressing questions that not even Titan can answer.



Summit will help Princeton University's Jeroen Tromp map the Earth's interior using earthquake data from around the world. Tromp and his team have already been using the process, known as seismic tomography, on Titan. Image credit: David Pugmire, ORNL

Summit, which will be available to users in 2018, will be another five to 10 times more powerful than Titan. That means it will have a peak performance somewhere between 150 and 300 petaflops. For the Oak Ridge Leadership Computing Facility, however, that's not really the point.

"We really don't like to talk about it in terms of peak performance, because peak performance really is not the most important thing," said OLCF Project Director Buddy Bland. "Peak performance is just the biggest number on your speedometer. It doesn't say how fast your car will really go. We selected the system

Continued on page 8

Image credit: Andy Sproles, ORNL

Titan has a very good year

As we prepare for Summit, the world's second fastest supercomputer is breaking scientific barriers right now

Early Summit projects

To help researchers make the most of Summit from day one, the Center for Accelerated Application Readiness brings application developers together with experts from the Oak Ridge Leadership Computing Facility and hardware makers IBM and NVIDIA. Their work will identify the best development strategies for Summit and facilitate early achievements on the system.

CAAR will focus on 13 projects encompassing a wide range of scientific disciplines and computational approaches. They include

- A climate code to couple atmospheric, land, ocean and ice models, focusing on land-ice interactions along the coasts of Greenland and Antarctica.
- Chemistry codes to promote safer handling of nuclear material, improve analysis of large molecular systems and analyze molecules that protect the cells in your body.

Continued on page 8

by Leo Williams
williamsjl2@ornl.gov

Summit won't be open to users for another three years, but let's not forget that ORNL already has the world's second-fastest computer—the 27 petaflop Titan.

Titan has been ranked either first or second in the world since researchers began using it in 2012. In fact, Titan delivered more computing power to researchers in the past year than ever before.

How fast is Titan? Imagine a million people doing one calculation each, every second, for a million years. When their time ran out, they would have done more than 30 million million million calculations. Titan would get through that workload in just under 20 minutes.

As a result, Titan has enabled breakthrough research from the practical to the profound. On the practical side, the largest, most accurate simulation to date of combustion will save both money and the environment by making our vehicle engines more efficient (see "The complexities of engines," page 10). Turning to the profound, simulations showing how our own Milky Way galaxy assembled over 10 billion years help explain how we got here (see "Team builds the Milky Way, star by star," page 11).

Other researchers have broadened our knowledge of high-temperature superconductors, materials with the potential to rewrite the rules of energy production and distribution (see "Superconductor simulated without cutting corners," page 9). Still others are expanding our knowledge in materials research, physics, biology and all areas of computational science.

They had these opportunities because the OLCF does a stellar job keeping Titan happy and productive. Not only were there no unscheduled outages last year—an impressive feat for a system of Titan's size and complexity—but all 18,000-plus nodes stayed busy. On top of that, most of the simulations run on Titan—62 percent to be precise—were massive, taking up 20 percent or more of the machine.

"We've had a great year," said OLCF Director of Science Jack Wells. "We've delivered more time—more capability—to users than ever before. We've delivered a higher percentage of big jobs than ever before, and at the same time we've had very high utilization. It's hard to do a good job at both, but we've done that."

(Summit: continued from page 6)

based on its predicted performance on full applications."

Getting ready for Summit

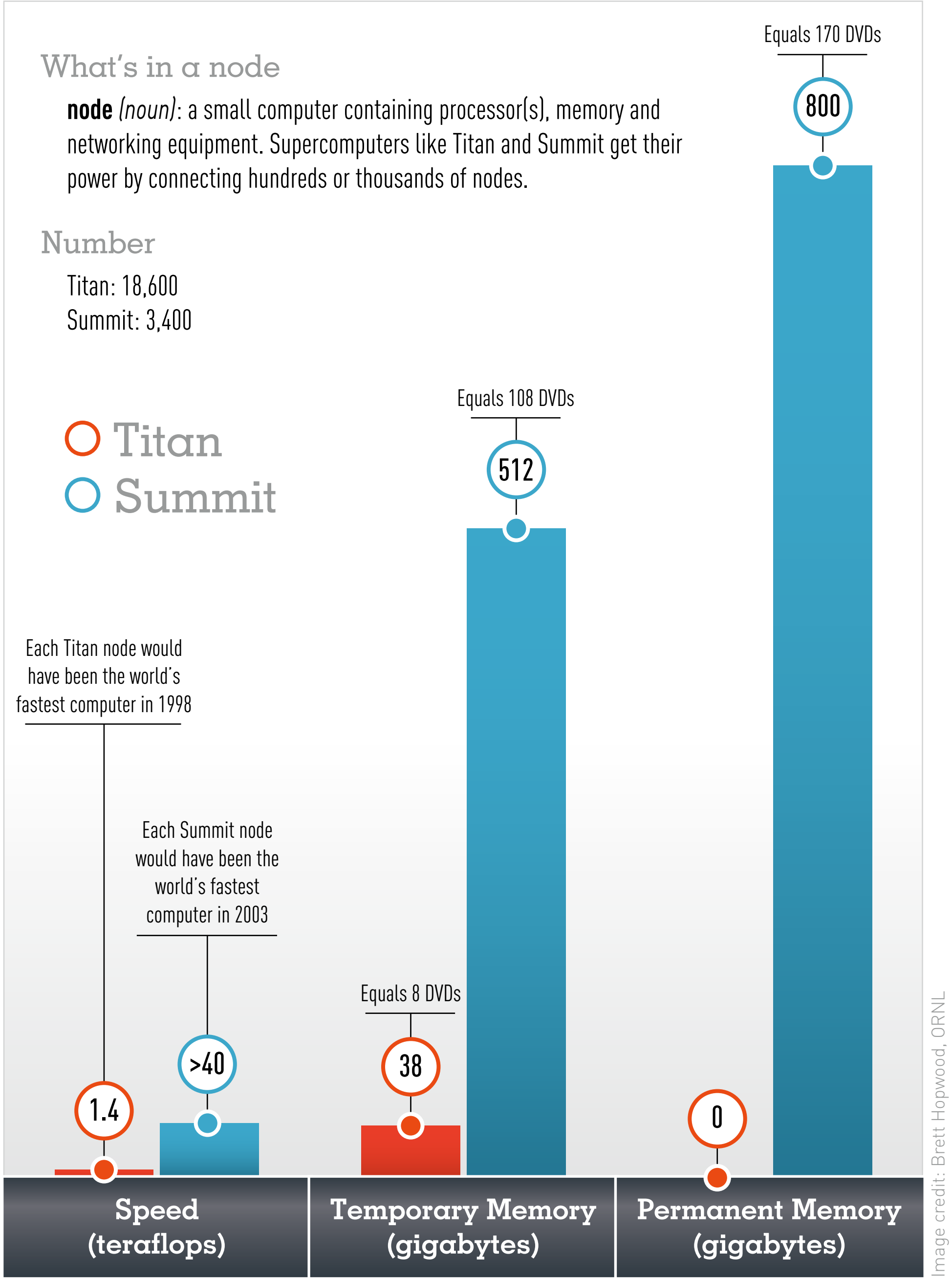
The drive to prepare applications for Summit will begin with the Center for Accelerated Application Readiness (see "Early Summit projects," page 7). CAAR will include 13 advanced applications chosen for their potential to produce scientific breakthroughs on the new machine. Application developers will work with teams that include experts from the OLCF, IBM and NVIDIA. Their goal will be both to optimize the applications for use on Summit and to develop best practices for developers preparing to run on the machine.

Their job will be made a little easier by the architecture OLCF officials picked for Summit. In choosing a system containing CPUs and GPUs, they are following the same path they started down with Titan. Summit will have fewer nodes (3,400, compared to 18,600 on Titan), and the nodes will be much more powerful. It will be able to perform many more calculations simultaneously, meaning developers will have to divide computing jobs into more and smaller pieces in a process known as parallelism.

A familiar process

Still, the process is fundamentally similar.

"For users who are running effectively on Titan and taking advantage of the GPUs, I think moving to Summit will be relatively easy," Bland said. "But it's only relatively easy. You still have to find more parallelism in the code."



Footnote: 1 teraflop = 1,000,000,000,000,000 calculations/second.

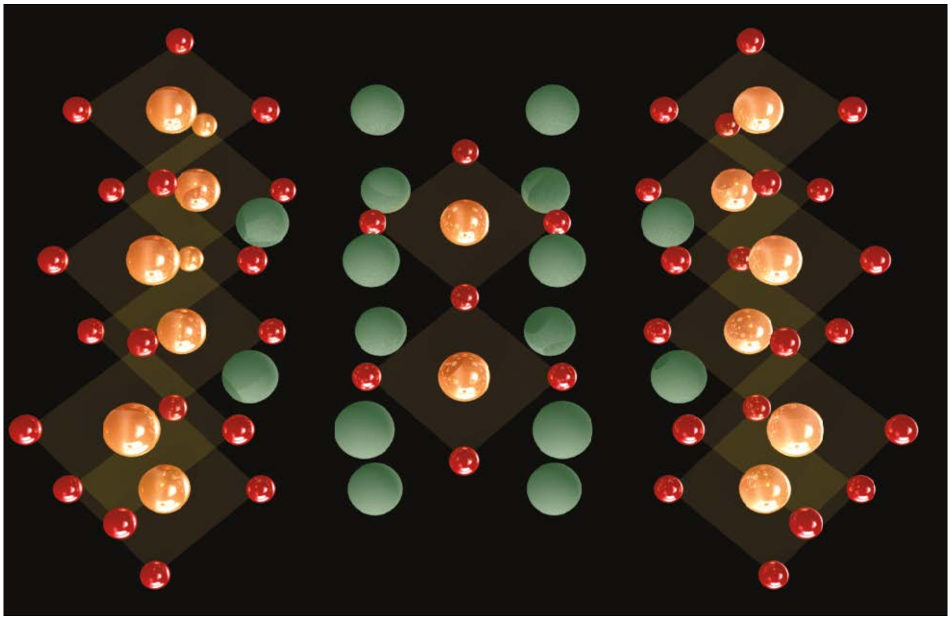
(Early Summit: continued from page 7)

- Astrophysics codes to advance our understanding of supernovas and cosmological structure.
- Fusion codes for understanding the conditions needed to run a fusion reactor and the complicated phenomena found at a fusion plasma's edge.
- A biology code to increase our understanding of communication between brain cells.
- A nuclear physics code that will enhance our understanding of nuclear decay and nuclear energy.
- A materials code that may help in the development of high-temperature superconductors.
- A combustion code that will enable realistic, high-fidelity simulations that identically match engine conditions.
- A seismology code that will create a high-fidelity picture of the Earth's interior.

For more information: http://go.usa.gov/3ZHUA

Superconductor

simulated without cutting corners



Superconducting material containing copper and oxygen with calcium (Ca_2CuO_3, right and left) and strontium (Sr_2CuO_3, center). Image credit: Foyevtsova, et al. PRX (2014)

by Eric Gedenk
gedenked@ornl.gov

DOE has long valued research on materials at the subatomic level. In fact, it considers a better understanding of electron structure in novel materials to be one of its grand challenges.

Improvements in our ability to predict the behavior of superconductors will allow scientists to expand research into a wide range of applications, including energy storage, catalysis, energy production, and metals that can be used as structural materials.

No assumptions

In keeping with this priority, a group led by ORNL's Fernando Reboredo and Paul Kent has advanced our understanding of superconductivity, performing the first simulation of copper-containing superconductors that doesn't rely on assumptions. These materials, known as cuprates, are among the most promising high-temperature superconducting materials.

"The goal of this research was to calculate the so-called exchange coupling, or interaction between adjacent copper molecules, from first principles."

When a simulation is performed from known laws of nature without using assumptions or models, it is considered ab initio (or "from first principles"). While such simulations are more reliable than the alternative, they typically demand an enormous amount of computing power.

"The goal of this research was to calculate the so-called exchange coupling, or interaction between adjacent copper molecules, from first principles," Kent said. "The challenge is that metal oxides are very difficult to predict, and our method had never been applied to this class of materials before."

Many materials scientists use density functional theory—a method using mathematical functions to compute electron behavior—to model subatomic interactions for these materials. Though DFT can offer accurate simulations, it has a difficult time simulating "d electrons," a type of electron important in chemical bonds. To accurately simulate d electron-rich copper oxides, the team needed another method.

Using quantum Monte Carlo

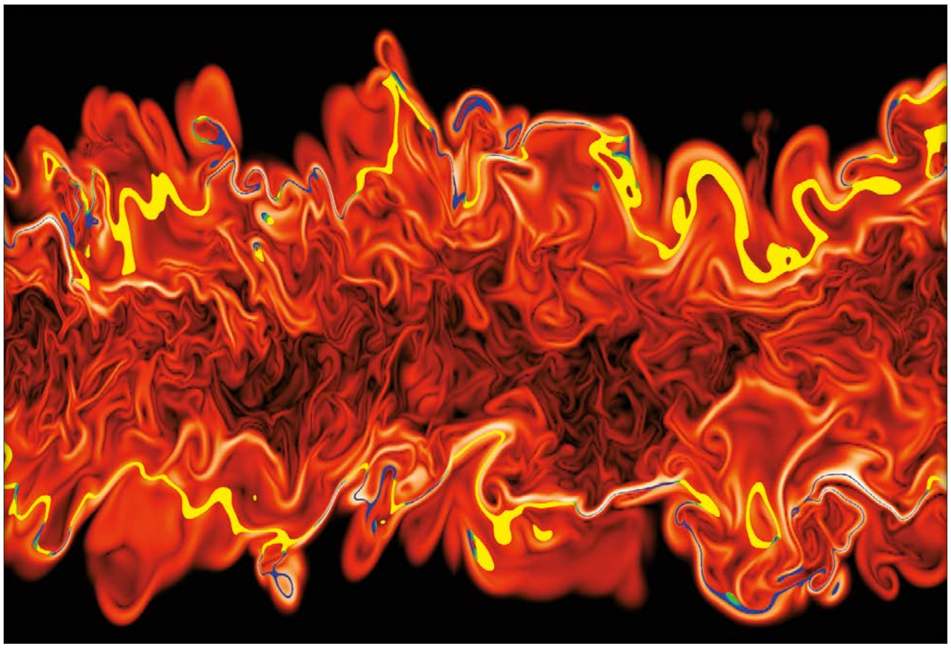
To overcome this obstacle, the team used an approach known as "quantum Monte Carlo." Instead of relying on mathematical functions, quantum Monte Carlo uses statistical data and random numbers to plot electrons in a simulation. While it is more computationally demanding, this approach also allows the researchers to perform ab initio simulations far more accurately than with DFT.

As computing power increases, the team will be able to simulate even heavier materials that could be used for large-scale superconducting applications.

For more information: http://go.usa.gov/3WNhP

Titan simulates

the complexities of engines



Direct numerical simulation of a turbulent dimethyl ether jet flame. The burning (yellow) and extinguished (blue) regions are superimposed. Image credit: Hongfeng Yu, University of Nebraska

by Gregory Scott Jones
ORNLReview@ornl.gov

Despite the rush to green energy technologies, traditional combustion engines will be an economic reality for years to come, in part because they have the potential to employ low-carbon and renewable fuels.

Nevertheless, we can improve the efficiency of combustion devices to help reduce our reliance on fossil fuels and the amount of carbon released into the atmosphere. Considering that Americans use two-thirds of their petroleum for transportation, such an improvement would be very helpful.

Better fuel efficiency

"If low-temperature compression ignition concepts are widely adopted in next-generation automobiles, fuel efficiency could increase by as much as 25 to 50 percent," said Jackie Chen, a researcher with Sandia National Laboratories who uses Titan to study the combustion of a wide variety of fuels.

Recently, Chen's team member Ankit Bhagatwala simulated a jet flame burning dimethyl ether to probe the fundamental physics of local extinction (where parts of the flame burn out) and reignition. If researchers can find ways to minimize flame extinction, they will also boost engine efficiency and reduce harmful emissions.

But the computational challenge is daunting. Even a system as powerful as Titan can't perform a direct numerical simulation of a jet flame that includes all of the relevant conditions—heat, chemistry and air flow—across all relevant scales. Chemical properties manifest on scales ranging from billionths to thousandths of a meter, while the effects of an engine valve's motion can be seen at scales ranging from hundredths to millionths of a meter.

Higher Reynolds number

Researchers must therefore simulate the jet flame at a lower Reynolds number (a measure of the mixing intensity and dynamic range of turbulence) that matches combustion's critical thermal and chemical conditions.

The team's latest Titan simulations delivered its highest Reynolds number to date. In fact, Titan and the team's application, known as S3D, pair so well that the application is six times faster than on Titan's predecessor, Jaguar.

The Titan simulations also included more chemical molecules known as species—in this case, 30—to model the combustion of dimethyl ether. The more species the simulation can include, the closer it can get to simulating realistic fuels, including biofuels.

The increased Reynolds value also allows the team to resolve a wider range of turbulence scales in space and time, a major breakthrough when trying to match experimental conditions and evaluate turbulent mixing and combustion models.

Specifically, the team wanted to know the dependence of reignition on the local mixing rate, or the rate of fuel and air mixing during the combustion process.

Better engine designs

"We found that oxygenated fuels such as DME [dimethyl ether] generate considerably more stable intermediates such as formaldehyde, rendering the flame more robust to local extinction than conventional hydrocarbons such as methane," Bhagatwala said.

Ultimately, more accurate combustion models, analyzed by direct numerical simulations and experiments, will be used to optimize engine design and improve the efficiency of combustion engines and devices.

For more information: http://go.usa.gov/3WNF9

Team builds

the Milky Way, star by star

Visualization of the Milky Way galaxy's formation. Image credit: SURFsara Amsterdam; Jeroen Bédorf, Leiden Observatory, the Netherlands; and NVIDIA

by Eric Gedenk
gedenked@ornl.gov

If you took a photograph of the Milky Way from a distance, the photo would show a spiral galaxy with a bright, central bulge of dense star populations.

The Sun—very difficult to see in your photo—would be outside this bulge, near one of several spiral arms composed of stars and interstellar dust. Beyond the visible galaxy would be a dark matter halo—invisible to your camera but important nonetheless because it keeps everything together by dragging down the rotational velocity of the bulge and spiral arms.

If you wanted a video of the Milky Way forming, you would have to go back 10 billion years, to a time when the galaxy was largely unrecognizable. But then you would have to wait about 5 billion years to witness the formation of our own solar system. By this point, 4.6 billion years ago, the galaxy would look almost like it does today.

"The grand structure of the galaxy has emerged from the self-organization of the stellar distribution over the past 10 billion years to eventually look like the Milky Way in the photo," said Simon Portegies Zwart of Leiden Observatory in the Netherlands.

This is the timeline he and other researchers from the Netherlands and Japan are seeing emerge when they use supercomputers to simulate the Milky Way's evolution.

The team's effort is impressive. The challenge of computing galactic structure on a star-by-star basis is, as you might imagine, the sheer number of stars—at least 100 billion in the Milky Way. The team needed at least a 100 billion-particle simulation to connect all the dots.

Gordon Bell nominee

Before development of the team's code, known as Bonsai, the largest galaxy simulation topped out around 100 million—not billion—particles. So it's no surprise the team earned a nomination for the 2014 Gordon Bell Prize, which recognizes outstanding achievement in high-performance computing.

"We don't really know how the structure of the galaxy came about," Portegies Zwart said. "What we realized is we can use the positions, velocities, and masses of stars in three-dimensional space to allow the structure to emerge out of the self-gravity of the system."

The code was able to make use of 96 percent of Titan's GPUs, enabling the simulation of a 242 billion-particle Milky Way over the course of 8 million years. Along the way, the team took Titan up to 25 thousand trillion calculations a second, or 25 petaflops.

Satellite comparisons

The team aims to compare simulation results to new observations coming from the European Space Agency's Gaia satellite, which launched last year. The Gaia mission is currently cataloguing star measurements—including distances, velocities, and stellar type—of one billion Milky Way stars.

Gaia will also provide data on stars farther than Earth's Solar Neighborhood, or only stars within tens of light-years. When compared with Bonsai simulations, these new observations will help researchers better understand larger galaxy dynamics, such as the interaction of the bar and spiral arms, in addition to local dynamics taking place around the Solar Neighborhood.

For more information: http://go.usa.gov/3WPNd

Sleuthing with neutrons

ORNL's head of neutron sciences explains how these fundamental particles are uniquely illuminating

by Katie Bethea
betheakl@ornl.gov

Paul Langan is the associate laboratory director for neutron sciences at Oak Ridge National Laboratory. He came to ORNL in April 2011 as a senior scientist and director of the Center for Structural Molecular Biology. In October of that year he became founding director of the Neutron Sciences Directorate's Biology and Soft Matter Division. In each role Langan has partnered with other ORNL directorates to build strong multidisciplinary research programs that exploit the neutron scattering capabilities at ORNL.

Langan's most recent research accomplishments have been in applying neutrons to study enzyme mechanism and drug binding, developing novel technologies and computational methods for neutron macromolecular crystallography, integrating neutron scattering with high-performance computing, and providing a detailed understanding of the cellulose and lignin components of cellulosic biomass.

What about neutrons makes them so interesting across a range of disciplines?

Neutrons are an essential probe for materials research because they provide unique information. In particular they have energies that are well matched to studying huge ranges of length and time scales.

Unlike photons and electrons, which are other essential probes for materials, neutrons are fundamental particles that interact through the strong nuclear force and are therefore sensitive to light elements and isotopes. They are uncharged and therefore highly penetrating, which allows the use of complex sample chambers to look at materials under extreme conditions. Because they are neutral, that means they don't cause direct radiation damage, which is important for studying functioning biological samples. Finally, they have spin and are therefore sensitive to magnetism.

Our users and staff are using these unique characteristics of neutrons for cutting-edge research. For example, they are studying the synthesis of a new type of diamond thread material that is formed at high pressures, which could have important industrial application in transportation or aerospace manufacturing. These diamond-like threads could be the first member of a whole new class of tunable nanomaterials. They are nondestructively studying parts built through additive manufacturing to improve the reliability of the manufacturing process. They have recently used neutrons to reveal the earliest structural formation of the disease type of the protein huntingtin, and that research is moving forward to study protein malformation responsible for Alzheimer's and Parkinson's diseases. They are studying a number of proteins that are important drug targets against several diseases such as AIDS and cancer, so that better drugs can be made. And they are using neutrons to study the intranozzle fluid dynamics of fuel injectors while they operate. These are just a few examples from the hundreds of experiments that researchers carry out each year at the Spallation Neutron Source and the High Flux Isotope Reactor.

Paul Langan, associate director for neutron sciences. Image credit: Genevieve Martin, ORNL

"I see Oak Ridge becoming a place where the best scientists want to come and work with us because they know we have the best neutron tools to solve the most important research problems that we face as a nation."

The primary mission of the Neutron Sciences Directorate is to deliver the scientific tools that provide solutions to U.S. energy challenges that make up the core missions of the DOE Office of Science. The scientific breakthroughs that will transform our future are accelerated by the availability of advanced research user facilities like SNS and HFIR. Neutron beams suitable for scattering experiments cannot be generated in small-scale academic or industrial laboratories; thus large-scale user facilities are the only means of providing neutron beams to the scientific community to access their unique possibilities. We are using our neutron facilities to address four science priority areas: quantum materials, materials synthesis and performance, soft molecular matter, and biosciences. A couple of years ago we described what our plan is to further develop our neutron facilities so that they can have higher impact in these priority areas of science, our "strategic science plan."

As a neutron scientist yourself, what science challenges do you think neutrons can address?

I don't see myself as a neutron scientist, but as a scientist who uses neutrons along with other complementary experimental methods to answer questions and solve problems. Researchers define a scientific problem and then use whatever experimental methods are best matched to solve that problem. Neutron scattering is one of these experimental methods, but it is an essential one, because neutrons see things that others can't. I see addressing and solving big science challenges as central to our mission. We met with science leaders from across the country last year to help define what some of those grand scientific challenges are. The workshops sought to outline the most pressing challenges in the fields of quantum materials, biosciences, soft molecular matter, materials synthesis and performance, engineering systems, and modeling and simulation. With those challenges defined, we are able to see clearly what further neutron technologies and innovations we will have to develop at Oak Ridge in order to solve the most important science problems over the next few years. We will be able to address some grand challenges at our present two neutron sources: HFIR and the first target station at the SNS. However, other emerging challenges will require the construction of a second target station at the SNS, one that is optimized for looking at complexity in matter and hierarchical systems.

Gaining a predictive understanding of complex systems is a major challenge in all of our science priority areas that is likely to increasingly dominate the next decade. Oak Ridge is really well positioned to make an impact not only because we have world-leading neutron sources, but also because we have powerful high-performance computing resources. Computing is needed to interpret the results from neutron experiments on complex systems, so I would like to work towards using neutrons and computing as a new integrated tool that can be applied with high impact across a range of different research problems. Construction of the second target station is part of a facilities road map that we have developed that will position Oak Ridge in the world as a truly unique center for neutron science.

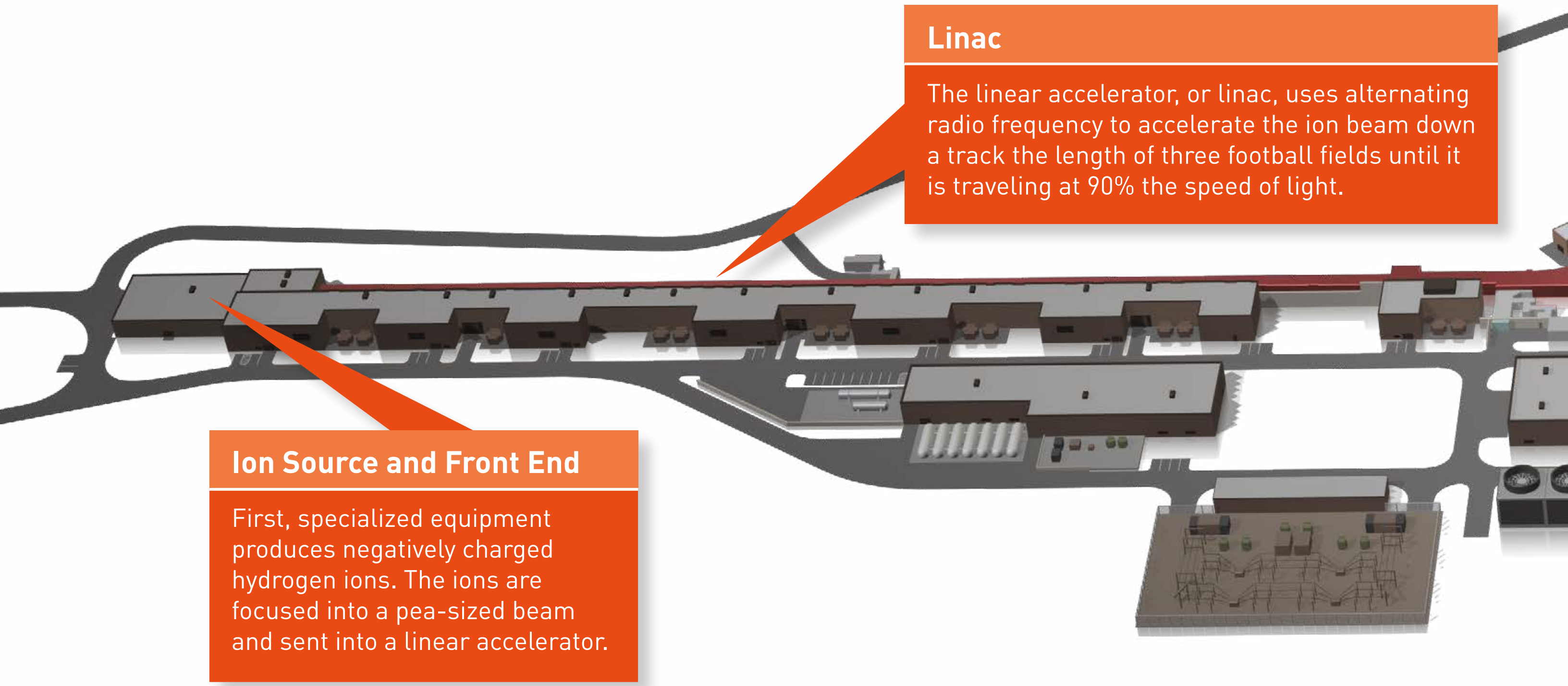
What's the future of neutron science at ORNL?

HFIR and SNS are world-leading neutron scattering facilities—in my opinion they are also two of our nation's most significant technological achievements. I'm very proud of that. But I don't think we've reached our full potential yet. The mission of this organization—the reason we're here—is to deliver high-impact science. Our biggest scientific breakthroughs and technical successes lie in the future. That's what motivates me. HFIR provides the world's brightest beams of continuous cold neutrons. SNS provides the world's most intense beams of pulsed neutrons. Together the SNS and HFIR provide neutron scattering instruments that enable science across a large range of different areas of science. I see Oak Ridge becoming a place where the best scientists want to come and work with us because they know we have the best neutron tools to solve the most important research problems that we face as a nation. We can make a difference to our nation's industrial competitiveness, our health and well-being, and also the major challenges we face in energy and security.

ORNL's Spallation Neutron Source

Spallation Neutron Source

We make neutrons so scientists can solve problems

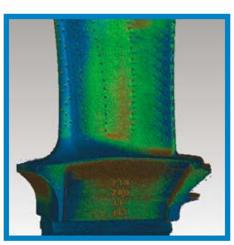


Neutrons are a precious scientific resource—electrically neutral, strongly penetrating, and energetically well matched to elementary excitations in matter. They see atoms and ions and differences in isotopic composition. They follow motions. And they reveal magnetic and electronic properties that are all but invisible to electrons and photons.

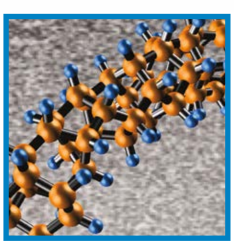
Neutrons can probe the enormous range of length and time scales important to 21st century materials and systems, looking deep inside to examine the physical properties that underpin new devices and technologies.

The Spallation Neutron Source at ORNL is the world's most powerful source of pulsed, accelerator-based neutrons. Its primary mission is to deliver scientific tools for meeting America's most important energy challenges.

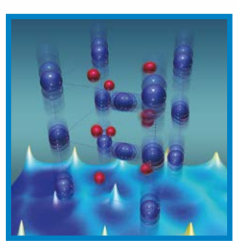
Neutrons are...



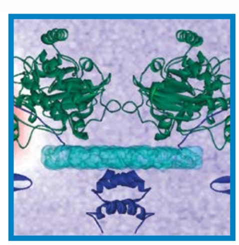
Peering deep inside 3-D printed turbine blades.



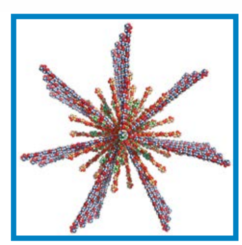
Confirming the structure of super strong nanothreads.



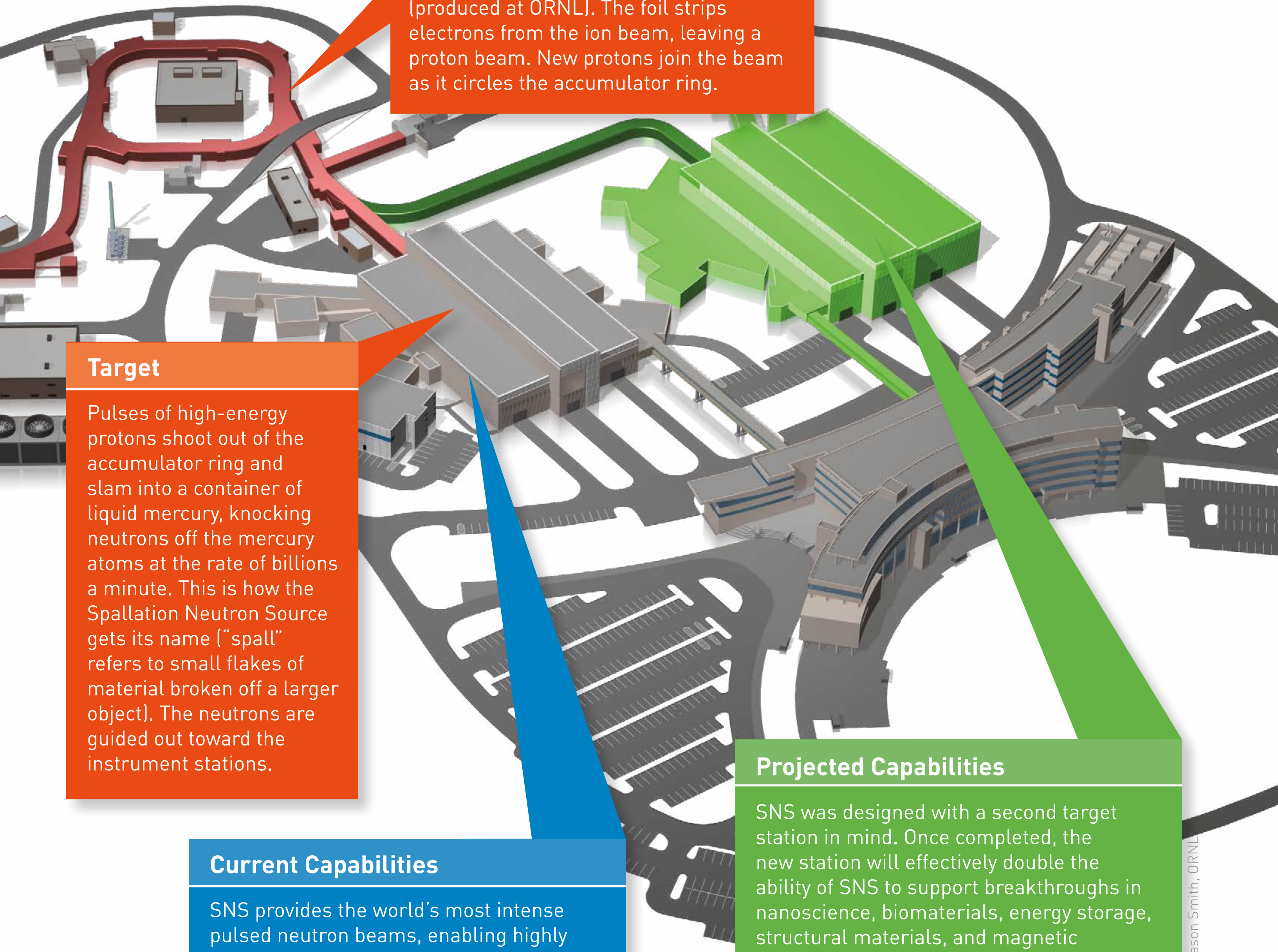
Analyzing atomic vibrations in metals.



Resolving protein structure for future drug development.



Designing future materials at the molecular level.



Accumulator Ring

As the beam enters the accumulator ring, it goes through foil made of diamond (produced at ORNL). The foil strips electrons from the ion beam, leaving a proton beam. New protons join the beam as it circles the accumulator ring.

Target

Pulses of high-energy protons shoot out of the accumulator ring and slam into a container of liquid mercury, knocking neutrons off the mercury atoms at the rate of billions a minute. This is how the Spallation Neutron Source gets its name ("spall" refers to small flakes of material broken off a larger object). The neutrons are guided out toward the instrument stations.

Current Capabilities

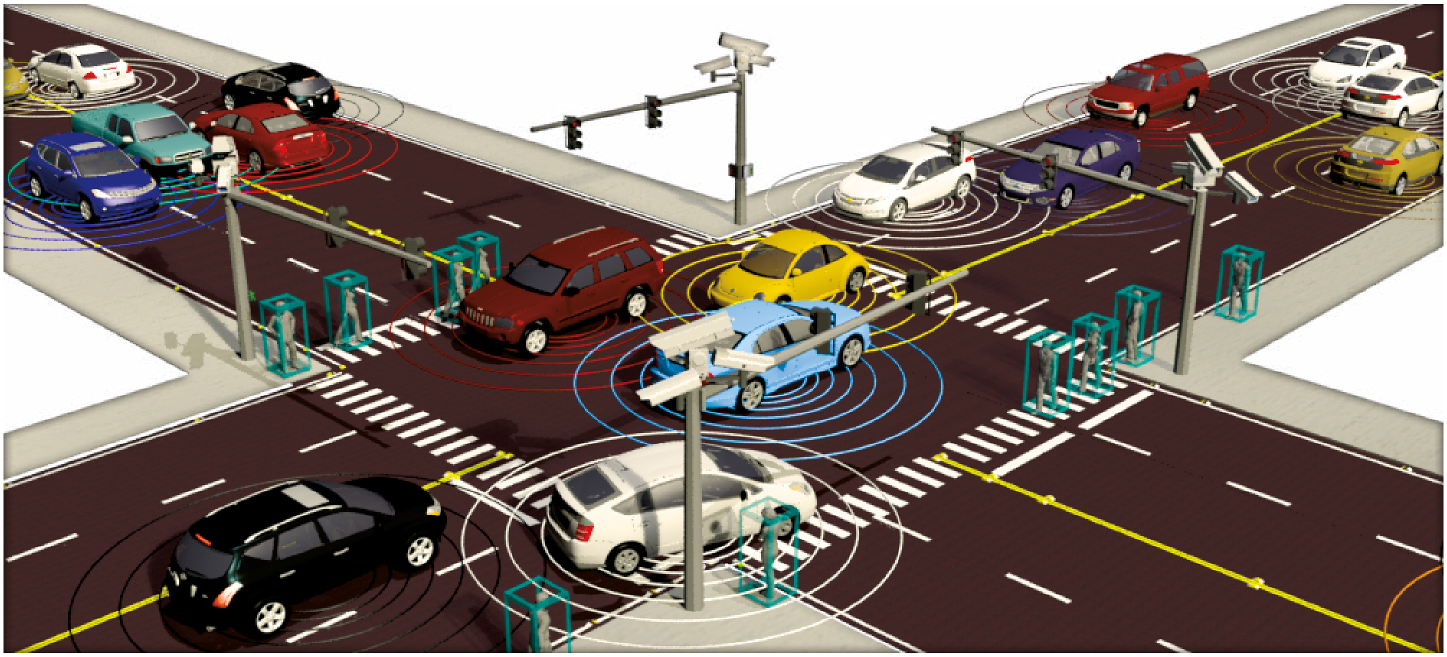
SNS provides the world's most intense pulsed neutron beams, enabling highly sensitive measurements that would be impossible at a less powerful facility. Each year the facility provides 4,500 hours of beam time, allowing more than 1,500 researchers to conduct 450 experiments on its 18 instruments.

Science priorities at the SNS include
- quantum materials
- materials synthesis and performance
- soft molecular matter
- biosciences

Projected Capabilities

SNS was designed with a second target station in mind. Once completed, the new station will effectively double the ability of SNS to support breakthroughs in nanoscience, biomaterials, energy storage, structural materials, and magnetic systems. It will also allow researchers to study the properties of materials that have never been studied before.

Image credit: Jason Smith, ORNL



Visualization of an ORNL connected vehicles simulation using decentralized control algorithms developed by researchers with the lab's Urban Dynamics Institute.
Image credit: Andreas Malikopoulos, ORNL

Framework helps cars, traffic lights communicate

by Katie Elyce Jones
ORNLReview@ornl.gov

Drivers trying to get to work or home in a hurry know traffic congestion wastes a lot of time, but it also wastes a lot of fuel. In 2011, congestion caused people in US urban areas to travel an extra 5.5 billion hours and purchase an extra 2.9 billion gallons of fuel costing $121 billion. But despite the tangle of vehicles at busy intersections and interstate ramps, most of the country's highways are open road, with vehicles occupying only about 5 percent of road surface.

Scientists with ORNL's Urban Dynamics Institute are working to reduce travel time and fuel consumption by developing a computational framework for connected vehicle technologies that facilitate vehicle-to-vehicle communication, as well as communication between vehicles and traffic controls such as traffic lights. Researchers envision vehicles exchanging information—such as location, speed, and destination—to generate individualized instructions for drivers.

"By telling drivers the optimal speed, the best lane to drive in, or the best route to take, we can eliminate stop-and-go driving and improve safety," said Andreas Malikopoulos, UDI deputy director and principal investigator of the Laboratory Directed Research and Development project.

First, the project team is developing decentralized control algorithms that govern how vehicles will communicate locally on each road but act globally to optimize traffic flow across a city. The computational framework uses "decentralized control" algorithms because, realistically, all the vehicles in a city cannot communicate information to a central control center.

"The first phase is an exploratory project. We'll validate our framework through simulation," Malikopoulos said.

The second phase of the project will connect the team's communication framework with a transportation analysis simulation system that uses data analytics to simulate traffic conditions in real urban settings. Simulations will predict and plan traffic flow based on large-scale data, such as the layout and population distribution of the area that reflects driver activities (for example, school zones are likely to be busier early in the morning, whereas entertainment districts are likely to be congested on weekends).

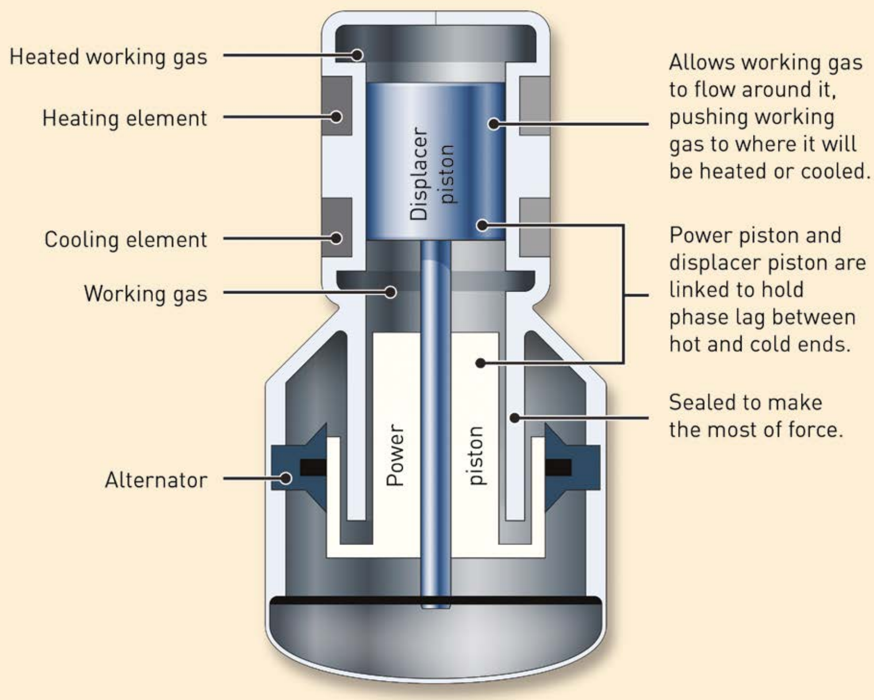
Phase two simulations also will allow the team to begin exploring questions related to cyber security and possible incentives for drivers to follow connected vehicle instructions, such as digital ticketing.

For more information: http://go.usa.gov/3Wy59

"By telling drivers the optimal speed, the best lane to drive in, or the best route to take, we can eliminate stop-and-go driving and improve safety."

Heat engine gets modern makeover for car and home

How a Stirling engine works



1. Heated working gas pressure rises; gas expands, pushing the power piston downward.
2. Displacer piston pushes working gas toward cool side.
3. Cooled working gas contracts; lower air pressure permits power piston to move upward.
4. Displacer piston pushes working gas toward hot side.
5. Repeat step 1.

...

6. Motion of power piston drives alternator and creates electricity.

Image credit: Brett Hopwood, ORNL

by Katie Elyce Jones
ORNLReview@ornl.gov

ORNL researchers are using 3D printing to put a 21st-century spin on a 19th-century technology.

Researchers with the lab's Fuels, Engines and Emissions Research Center will integrate an external combustion heat engine known as a Stirling engine into an ORNL 3D printed vehicle, creating a prototype range-extended electric vehicle that can also provide auxiliary power for homes and buildings. This vehicle will be used for researching integrated energy applications that connect vehicles, buildings and small power sources such as generators.

Two centuries of technology

Although Stirling engines have been around for about 200 years, they are not typically used in automobiles because they respond to load changes more slowly than internal combustion engines.

"An internal combustion engine is an open cycle where the working fluid is inducted into the engine, combustion occurs, work is done, and the exhaust gases are pushed out of the engine," said Robert Wagner, director of the research center. "A Stirling engine is a closed cycle where the working fluid is sealed within the engine and heat from an external source drives the engine."

Today's Stirling engines often are used in applications where a large differential temperature is possible between the external heat source and the environment, such as in spacecraft where there is a high-temperature heat source like plutonium against the low temperature of space. The engine's ability to run off of different heat sources makes it attractive for clean energy applications aimed at easing petroleum and coal power dependence.

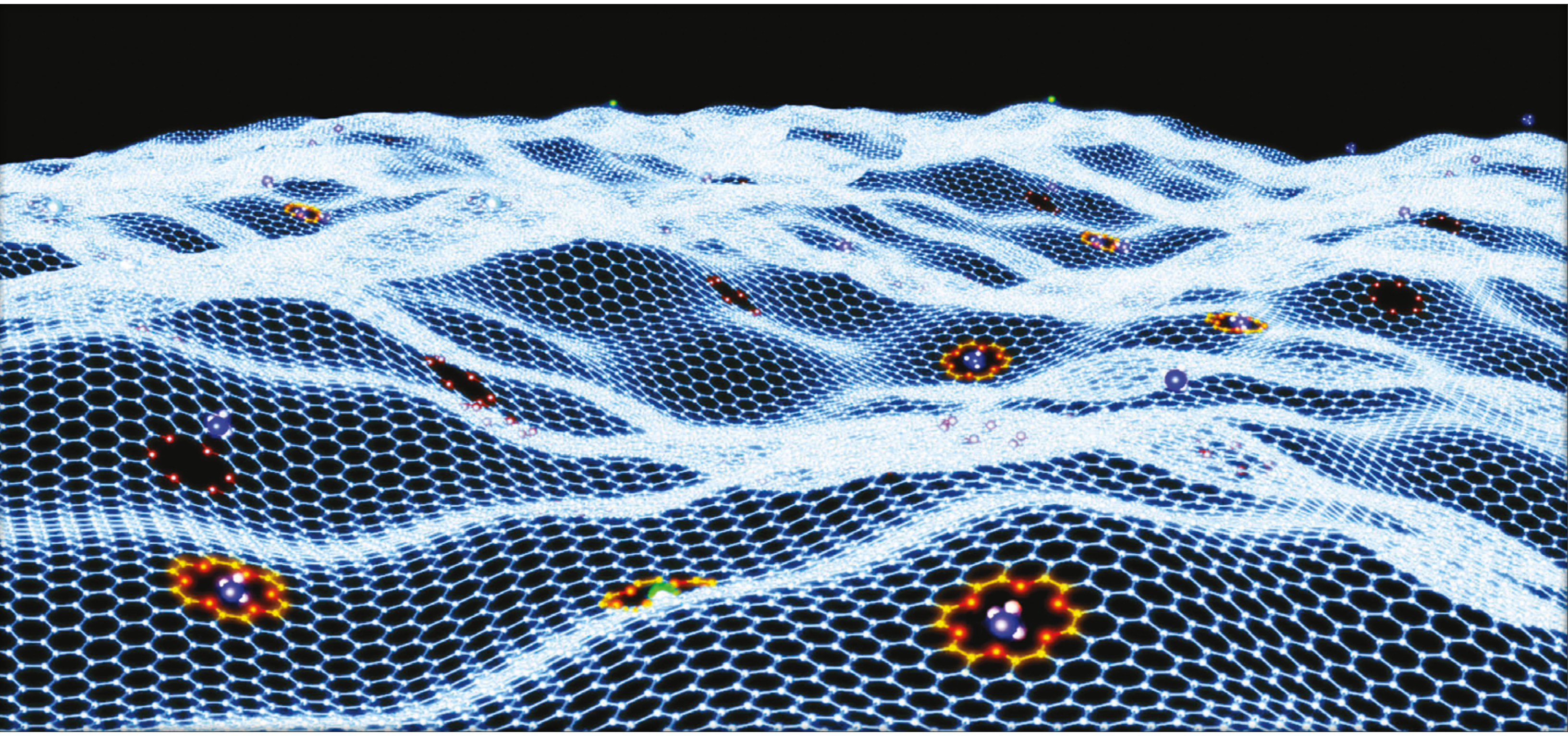
Comprehensive testing

Using natural gas as the heat source, the team will initially test the engine under a range of conditions in a dynamometer cell at the research center.

Then the engine will be integrated into an EV powertrain and run through simulated drive cycles, allowing researchers to optimize the electrical controls to manage acceleration and buffer the slow response time of the Stirling engine so it responds more quickly to driver demands. The engine tests will advance from the dynamometer to the powertrain to the 3D printed car, where it will be integrated with an EV drive system for road tests. The team will also use additive manufacturing tools available at ORNL's Manufacturing Demonstration Facility to print specially designed parts that optimize heat transfer and reduce weight.

"At that point we should have a functional range extender EV," Wagner said. "Then we'll work with ORNL's Integrated Energy Systems team to develop control systems so that it can interact with a building as well as the local grid."

For more information: http://go.usa.gov/3E2qd



An ORNL-led team has discovered a way to make graphene useful in diverse applications by taking advantage of crown ethers in its grid-like framework. Image credit: Oak Ridge National Laboratory

Researchers build a better atom trap

by Dawn Levy
levyd@ornl.gov

An ORNL-led team has found a way to create strong, specific electrostatic binding of ions and molecules. The discovery may advance chemical separations, sensing and catalysis.

The cornerstone of the finding is ethers—molecules in which an oxygen atom bridges two carbon atoms. They are building blocks of common solvents, propellants, cosmetics and pharmaceuticals. Link them in large rings, and they gain new powers as atom traps.

Called crown ethers, these ringed "host" molecules have cavities for capturing "guest" ions and molecules. Separately weak interactions, such as the electrostatic bond between an ether oxygen atom and a metal ion, organize in crown ethers to collectively achieve strong, selective binding that may become useful in metal extraction, environmental cleanup, medicine and other fields.

But a problem has prevented traditional crown ethers from achieving their full potential. They are flexible, so opposite charges on the host and guest rarely line up directly. That limits crown ethers' strength and affinity for binding specific metal atoms.

The ORNL–led team solved that problem when it discovered crown ethers within an ultra-strong and light material—graphene, a one-atom thick sheet of carbon constrained in a honeycomb pattern.

When crown ethers formed in graphene, the framework forced the ether rings to lie flat. Compared to the flexible rings of traditional crown ethers, the resulting rigid rings of crown ethers in graphene were better at trapping atoms of certain sizes, making them more effective for specific uses. Moreover, binding strength improved because constraining the crowns in two dimensions forced all oxygen charges to point toward the centers of the cavities, optimizing binding potential.

"We're the first to see crown ethers in graphene," said Matthew Chisholm, leader of ORNL's Scanning Transmission Electron Microscopy Group. "Our calculations based on these observations indicate unprecedented selectivity and binding strength."

This advance may herald a new reign for crown ethers in nuclear-waste cleanup, recycling of rare-earth elements, energy production in durable lithium-ion batteries and other vital applications.

For more information: http://go.usa.gov/3W9Zd

Penciling patterns

in polymers at the nanoscale

by Morgan McCorkle
mccorkleml@ornl.gov

ORNL researchers got a surprise recently when they used one of the lab's powerful atomic force microscopes to measure the conductivity of a thin liquid film. Instead of a straightforward measurement, their most interesting discovery was that the microscope could etch patterns on the film's surface at an almost unbelievably small scale.

"We were expecting to measure ionic conductivity, and instead we found that we were forming holes on the surface," said ORNL's Vera Bocharova, corresponding author on a study published in Advanced Functional Materials. "Then we started to think about how this might have great applications in nanofabrication."

The researchers were working with polymerized ionic liquids. Because they conduct charged atoms, and because they have a unique structure, these materials have potential applications in technologies such as lithium batteries, transistors and solar cells. They were only recently discovered, however, so they are not well understood.

The group's work with an atomic force microscope suggested that the equipment can be used to fabricate materials very, very finely. To this point, the dominant technology used by industry for nanofabrication is nanolithography, but nanolithography can't get small enough for everyone. Researchers are looking for ways to precisely fabricate increasingly smaller devices.

"This study is part of our search for alternative methods and materials that can be used to create smaller-sized objects," Bocharova said. "For example, our technique might be interesting for the miniaturization of semiconductor technology."

Similar atomic force microscopy techniques have been used to study and produce patterns in nonconductive polymers, but the ORNL study uncovered several differences in the application to polymerized ionic liquids.

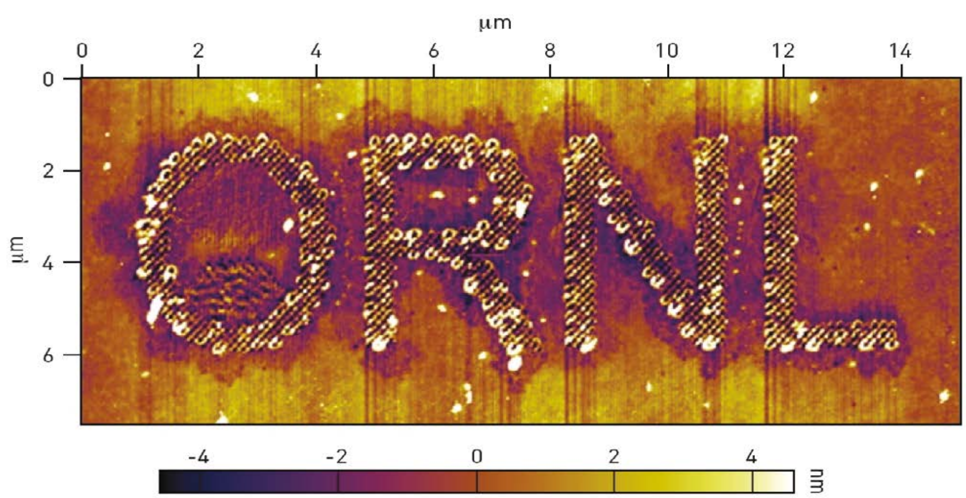
"In comparison to nonconductive polymers, we have to apply less bias—4 volts instead of 20 volts—to generate the holes, which is good in terms of energy savings for future applications," Bocharova said.

The researchers plan to continue refining the technique's capabilities and their understanding of the polymerized ionic liquids' properties.

"Right now the size of the formed features is in the range of 100 nanometers, but it's not the limit," Bocharova said. "We believe it's possible to change the experimental setup to advance to lower scales."

For more information: http://go.usa.gov/3Cefm

"Then we started to think about how this might have great applications in nanofabrication."



Oak Ridge National Laboratory researchers used atomic force microscopy to draw nanoscale patterns in a polymerized ionic liquid.

ORNL researcher Kaushik Biswas analyzes the thermal performance of a 2-by-2 foot composite panel covered with smaller modified atmosphere insulation panels separated by foam insulation. Image credit: Jason Richards, ORNL

Collaboration works to keep the warm side warm and the cool side cool

by Chris Samoray
ORNLReview@ornl.gov

Inadequate insulation is a major cause of wasted energy, undermining the effort we put into creating comfortable indoor environments. In fact, about 6 percent of U.S. energy consumption goes to making up for heat lost through building roofs and walls.

That's why ORNL researchers are collaborating with industry to develop a high-performance, cost-effective material that nearly doubles the performance of traditional insulators.

Commercial buildings are typically insulated with foam boards, while residential structures generally use spray foam. These technologies are affordable, but they don't insulate as well as we might like, because of their low heat transfer ratings, or R-values.

The solution being developed by ORNL, NanoPore and Firestone Building Products is a composite foam board containing "modified atmosphere insulation" cores.

A vacuum in MAI panels is produced by filling the porous core with a condensable vapor, which then condenses to liquid that occupies a fraction of its original volume, leaving the remaining space a vacuum. The MAI sealing process is comparable to that used in sealing potato chip bags.

The nanoporous structure and vacuum within the MAI cores help to reduce two of the three modes of heat transfer in insulation materials: solid conduction and gas/vapor conduction. The third mode of heat transfer, radiation, can be reduced by adding opacifiers to the core, which can potentially further increase the R-value.

For more information: http://go.usa.gov/3xAbG

Cheap sensors improve indoor environment

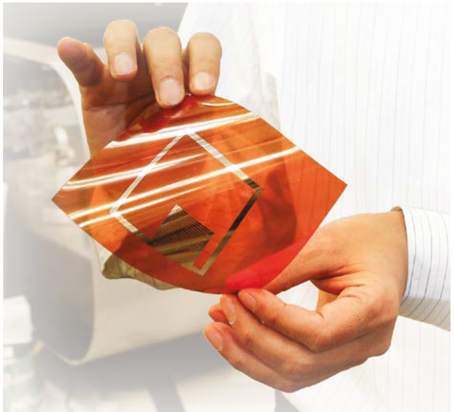
by Sara Shoemaker
shoemakerms@ornl.gov

Regulating comfort in small commercial buildings could become more efficient and less expensive thanks to an innovative, low-cost wireless sensor technology being developed by researchers at ORNL.

Buildings are responsible for about 40 percent of the energy consumed in the United States. Studies indicate that advanced sensors and controls have the potential to reduce that energy consumption by 20 to 30 percent.

"It is widely accepted that energy-consuming systems such as heating, ventilating and air conditioning units in buildings are under-, or poorly, controlled, causing them to waste energy," said Patrick Hughes, director of ORNL's Building Technologies Program. "Buildings could increase their energy efficiency if control systems had access to additional information."

Collecting data such as outside air and room temperature, humidity, light level, occupancy and pollutants is currently cost-prohibitive, whether the information is gathered by inexpensive conventional



ORNL researchers are experimenting with additive roll-to-roll manufacturing techniques to develop low-cost wireless sensors. ORNL's Pooran Joshi shows how the process enables electronics components to be printed on flexible plastic substrates. Image credit: Jason Richards, ORNL sensors that must be wired, or by wireless sensors that go for $150–$300 per node.

ORNL's new wireless sensor prototype could reduce costs to $1–$10 per node by leveraging advanced manufacturing techniques such as additive roll-to-roll manufacturing. This process enables electronics components such as circuits, sensors, antennae, and photovoltaic cells and batteries to be printed on flexible plastic substrates (base materials). The nodes can be installed without wires using a peel-and-stick adhesive backing.

Promising applications

"If commercially available at the target price point, there would be endless application possibilities where the installed cost to improve the control of energy-consuming systems would pay for itself through lower utility bills in only a few years," Hughes said.

The ultra-low-power smart sensors collect and send data to a receiver, which can capture data from many different peel-and-stick nodes and provide information to the energy-consuming system. The more information received, the better the building's energy management.

Both new construction and retrofitted buildings can benefit from ORNL's smart sensors.

"This technology provides the information that enables ongoing continuous commissioning, fault detection and diagnosis, and service organization notifications when needed," said ORNL's Teja Kuruganti, principal investigator on the low-cost wireless sensors project.

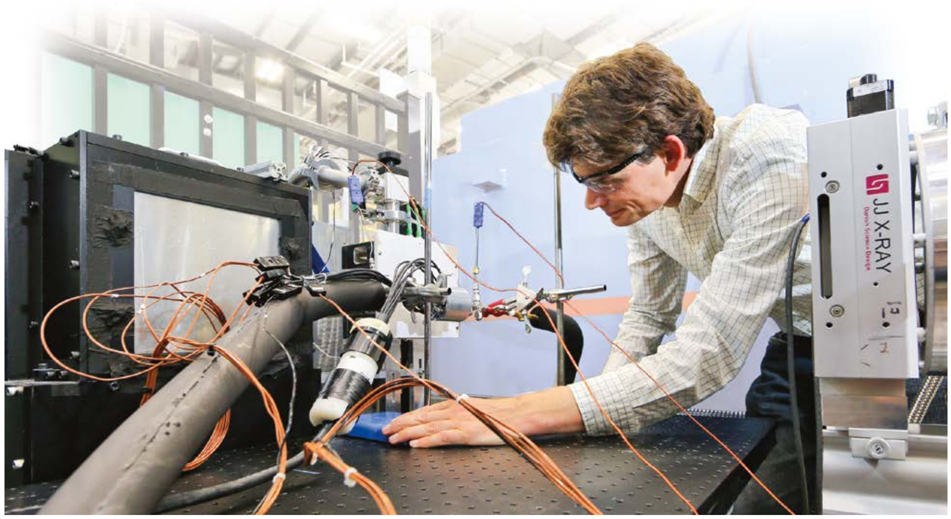
Making the sensors available

ORNL recently established a Cooperative Research and Development Agreement with Molex, a premier international electronics manufacturer, to make the low-cost wireless sensors commercially available.

The research team used ORNL's Nanoscale Science and Technology Laboratory cleanroom facility to select the best substrate material.

For more information: http://go.usa.gov/3a3Pw

Researchers use neutron imaging to peek inside heat exchanger



To observe the effects of heat on refrigerants, ORNL researcher Patrick Geoghegan used the High Flux Isotope Reactor to capture undistorted neutron images. Image credit: Jason Richards, ORNL

by Chris Samoray
ORNLReview@ornl.gov

Scientists have long noted that observation can alter results. Imagine how true this becomes when the process of observation involves removing parts from your equipment.

ORNL researchers have overcome this challenge in at least one case, using neutron imaging at the lab's High Flux Isotope Reactor to capture undistorted snapshots of refrigerants flowing through small heat exchangers.

Heat exchangers are used in applications from the personal (space heaters, air conditioners) to the industrial (petroleum refineries, sewage treatment plants). As the name implies, their job is to move heat toward where it's wanted or away from where it's unwanted.

To get a better understanding of heat exchangers, the researchers made use of another ORNL strength: additive manufacturing, also known as 3D printing. The apparatus they printed contained small, compact tubes known as microchannels, designed so that the process of heat transfer can be viewed and analyzed using neutrons produced at HFIR.

"That's what we're trying to understand—what does the refrigerant look like on the inside of these channels?" said Patrick Geoghegan, a researcher with the Buildings Technologies Research and Integration Center.

Up to this point, the usual mode of operation was to cut off the top of a larger heat exchanger tube, cover it with Plexiglas, and then peer inside as it was heated, a method that could tarnish the results.

The team found that the microchannels were very effective at their jobs. Even though the refrigerant contained both liquid and vapor, the liquid did not sink to the bottom of the microchannel under most circumstances. Rather, surface tension caused the liquid to stick to all sides, ensuring good heat movement.

"The beauty with microchannels is that surface tension comes into play, and surface tension holds the refrigerant liquid onto all the surfaces of the microchannel," Geoghegan said. "The entire area is still available for heat transfer, and that's what you want."

For more information: http://go.usa.gov/3xG4x

US ITER pushes ahead

The United States is a major participant in the ITER fusion reactor, an experimental reactor intended to demonstrate that the process that powers stars can also produce clean energy on Earth. The U.S. contribution to this international collaboration is coordinated by DOE's Office of Science and headquartered at ORNL.

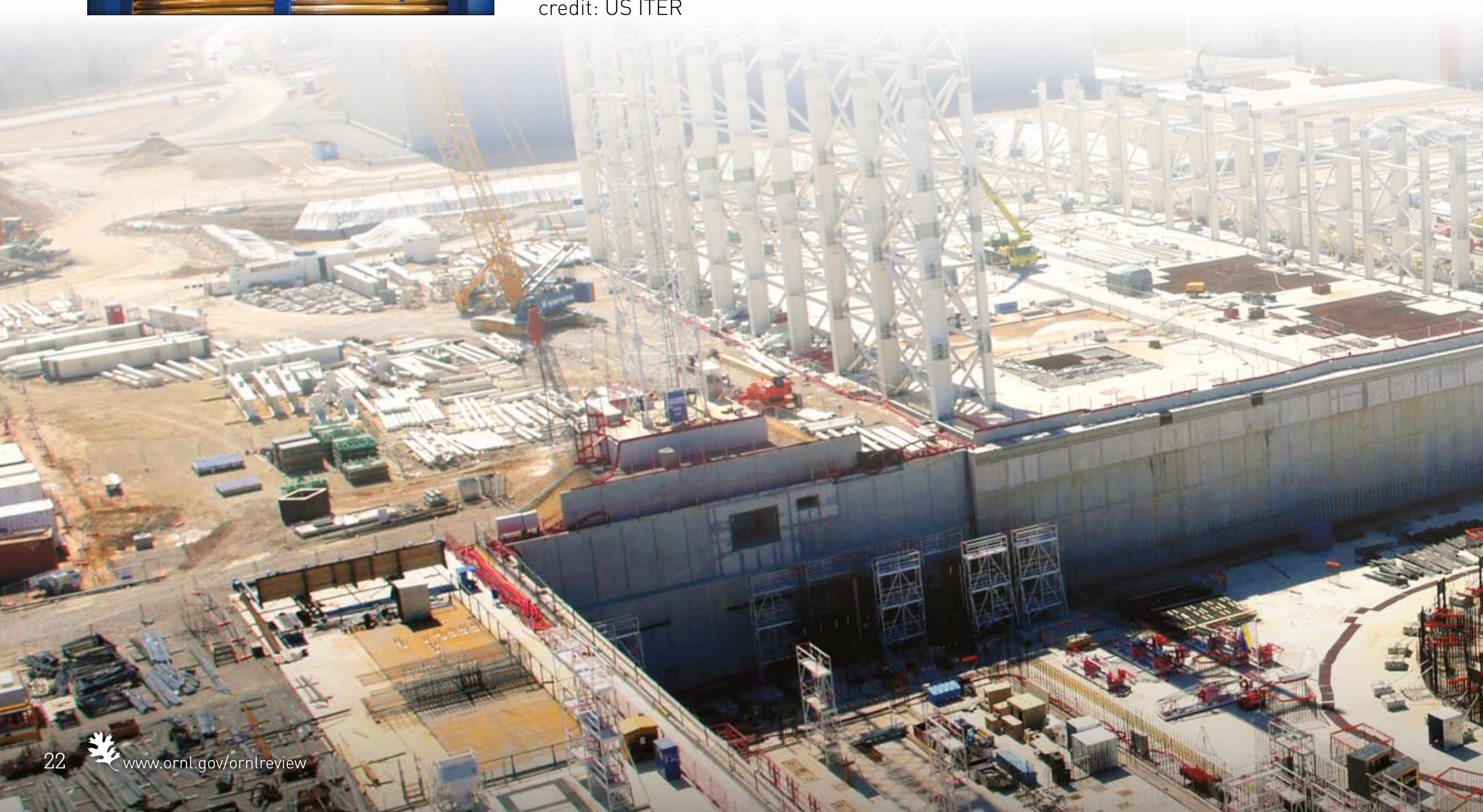
As part of its participation, US ITER is producing and delivering some unique and massive components for the reactor.

by Lynne Degitz
degitzlk@ornl.gov

Magnet systems: toroidal field conductor

The U.S. is providing 8 percent of ITER's toroidal field magnets, for a total of over 4 miles of conductor, and will complete its conductor deliveries by 2016. Five other ITER partners—China, the European Union, Japan, Korea and Russia—are also contributing toroidal field conductor. The toroidal field coils will produce a powerful magnetic field of up to 11.8 tesla around the ITER tokamak torus to confine the plasma particles.

The January toroidal field conductor delivery to the European Union winding facility in La Spezia, Italy, was the first U.S. shipment of "active production" conductor which will be installed in the ITER machine. Earlier U.S. deliveries of toroidal field coil magnets were used to verify the manufacturing and winding process. The production conductor will be wound into coils and inserted into a D-shaped winding pack before installation. Image credit: US ITER



Tokamak cooling water system: drain tanks

A 61,000 gallon, 73.5 metric ton drain tank undergoes final testing at Joseph Oat Corporation in Camden, N.J. Two drain tanks have completed fabrication and been delivered to the ITER site. Three more tanks will be delivered this year. The tanks provide storage for ITER's tokamak cooling water system. Image credit: US ITER

Central solenoid: magnet modules

Fabrication of the first superconducting magnet module for the central solenoid has begun at General Atomics' Magnet Technologies Center in Poway, Calif. The central solenoid is the heartbeat of ITER: The 1,000 metric ton magnet induces the majority of magnetic flux charge needed to initiate and maintain plasma current. Image credit: General Atomics

Site power: substation transformer

The main body of an 87 ton high-voltage substation transformer is off-loaded at Fos-sur-Mer, France, the industrial port of Marseille. Three more transformers have since been delivered to the ITER site. The equipment is necessary to power up the steady-state electrical network by October 2015. Image credit: ITER Organization

The ITER site in mid-April 2015. The dark circle near the middle of the photograph is the tokamak pit of the tokamak building. Behind it are pillars for the assembly building. Image credit: ITER Organization

Distinguished

Susan Solomon

Susan Solomon is the Ellen Swallow Richards Professor of Atmospheric Chemistry and Climate Science at the Massachusetts Institute of Technology. In the mid-1980s she led expeditions to Antarctica that confirmed a growing hole in the Earth's ozone layer and laid the blame on the human use of chlorofluorocarbons.

She delivered the Eugene Wigner Distinguished Lecture on Dec. 10, 2014 focusing on "Ozone Depletion at the Ends of the Earth: A Science and Policy Success Story." We asked about her experience working on a high-profile scientific problem and the lessons she drew from it.

1. You led the Antarctic expedition that confirmed a growing hole in the ozone layer and linked it to chlorofluorocarbons. What lessons can we learn from that experience?

One of the important ones is the role of long-term monitoring. If we're making changes in our environment, it's very important to make sure that we create and maintain a network that allows us to know what it used to be like and whether it's changing. Also, when we put material into our environment, it's really important to look at how long that stuff is going to live. In the case of the ozone hole, the molecules that are causing it have lifetimes of the order of 50 to 150 years. So, if we made a mistake, we're going to live with it for a very long time.

2. How did that experience influence how you later approached your career?

The great thing about the work that I did there was that it allowed me to become exposed to how science is used. The work that I was doing scientifically was of interest to people who were trying to formulate policies around ozone depletion, so I got to talk to those people and understand how they think.

3. How should scientific research guide public policy in areas such as climate research?

Scientific research is an input to public decision-making, but it's not the only input. I think that scientific research can do its best job in serving the public and serving the needs of decision-making by providing the best policy-relevant information we can, which means providing options.

The other thing is to help people understand the difference between the fundamental science and levels-of-detail questions that may remain. In the case of DDT and long-lived pesticides, there was a fundamental fact: These things are long lived. There was also another fundamental fact: They are retained in the human body. There's a lot of uncertainty regarding very, very important additional questions, but there are distinctive science fundamentals that we actually know extremely well.

4. Why was it important to visit ORNL, meet with researchers here and participate in the Wigner Lecture Series?

I think it's a great place, this institution. There's lots of wonderful laboratories at various government agencies around the country, and it's really important that the academic and government and industry communities in science communicate with one another and work together.

The Eugene P. Wigner Distinguished Lecture Series in Science, Technology, and Policy gives scientists, business leaders and policy makers an opportunity to address the ORNL community and exchange ideas with lab researchers. The series is named after Eugene Wigner, ORNL's first research director and recipient of the 1963 Nobel Prize in Physics.

Lecturers

Ada Yonath

Ada Yonath serves as director of the Helen and Milton A. Kimmelman Center in Rehovot, Israel. In 2009 she received the Nobel Prize in Chemistry for her pioneering work in the structure and function of the ribosome.

Yonath delivered the Jan. 15 Eugene P. Wigner Distinguished Lecture on the topic "Combating species-specific antibiotics resistance and thoughts about origin of life." We asked about her research and the environment for women in science.

1. Why do diseases become resistant to antibiotics?

We are talking only about bacterial diseases, infectious diseases. They're made by bacteria, and bacteria want to live. If we take antibiotics, bacteria die, and they don't want to. They are cleverer than us, they have been on Earth before us, and they are with us. There were mammoths and dinosaurs, but they're all gone. Bacteria are still here. They are with us, and the pessimists say they will be here after us. But so far, what they're doing, the way they behave, they want to live. So they become resistant. It's not that the diseases are resistant; it's the bacteria.

2. You say the world seems to be headed for a "post-antibiotic era." What would such an era look like?

Like before antibiotics. This is before the middle of the last century. Antibiotics have been used only from the middle of the last century. Before that, people died from infectious diseases that don't count today. They died at 35 or 40, before antibiotics. Look at Mozart, Schubert—they died when they were not even 40 years old from infectious diseases. Maybe we all want to be Mozart, but that's not the only way.

3. What can we do about it?

Try to make better antibiotics. I'm not sure we can cure everything, that we can win the game against bacteria, but we can try to control it, to make the appearance of resistance more controllable. We can look for new antibiotics, not overuse antibiotics, not use antibiotics where they are not needed. If possible, if somebody has an idea for something completely new, I would love that.

4. You are only the fourth woman to win the Nobel Prize in Chemistry and the first from the Middle East to win a Nobel Prize in the sciences. How do you see the climate for women in the sciences?

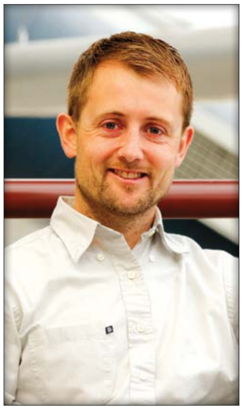
First of all, sciences are also physiology, medicine, and there are more women there. Second, I don't think that the committee in Stockholm is against women. I don't think they had 46 years until they found a woman. I just think that there are less women in science—surely less in chemistry. The society is still not encouraging women to go into science. Until now nobody said it clearly; they said it indirectly. They penetrate into the heads of young girls that it's no good to be a scientist, no good to be a scientist and a mother. They just implant it into the girls. So this has to be changed. I don't think that in science there is something against women. Many women say that it's a society made up of men and they're against women; I didn't feel it. I went in from a poor family, and I was in, and I never felt that being a woman made a difference. There is a difference, but it's in the number of females that go in and the number of females that stay. They study but go on to do other things, things that are related to science, but not always in science. So I think that this is the main problem, that there are not enough girls, not enough young girls or young scientists. I think that once they are in, they have the same chance. It's difficult to be a scientist, but not only for women, also for men. If you look at the proportion of how many men are there and how many female, I think the females are not doing so badly. Maybe not as good, but not so badly. More women, more prizes.

5. Why was it important to visit ORNL, meet with researchers here, and participate in the Wigner Lecture Series?

First of all, I'm trying to visit every university or research center that I think has a meaning, that has the quality and contributes. I've never been here, but I heard about it. I know there are three new beam lines here now, and I just wanted to see what's going on.

ORNL is proud of its role in fostering the next generation of scientists and engineers. We bring in talented young researchers, team them with accomplished scientists and engineers, and put them to work with at the lab's one-of-a-kind facilities. The result is research that makes us proud and prepares them for distinguished careers.

We asked some of these young researchers why they chose a career in science, what they are working on at ORNL, and where they would like to go with their careers.



Ryan Cooper

Postdoc affiliated with Materials Science and Technology Division
Ph.D. from Columbia University

What are you working on at ORNL?

I focus on the mechanical properties of materials in energy production. I measure thermomechanical properties of porous microcracked ceramics for diesel particulate filters that can be used to predict lifetimes of devices.

I'm also involved in next generation coal power plant research with nickel-based superalloys, which can raise the efficiency of coal power plants by more than 30 percent.

What would you like to do in your career?

Currently, I'm part of the ORNL Post-doctoral Association and serve as the Professional Development Chair.

Looking forward, I would like to continue doing science, specifically, looking at multiscale problems such as those seen in the fracture, creep and fatigue properties of metals. Ultimately, I would like to become a recognizable expert in the field of multiscale material characterization.

Why did you choose a career in science?

I always idolized the scientists in televisions shows and other stories—Donatello in "Teenage Mutant Ninja Turtles" and Egon Spengler in "Ghostbusters"—and the idea of science always appealed to me.

In undergraduate and graduate school I approached problems in a systematic, analytic way, which has led to my current position as a researcher here at ORNL.

Nannan Jiang

Graduate Student, Ph.D. in Energy Science and Engineering at Bredesen Center
Biosciences Division, Center for Environmental Systems Microbiology

What are you working on at ORNL?

I'm working on the microbial bioremediation of environmental pollutants. I'm interested in using genetics and synthetic biology to study the genes responsible for degrading toxic compounds and heterologously expressing them in different hosts.

The technique allows for investigation of novel gene combinations not yet tested by nature and could help increase the rates of pollutant degradation.

What would you like to do in your career?

Researchers enter science to create an impact on society while also fulfilling personal curiosities, but since the impact of research can be slow to observe, I've also enjoyed STEM outreach, which creates impact today.

Through outreach, I can help expand the impact factor from the lab to society, and the ultimate goal is to benefit society and have fun doing it.

I intend to push science forward.

Why did you choose a career in science?

I've been interested in science since high school, and I'm forever indebted to my university advisers who've given me the skills to pursue my passion.

In college, I worked in a greenhouse germinating corn seeds and interned through the Howard Hughes Medical Institute, where my interests became more defined.

Lindsay Kolbus

Postdoc—Doctorate from Virginia Tech in geosciences with concentration in mineral physics/crystallography
Chemical Engineering Materials Division, Engineering Materials Group

What are you working on at ORNL?

I work on additively manufacturing nickel super-alloys to determine residual stresses and microstructure. I also do some work on shale cores using neutron imaging and look at fluid uptake rates in fractured shale cores with the goal of providing information to energy companies and making the hydraulic fracturing process more efficient and environmentally sound.

What would you like to do in your career?

There's also a lot of potential for career development in the neutron sciences here, and I would like to stay in the ORNL group I'm with now. They're really good people who do great science.

I feel that my Ph.D. work and the skills I've gained at the lab are value assets for the group, but there's more work that needs to be done and I would like to be part of it.

Why did you choose a career in science?

I thought I would go into teaching, but one of the general education classes I took was intro to geology.

My professor hooked me in. I did an undergrad project and got kind of addicted to the rewards that science and research bring.

Mallory Ladd

Ph.D. student, Energy Science and Engineering
University of Tennessee, Knoxville

What are you working on at ORNL?

I work with the vegetation and biogeochemistry teams on ORNL's NGEE-Arctic project (Next Generation Ecosystem Experiments). I'm interested in using high-resolution mass spectrometry to look at the rates and controls of nitrogen availability and how that feeds back to the vegetation, decomposition rates and greenhouse gas release from permafrost soils.

What would you like to do in your career?

After I finish my dissertation and potentially a post-doctoral position, I'd eventually like to use my scientific base to work with energy policy makers to frame questions and issues, consider solutions, and implement specific outcomes.

Why did you choose a career in science?

When I was young I relentlessly asked "Why?" to anything and everything. I think my science classes were some of the first ones that started leading me to answers. In college, I learned that a degree in science really opened up a lot of different doors. You could take that knowledge base and apply it to a lot of different careers. Also, I think there was a part of me that wanted to prove that anyone, especially girls, can do math and science, too.

Kaitlin Palla

Biosciences Division and Plant Systems Group
Master's from Purdue University, applying for Ph.D. at Bredesen Center among others

What are you working on at ORNL?

I'm involved with the Crassulacean Acid Metabolism project, and what I do is work with plant tissue culture. We're trying to make plants more water efficient for bioenergy purposes so that they can be planted on marginal lands or in areas that don't really have a lot of natural water resources.

What would you like to do in your career?

I love science and research, and definitely want to stick with plants. I think there's just so many crazy, amazing things that you can do, especially with the genetic engineering—it's going to be the new plant breeding of the future. I think the bioenergy side of the lab is just rife with possibilities and completely fascinating, too, and that's where I'm kind of getting drawn in with my research. We'll see if it clicks.

Why did you choose a career in science?

When I was in elementary school my friend's dad helped us set up an experiment for our science fair project. He gave us duckweed and petri dishes to use and showed us how to record our observations, and how to use pH strips to test our solutions. We got to wear lab coats and make different pH solutions out of various home-sourced chemicals. It was thrilling for fourth-grade me, and it's when I first really fell for science.

Gautam S. Thakur

Postdoc research associate, Computational Data Analytics Group
Ph.D. from University of Florida-Gainesville

What are you working on at ORNL?

My work allows for research in realistic and data-driven activity modeling in urban dynamic systems. I study the structure, function and science of such networks using a combination of empirical methods and visualization techniques. My current research focuses on urban dynamics and health care.

In health care, I'm designing high-resolution health care data for the United States population. With urban dynamics, I'm working to create a hybridized causality model that tries to map population dynamics with transportation.

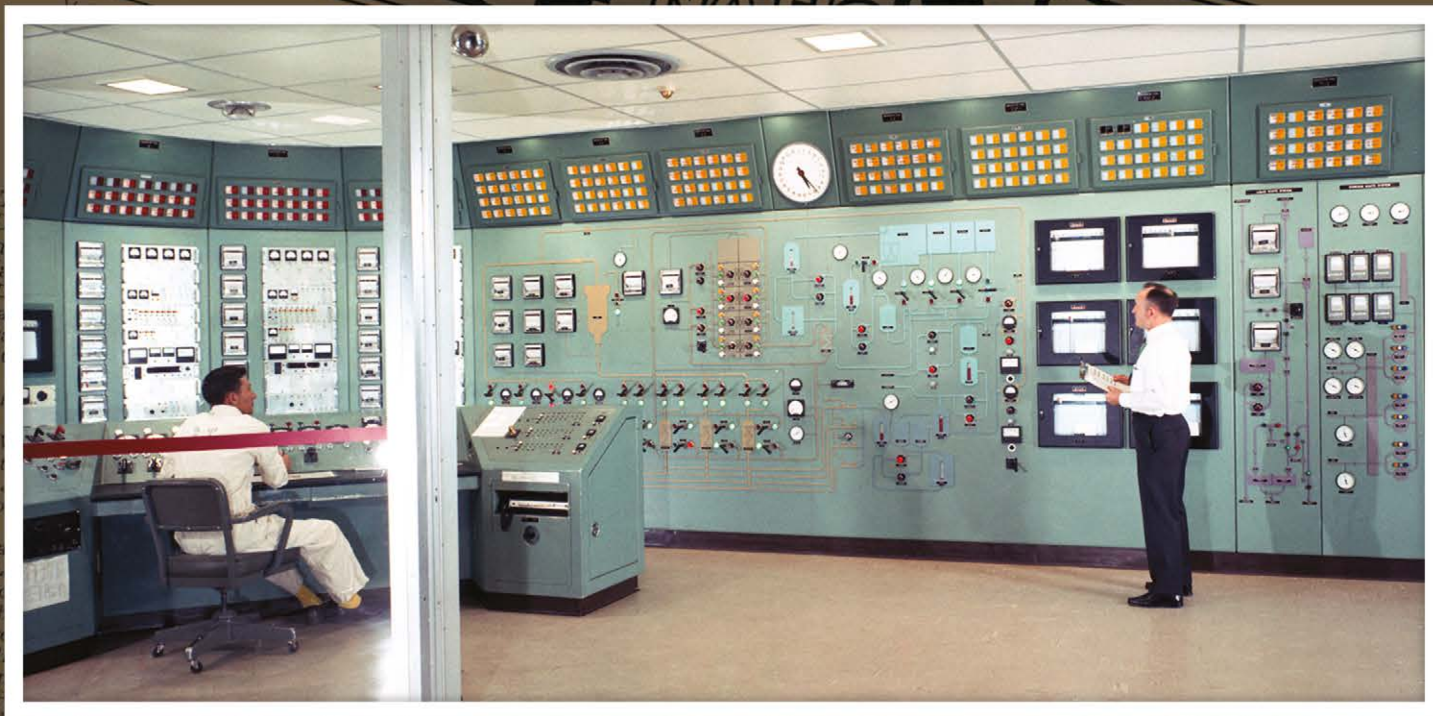
By exploring the data, I try to design new models and analytic techniques to find solutions otherwise impossible to solve using traditional approaches like theoretical models.

What would you like to do in your career?

My biggest motivation is to work on real problems, such as creating design patterns of non-conforming events to improve urban dynamic systems. For example, the urban system has to be more adaptive to small changes such as sudden snowfall, which can cause millions of dollars of damage. How can you best adapt to these nonconforming events? I call it "Adaptive Urban Dynamics."

Why did you choose a career in science?

I thought, "you can be a scientist or you can be anything in the world." And the simple reason is that I chose to be a scientist. I love being inventive in science, and I think that's what I'm designed for. I guess it's just what my DNA is encoded for.



HFIR turns 50

by Tim Gawne
gawnetj@ornl.gov

At 2:22 pm on August 25, 1965, the High Flux Isotope Reactor achieved criticality for the first time. Just over a year later, HFIR reached its design power of 100 megawatts, delivering the highest neutron flux of any research reactor in the world.

As its name implies, HFIR's primary mission was the production of isotopes for medical, research, and industrial applications. The reactor design was optimized to produce the highest possible neutron fluxes to support production of transcurium isotopes (i.e., isotopes of elements with atomic numbers higher than curium's 96) and studies of irradiated materials. HFIR's versatile design also provided capacity for the production of lighter radioisotopes and two facilities for neutron activation analysis. In addition—and at the insistence of then-ORNL Director Alvin Weinberg—four beam tubes were included to make the reactor's high-intensity neutrons available to neutron scattering researchers.

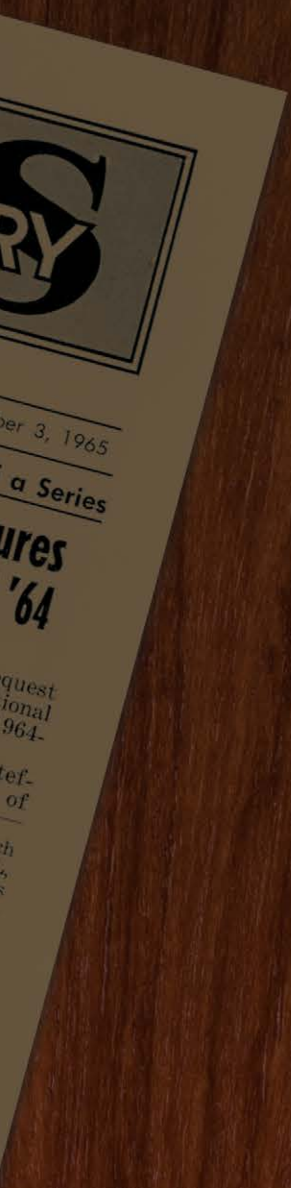
Neutron scattering experiments at HFIR have answered fundamental questions about magnetism and superconductivity, advanced our understanding of polymers, provided insights into biological structure and function, and revealed residual stress in engineered materials. Techniques and instruments developed to take advantage of HFIR's neutrons have been adopted by other research institutions, as well.

HFIR was recognized as a Nuclear Historic Landmark by the American Nuclear Society at a ceremony in April, the sixth ORNL facility to receive the ANS designation.

Today, HFIR routinely operates at 85 megawatts and remains a key national resource for isotope production, materials irradiation, and neutron activation analysis, but its primary mission is neutron science. At 50 years old, HFIR is one of the world's most powerful reactor-based sources of neutrons for research, delivering the brightest cold neutron source in the world and a thermal neutron flux on target equal to any in the world. With an array of new and upgraded instruments that enable studies of complex materials such as polymer blends, proteins and superconductors, HFIR continues to be a world-class platform for scientific discovery.

Each year, approximately 500 researchers use HFIR's unique capabilities for neutron scattering, isotope production, materials irradiation, and neutron activation analysis, and it is expected to continue supporting the delivery of breakthrough science for decades to come.

(Top) HFIR Control Room - circa 1966. (Middle) AEC chairman, G. T. Seaborg and ORNL director, Alvin M. Weinberg with dummy fuel cell. (Bottom) HFIR goes critical.



next issue

ORNL and economic development

www.ornl.gov/ornlreview

OAK RIDGE NATIONAL LABORATORY REVIEW
PO Box 2008, Oak Ridge, Tennessee 37831-6266

PRSRT STD
US Postage
PAID
Permit No. 3
Oak Ridge, TN

Editor—Leo Williams
Writers—Katie Bethea, Lynn Degitz, Tim Gawne, Eric Gedenk, Katie Elyce Jones, Gregory Scott Jones, Dawn Levy, Morgan McCorkle, Chris Samoray, Sara Shoemaker, Leo Williams
Designer—Brett Hopwood
Illustrators—Brett Hopwood, Jason Smith, Andy Sproles
Technical editor—Wendy Hames
Photographers—Carlos Jones, Genevieve Martin, Jason Richards

Phone: (+1) 865.574.8891
Fax: (+1) 865.574.0595
E-mail: ornlreview@ornl.gov
Internet: www.ornl.gov/ornlreview

Oak Ridge National Laboratory is managed by UT-Battelle, LLC, for the US Department of Energy under contract DE-AC05-00OR22725

ISSN 0048-1262