OAK RIDGE NATIONAL LABORATORY

Review

The origin of elements

OAK RIDGE National Laboratory

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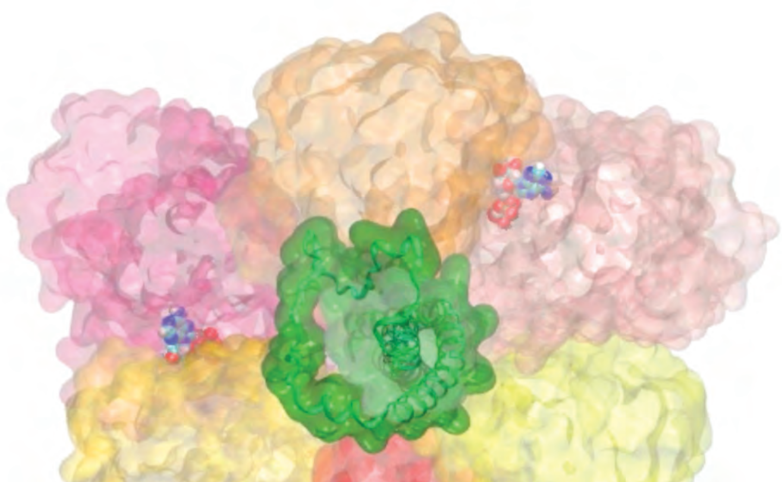


On the Cover

DOE Office of Science Early Career Research Program award-winner Kelly Chipps.

Solving the country's biggest problems

When I came to ORNL in 1987, the enormous potential present in the lab and its accomplished staff quickly became clear.

I arrived as a postdoctoral fellow in the Metals and Ceramics Division, recruited by group leader and future Corporate Fellow Stan David into a collaborative environment that encouraged talented researchers to apply themselves to solving the nation's most challenging scientific and technical problems.

In my case, the mentoring and support so generously offered encouraged me to explore how high-performance computers could be used in developing and understanding materials and manufacturing processes. The results of this work led me to pursue more powerful computational resources and eventually to focus on securing and sustaining leadership-class computing capabilities for ORNL. Those efforts paid off. ORNL is home to one of the world's premier supercomputing facilities; our Titan system has been America's most powerful supercomputer for the past five years, and our next system, Summit, will be five to 10 times more powerful still.

Of course, the climate of cooperation at ORNL is not unique to computing. Smart people support each other across the lab, identifying important problems and pursuing creative solutions. Along the way they are making their mark in areas ranging from expanding our fundamental understanding of nature to delivering innovations with the potential to transform our energy system and enhance our quality of life. The benefits of their efforts can be seen not only in the growth of scientific knowledge, but also in an improving environment, stronger national security, better health care and a more efficient and competitive industrial sector.

In this issue of *ORNL Review*, we shine a spotlight on one of the fastest-growing areas of our research and development: additive manufacturing, also known as 3D printing.

Long the domain of tinkerers and designers, additive manufacturing is poised to make a substantial impact on industry in the United States and around the world. The reasons are easy to see: Additive manufacturing can be both more flexible and more efficient than traditional manufacturing technologies, free from production constraints and the materials waste of traditional "subtractive" processes.

To reach its potential, however, this approach must overcome a variety of challenges, from size and cost limitations to reliable quality control. This is where the unique breadth of ORNL's expertise pays off. Talented engineers are increasing the size and decreasing the cost of additively manufactured components, making the technology attractive for an increasingly wide range of products. Neutron scientists and computational researchers are demonstrating how we can analyze and even design the material properties of objects as they are being produced. Biomaterials researchers are demonstrating how we can use homegrown feedstocks to produce materials for additive manufacturing that promote local and regional economies while being friendly to the environment.

ORNL was created during a great national crisis—the second world war—in which failure would have been unthinkable. National needs have driven our work ever since, and we are uniquely positioned to take on the most important and difficult challenges today. My goal is for ORNL to be the premier research institution in the world, delivering and translating innovative breakthroughs that will secure our nation's energy future and mitigate national security threats.

I hope you enjoy this edition of the *ORNL Review* and learn more about the important work we are performing today.

Thomas Zacharia
Laboratory Director

Alex Zucker in 1964. Image credit: ORNL

Alex Zucker, former ORNL acting director, dies

Alex Zucker, who came to ORNL as a nuclear physicist and crowned a 40-year scientific and administrative career as acting laboratory director, died November 8. He was 93.

Zucker became acting director in 1988 after Herman Postma stepped down from the position to accept a post with Martin Marietta Energy Systems Inc., ORNL's contractor at the time. Zucker held the post until Alvin Trivelpiece was appointed the new lab director the following year, after which Zucker served as the lab's associate director of nuclear technologies.

From 1975 to 1992 he was also consulting editor for *ORNL Review*.

Zucker was born in what is now Croatia and came to the United States with his parents at age 14. He served in the U.S. Army in World War II's European theater. His decision on a postwar career in physics was bolstered by the revelation of the Manhattan Project at the war's end.

He arrived at ORNL's Electronuclear Division in 1950 and was assigned to the project to build the lab's 86-inch cyclotron. During that period he was asked to investigate a concern by a group of nuclear pioneers that included Edward Teller and Hans Bethe: Would a hydrogen bomb explosion ignite the atmosphere?

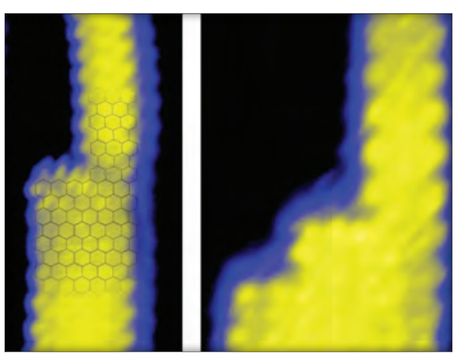
Having worked with cyclotrons for his Yale doctorate, Zucker used parts from calutrons to help develop an ion source that became the 63-inch cyclotron, which produced cross-section measurements that supported Bethe's calculations that no ignition would occur. Following that reassurance, Zucker's team turned the cyclotron into the world's first source of multi-charged heavy ion beams for a new field of studies in complex nuclei interactions.

As a manager, he was instrumental in bringing many projects to fruition, helping to overcome formidable administrative and budgetary hurdles. His managerial skills, for example, helped bring into being ORNL's Holifield Heavy Ion Research Facility and High Temperature Materials Laboratory.

Zucker's career as a science administrator extended beyond ORNL. He was executive director of the National Academies' Environmental Studies Board in the early 1970s and sat on the editorial advisory board of *Science* magazine. He was a fellow of the American Association for the Advancement of Science and the American Physical Society.—*Bill Cabage*

Preparing graphene for future electronics

An ORNL-developed approach creates seamless electrical contacts between precisely controlled nanoribbons of graphene, making the material viable as a building block for next-generation electronic devices.



An ORNL-led team formed seamless interfaces between graphene ribbons with different widths, creating a staircase configuration. Image credit: Chuanxu Ma and An-Ping Li, ORNL

In a recent study, an ORNL-led team grew the popular, atom-thick semimetallic graphene material as semiconducting ribbons, constructed from the bottom up using a precise number of atoms across and a precise molecular structure at the edge.

To make the approach more useful in electronics, the team focused on forming seamless interfaces between ribbons with different widths, which created a staircase configuration.

"This novel configuration allows us to adjust the energy gap, tune the energy level alignment and direct the flow of electricity through the materials," said An-Ping Li, ORNL coauthor of a study published in *Nano Letters* that describes the approach.—*Sara Shoemaker*

For more information: https://goo.gl/MSQ1Sz

ORNL researchers win nine R&D 100 Awards

ORNL researchers have received nine R&D 100 Awards in recognition of advancements in science and technology. The honorees were recognized recently at the 55th annual R&D 100 Conference, sponsored by *R&D Magazine*.

The awards, known as the "Oscars of Invention," honor innovative breakthroughs in materials science, biomedicine, consumer products and other fields, from academia, industry and government-sponsored research agencies. This year's nine honors bring ORNL's total R&D 100 awards to 210 since the awards' inception in 1963.

ORNL researchers were recognized for the following innovations:

ACMZ Cast Aluminum Alloys were developed by ORNL researchers with Fiat Chrysler Automobile U.S. and Nemak U.S.A.

ACMZ aluminum alloys are a new class of affordable, lightweight superalloys capable of withstanding temperatures of almost 100 degrees Celsius more than current commercial alloys while providing exceptional thermomechanical performance and hot tear resistance.

Common commercial alloys soften rapidly at high temperatures, limiting their use in next-generation vehicles, while other alloys that can withstand elevated temperatures are cost prohibitive and difficult to cast. ACMZ alloys were developed using a suite of atomic-level characterization and computation tools, resulting in a strong, stable and versatile material capable of withstanding the stressful conditions of next-generation high-efficiency combustion engines.

Additively Printed High Performance Magnets were developed by ORNL researchers and co-developed by Ames Laboratory, DOE's Critical Materials Institute, Magnet Applications Incorporated, Tru-Design and Momentum Technologies.

Additively Printed High Performance Magnets are the first rare earth bonded magnets created using the Big Area Additive Manufacturing method, allowing for rapid production with no size or shape limitations and minimal material waste. In contrast to more common sintered magnets that require the application of very high pressure to chemically reactive materials, bonded magnets are less expensive and resource-intensive to produce.

The magnet feedstock blends a magnetic powder with a nylon polymer, and the finished magnets demonstrate magnetic, mechanical and microstructural properties comparable to or better than bonded magnets created with traditional injection molding methods.

Filler Materials for Welding and 3D Printing were developed by ORNL in collaboration with the U.S. Army Tank Automotive Research, Development and Engineering Center.

The heating and melting processes of welding and metal additive manufacturing generate localized distortions and residual stresses in steel and other materials. These defects can cause the material to become brittle or crack, which can lead to catastrophic structural failure.

ORNL's innovative filler materials counterbalance how much the materials expand and shrink and control the residual stress and distortion of high-strength steel structures. The filler materials also do not require the costly, labor-intensive heat treatments normally needed to avoid cracking and material embrittlement, providing significant economic benefits while improving the stability and durability of welded and 3D-printed structures.

Safe Impact Resistant Electrolyte was developed by ORNL researchers and co-developed by the University of Rochester.

In typical automotive lithium-ion batteries, the liquid electrolyte—which conducts the electrical current—poses a fire risk in high-speed collisions and requires heavy protective shielding, decreasing the vehicle's range and efficiency. SAFIRE eliminates this risk by using an additive that transforms the liquid electrolyte to a solid upon impact. Blocking contact between electrodes prevents short circuiting and a potential fire. SAFIRE performs as well as conventional electrolytes under normal conditions and can significantly reduce electric vehicle weight and increase travel distance.

The **dropletProbe Surface Sampling System for Mass Spectrometry** was developed by ORNL researchers in coordination with SepQuant.

The system is a new means of surface sampling for mass spectrometry, a major scientific technique for measuring the masses of chemicals in a sample. The dropletProbe system provides rapid, simple chemical extraction and analysis for a host of scientific applications.

The system uses a liquid junction between the device and a surface to obtain samples for high-performance liquid chromatography and mass spectrometry analysis. It is a low-cost, low-maintenance and nondestructive method for sampling complex analytical surfaces, such as biological tissue samples, with a high degree of precision.

ACE: The Ageless Aluminum Revolution was submitted by DOE's Critical Materials Institute and was co-developed by ORNL, Eck Industries, Ames Laboratory and Lawrence Livermore National Laboratory.

Lightweight materials like aluminum alloys can help substantially increase the efficiency of vehicles and airplanes. ACE is a new family of aluminum alloys that exhibits better performance at high temperature, is easier to cast than previous alloys, and does not require a heat treatment. By combining aluminum and cerium, or a similar element, with traditional alloying materials, ACE is able to demonstrate high mechanical performance and resist corrosion.

ACE alloys remain stable at temperatures 300 degrees Celsius higher than leading commercial alloys and can withstand 30 percent more load before they deform. Manufacturers can successfully cast ACE alloys in a wide variety of structural components without energy-intensive heat treatments, which could significantly increase production output and reduce manufacturing costs, in some cases by almost 60 percent.

dfnWorks: A Computational Suite for Flow and Transport in Subsurface Fracture Networks was submitted by Los Alamos National Laboratory and co-developed with ORNL's Scott Painter.

dfnWorks is a software suite that generates 3D models of fractures in rocks and the way fluids move through those fractures. Research in hydraulic fracturing, safe nuclear waste disposal and underground carbon dioxide storage relies on this type of software. The models can be incredibly complex and often require a great deal of computational time and power to run.

Compared with similar programs, dfnWorks requires less time to run and allows scientists to model geological conditions they could not previously model. Scientists have used the software to model a variety of systems from a few millimeters up to kilometers in size.

Coating Solutions for Large-Format Additive Manufacturing was submitted by Tru-Design and co-developed with ORNL and Polynt Composites.

Large-scale 3D printing can quickly produce prototypes and molds used to manufacture parts, but these pieces are often neither smooth nor vacuum tight.

As a result, manufacturers can't use these molds, limiting the usefulness of 3D printing.

The Large Format Additive Coating Solutions—TD Coat RT and TD Seat HT—minimize this problem. They cover the rough exterior of a printed part and create an unbroken vacuum-tight seal. The coatings can be machined and finished for manufacturing tools and molding applications at a fraction of the cost of traditionally tooled metal parts.

Techmer Engineered Additive Manufacturing Materials was submitted by Techmer PM and co-developed with ORNL and BASF.

These materials are new filled plastic carbon fiber compounds that are specially designed for 3D printing. Manufacturers can use these 3D printed materials and an autoclave to produce molds for high-performance composite panels and parts.

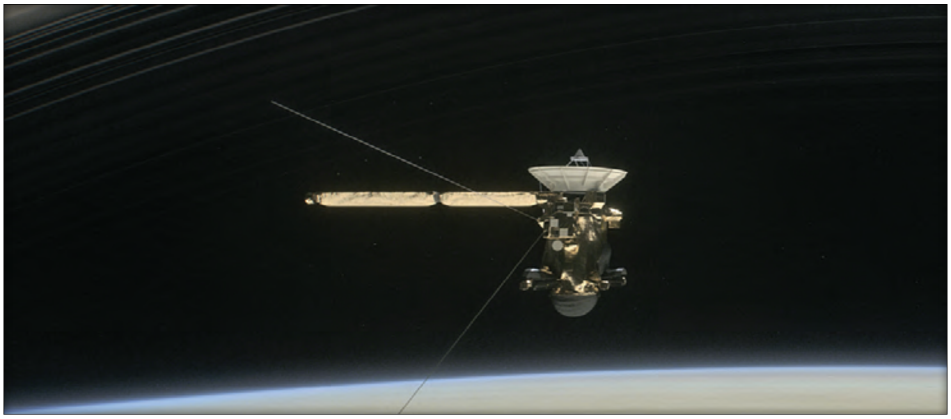
The company offers two types of TEAMM with different proportions of carbon fiber—25 and 50 percent—to provide a variety of mechanical properties for a range of applications. Using these compounds with an autoclave, aerospace companies can produce molds for a 10th of the cost and lead time compared to existing technology. Other applications include defense and high-end automotive markets.—*Sean Simoneau*

For more information: https://go.usa.gov/xnKf2

Cassini craft flew with ORNL-fabricated tech

An ORNL-fabricated component arrived this past September at the end of a fascinating ride, including a seven-year trek across the solar system and 13 more years orbiting a planet that has fascinated night sky gazers for centuries, even from three quarters of a billion miles away.

NASA's Cassini spacecraft lifted off from Earth in 1997 equipped with radioisotope thermoelectric generators—plutonium dioxide heat sources that provide electrical power for deep-space missions. Upon arrival in Saturn's orbit in 2004, Cassini began producing streams of data and close-up images of the planet, its moons and the famous rings.



A still from the short film "Cassini's Grand Finale" shows the spacecraft diving between Saturn and the planet's innermost ring. Image credit: NASA/JPL-Caltech

Those transmissions ended when Cassini burned up in Saturn's atmosphere.

ORNL's Radioisotope Power Systems program developed and fabricated the protective cladding for the RTG's plutonium dioxide fuel. The iridium alloy "clad vent sets" have been used in other deep-space missions including Galileo, Ulysses, Mars Curiosity and the New Horizons mission to Pluto and beyond. In fact, the RTGs make deep-space missions that venture beyond solar power's reach feasible.

The end of the Cassini mission was ordained primarily by the depletion of fuel for its rocket thrusters after 20 years. RTGs last longer. The two Voyager missions launched 40 years ago are still transmitting from interstellar space—although diminishing energy has forced controllers to decide which instruments can function. Both are expected to keep running at least one of their instruments until 2025 and may send signals until 2036.—*Bill Cabage*

AI researcher named ORNL's top scientist

Georgia Tourassi of ORNL's Computing and Computational Sciences Directorate has received the ORNL Director's Award for Outstanding Individual Accomplishment in Science and Technology.

ORNL Director Thomas Zacharia presented the top scientist award to Tourassi during the lab's annual Awards Night event.

The award recognized Tourassi for advancing the research, development and deployment of artificial intelligence in data-driven biomedical discovery and medical imaging, including applications for cancer diagnosis and management. She was also cited for her support of the missions of biomedical scientific societies and federal agencies and for mentoring students in biomedical science and technology.

Tourassi, who works in the Computational Sciences and Engineering Division and directs the laboratory's Health Data Sciences Institute, also received the Distinguished Researcher award.

Brian Weston of the Neutron Sciences Directorate's Research Reactors Division received the Director's Award for Outstanding Individual Accomplishment in Mission Support.

Weston, who also received the evening's Outstanding Individual Accomplishment in Mission Support award, was cited for

Georgia Tourassi

Brian Weston

distinguished contributions to the High Flux Isotope Reactor's outstanding performance, which has included providing seven operation cycles in each of the past two years and greater than 98 percent reliability for a decade. He was also recognized for sustained contributions to other laboratory and DOE projects.

Timothy Burress, Jason Pries, Lixin Tang and Randy H. Wiles received the Director's Award for Outstanding Team Accomplishment for their development of a low-cost, high-power-density prototype motor that is 75 percent more powerful than same-sized commercial motors. The prototype motor also contributes to national energy security by replacing magnets made from imported rare earth materials with magnets made from inexpensive ferrite, found in abundance in the United States. All four work in the Energy and Environmental Sciences Directorate's Electrical and Electronics Systems Research Division.—*Bill Cabage*

Five from ORNL named AAAS fellows

Five ORNL researchers have been elected fellows of the American Association for the Advancement of Science.

AAAS, the world's largest multidisciplinary scientific society and publisher of the *Science* family of journals, honors fellows in recognition of "their scientifically or socially distinguished efforts to advance science or its applications."

Budhendra Bhaduri, leader of the Geographic Information Science and Technology Group in the Computational Sciences and Engineering Division and director of ORNL's Urban Dynamics Institute, was elected by the AAAS section on geology and geography for "distinguished contributions to geographic information science, especially for developing novel geocomputational approaches to create high-resolution geographic data sets to improve human security."

Bhaduri's research focuses on novel implementation of geospatial science and technology, namely the integration of population dynamics, geographic data science and scalable geocomputation to address the modeling and simulation of complex urban systems at the intersection of energy, human dynamics and urban sustainability.

Sheng Dai, leader of the Nanomaterials Chemistry Group in the Chemical Sciences Division, was elected by the AAAS section on chemistry for a "significant and sustained contribution in pioneering and developing soft template synthesis and ionothermal synthesis approaches to functional nanoporous materials for energy-related applications."

Dai's research group synthesizes and characterizes novel functional nanomaterials, ionic liquids and porous materials for applications in catalysis, efficient chemical separation processes and energy storage systems.

Mitchel Doktycz, leader of the Biological and Nanoscale Systems Group in the Biosciences Division, was elected by the AAAS section on biological sciences for "distinguished contributions to the field of biological sciences, particularly advancing the use of nanotechnologies for characterizing and interfacing to biological systems."

Doktycz, also a researcher at ORNL's Center for Nanophase Materials Sciences, specializes in the development of analytical technologies for post-genomics studies, molecular and cellular imaging techniques, and nanomaterials used to study and mimic biological systems.

Bobby G. Sumpter, deputy director of the Center for Nanophase Materials Sciences, was elected by the AAAS section on physics for "distinguished contributions to the field of computational and theoretical chemical physics, particularly for developing a multifaceted approach having direct connections to experimental research in nanoscience and soft matter."

Sumpter's research combines modern computational capabilities with chemistry, physics and materials science for new innovations in soft matter science, nanomaterials and high-capacity energy storage.

Robert Wagner, director of the National Transportation Research Center in the Energy and Transportation Science Division, was elected by the AAAS section on engineering for "distinguished contributions to the fields of combustion and fuel science, particularly for seminal research on combustion instabilities and abnormal combustion phenomena."

Wagner is the lead of the Sustainable Mobility theme for the Urban Dynamics Institute and the co-lead of DOE's Co-Optimization of Fuels and Engines Initiative, which brings together the unique research and development capabilities of nine national labs and industry partners to accelerate the introduction of efficient, clean, affordable and scalable high-performance fuels and engines.

The new fellows will be formally recognized in February at the 2018 AAAS Annual Meeting in Austin, Texas.—*Sean Simoneau*

Budhendra Bhaduri

Sheng Dai

Mitchel Doktycz

Bobby G. Sumpter

Robert Wagner

Moving into the future with 3D printing

by Leo Williams
williamsjl2@ornl.gov

It's been more than three decades since inventor Chuck Hull created stereolithography, a process that produces 3D objects by hardening a liquid resin with an ultraviolet laser beam.

Devices using this process, widely considered the first 3D printers, are still in use today, but they are hardly alone. Not only has a wide variety of 3D-printing technologies been developed in recent years—some using metals, others high-tech plastics—but their applications have also expanded, taking them out of the design studio and into the factory.

Additive technologies have the potential to profoundly change the way manufacturing is done in many industries. They are relatively flexible, allowing manufacturers and researchers alike to create one-of-a-kind objects, and they don't penalize users for creating complex, intricate designs. In fact, 3D printers can create designs impossible by other methods.

These technologies are also efficient, using consistently less material than traditional processes and reducing waste.

"The average yield for a titanium component on an aircraft [made using traditional methods] is 10 percent," noted Bill Peter, director of DOE's Manufacturing Demonstration Facility located at ORNL. "For every 10 pounds of incoming titanium material, 9 pounds are removed and 1 pound ends up in the final component."

ORNL goes additive

ORNL has gone a long way toward demonstrating the value of additive technologies. In 2014 the lab designed and produced the world's first 3D-printed car with partners Local Motors and Cincinnati Incorporated. More recently it earned a Guinness World Record for the world's largest solid 3D-printed item, a trim-and-

See MOVING INTO THE FUTURE WITH 3D PRINTING, page 8

At ORNL's Manufacturing Demonstration Facility, from left, Polymer Materials Development Team leader Vlastimil Kunc, imaging scientist Vincent Paquit, Manufacturing Systems Research Group leader Lonnie Love, MDF Director Bill Peter, Deposition Science and Technology Group leader Ryan Dehoff, and Suresh Babu, Governor's Chair for Advanced Manufacturing at the University of Tennessee and ORNL. Image credit: Carlos Jones, ORNL

Printing better materials

by Leo Williams
williamsjl2@ornl.gov

On the surface, additively manufactured parts may seem like just a series of really small welds, but the minute details of exactly how you print a component play a significant role in its performance.

The approach is substantially different from that of traditional manufacturing, where the links between processing and properties are well understood, and the goal is to produce materials that have a uniform, or equiaxed, structure.

"We often cast and then forge the material to produce an equiaxed grain structure so that it has uniform material properties in all directions," ORNL Deposition Science and Technology Group Leader Ryan Dehoff said of the traditional process. "The challenge is getting the final geometry from the material.

> *"The chief technology officer said, 'I've spent 30 years of my career trying to accomplish site-specific microstructure control, and you have proved the holy grail of metallurgy is now possible.'"*
>
> — ORNL Deposition Science and Technology Group leader **Ryan Dehoff**

"Additive manufacturing is just the opposite; we can now accomplish complex geometries. The challenge is understanding how the complex thermal cycles affect the mechanical properties of the material."

Much of the difference between the two approaches lies in the crystalline structure of a metal. In many traditional manufacturing processes, crystals are randomly oriented, making the bulk material equally strong in every direction. If, however, the crystals are aligned, that material becomes extra strong in one direction at the expense of strength in others. The extreme case is referred to as a single crystal, where there's only one crystallographic orientation.

Researchers at ORNL have figured out how to control the material's crystal structure at a very local level by incorporating advanced materials theory into the additive manufacturing process. Such an ability is unprecedented.

"Now we can control the material response to a degree that was never possible before," Dehoff explained. "The first time I openly disclosed this new capability, we were with a Fortune 100 company, and the chief technology officer said, 'I've spent 30 years of my career trying to accomplish site-specific microstructure control, and you have proved the holy grail of metallurgy is now possible.'"

The work highlights the benefits of collaboration between specialties across the lab.

Ryan Dehoff, ORNL Deposition Science and Technology Group leader.
Image credit: Carlos Jones, ORNL

At the core is supercomputing.

Significant advances were made when Naren Raghavan, a student with the University of Tennessee's Bredesen Center for Interdisciplinary Research and Graduate Education at ORNL and part of the manufacturing team, worked with computational scientist John Turner and colleagues. The result was a high-performance computational platform that allowed researchers to understand the fundamentals of the process and apply them to more complex parts, controlling local properties and performance.

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drill tool for evaluation by The Boeing Company. Along the way ORNL has printed vehicles, buildings, heavy machinery, and even a submersible.

These demonstrations illustrate the possibilities of large-scale additive manufacturing, but they are not an end in themselves. Rather they set the stage in areas such as advanced materials research, the development of physics-based computational simulation, and the creation of controls and sensors that provide real-time quality control in the deposition process, helping to pave the way for the next generation of additive manufacturing.

> *"One machine and a fairly small area is able to manufacture a broad spectrum of applications."*
>
> — ORNL Manufacturing Systems Research Group leader **Lonnie Love**

ORNL has worked with additive technologies for years, but only recently has the lab put an intense focus on applying its scientific expertise to some of additive manufacturing's largest challenges.

"The challenges in additive manufacturing have changed," said Ryan Dehoff, leader of the lab's Deposition Science and Technology Group. "Five years ago the focus was on creating complex geometries. Today additive processes are required to be faster, larger, and use an increased range of materials" (see "Printing better materials," p. 7).

Many of these applications, in fact, require new and unique materials designed specifically for the complexities of additive manufacturing, including high-temperature metals and lightweight reinforced carbon fiber composites. ORNL researchers and colleagues discussed one promising application—the use of functional materials such as rare-earth magnets—in *Nature Scientific Reports* (see go.usa.gov/xngZc).

To reach its full potential, additive manufacturing must also go bigger, faster and cheaper. And manufacturers need a way to both ensure and verify the quality of each printed component (see "Controlling the quality of printed parts," p. 11).

Getting bigger and faster

ORNL has done much to overcome the size limitations inherent in conventional 3D printing. By incorporating robotic arms on a gantry system, ORNL researchers can deposit material faster while maintaining print quality. Because robots have substantial freedom of movement, these systems overcome some of the limitations of conventional 3D printing by, for instance, emulating the process a person might use to create an object by hand.

"One of the problems we have with traditional gantry systems is that when you're growing a part, you can't defy gravity," explained Lonnie Love, leader of ORNL's Manufacturing Systems Research Group. "One thing I can do with a robot is tilt the part or apply pressure.

Lonnie Love, ORNL Manufacturing Systems Research Group leader. Image credit: Carlos Jones, ORNL

"If you look at how humans make clay pots, you defy gravity all the time by supporting the material while it's being formed. Again, imagine having multiple robots that can support the material while it's setting, and then when it's stiff enough they can let it go."

In thinking big, however, Love's team is not giving up on gantries altogether. Rather than being a component within a printer, they become the means of moving that printer.

"When you want to make something massive, you want this robot to be on a rail," he said. "Imagine a robot that's on a moving base that can move forward, backward, side to side, up and down. Now you're not limited in terms of the size of part you want to make."

Another obstacle to the widespread use of additive manufacturing is its expense. Between the cost of materials going into the process, the cost of the machine itself and the slow pace of printing, parts coming off a conventional 3D printer end up costing as much as $1,000 a pound, Love said.

Few industries can support such a cost, with aerospace and medical applications being potential exceptions.

The Big Area Additive Manufacturing system—developed through a collaboration with Cincinnati Incorporated—works to overcome the speed and cost challenges by depositing commodity materials and doing it faster than earlier systems. Like those systems, the BAAM machine melts a carbon-reinforced polymer to create products, but instead of pushing and melting a plastic wire, it relies on pellets of the material fed with a screw extruder.

"There's a fundamental limit on how fast you can heat the wire and melt it," Love said. "By going from a heated tube and wire to a pellet and screw, you go from a limit of one cubic inch an hour to printing as fast as you want."

By using this new system and reinforcing the material with carbon fiber, he said, researchers were able to bring the cost of a final part from $1,000 a pound to around $20 a pound.

"Now it gets to be pretty exciting," he said. "It opens up other applications where traditionally you would never think about 3D printing."

Controlling quality and making a difference now

One goal for researchers working in additive manufacturing is to produce parts that can go into high-performance applications such as aircraft. The challenge in this case is quality control. In essence, one of the great strengths of additive manufacturing—the uniqueness of every component that comes off a 3D printer—is a potential roadblock because it means a close analysis of one part is no guarantee that the next part will be acceptable.

Before 3D-printed parts are used in critical areas of a plane, manufacturers will have to be able to perform rigorous quality control on every part that's produced. ORNL is applying its expertise in materials, data and neutron science to overcome this challenge, but researchers stress that additive manufacturing is already prepared to make a big splash in many other areas.

Love said one major example is the tool-and-die industry, which has largely left the United States. Additive manufacturing has the potential to bring that business back home, creating jobs while saving manufacturers millions of dollars.

"What we're showing is the killer application for 3D-printing today is printing tools, molds, and dies," he explained. "Usually these things take months, if not years, and cost hundreds of thousands of dollars. They're one-of-a-kind parts, which is what additive is really good at."

As an example he pointed to a mold printed at the Manufacturing Demonstration Facility for the Marine Corps air station at Cherry Point, North Carolina. The mold would typically take months to produce, Love said, but in this case the Manufacturing Demonstration Facility had specifications on a Monday and was able to deliver the finished mold that Friday.

"The customer called the next week and asked how long it took to make the mold and how much it cost. I said, 'Seriously, it took longer and cost more to ship it than it did to make it.'"

Love continued: "The automotive industry pays hundreds of millions of dollars for every model of car to make its tooling for a production line. If you ask yourself why the United States will sell SUVs when gas is $5 a gallon and smart cars when gas is $2, it's because energy policies change faster than the automotive industry can change the model of a car."

The future of 3D printing

ORNL is well placed to contribute as additive manufacturing moves into critical applications and plays an increasingly large role in manufacturing in general. As DOE's largest science and energy national laboratory, ORNL can exploit a range of complementary strengths—in manufacturing, materials science, computation and data analysis, and neutron science—to prepare additive manufacturing for the big time.

"That's what's amazing about this one facility," Love said. "ORNL can model the process, can make parts, and then can measure and validate them. Nowhere else in the world can you do this. That's why overnight we've become the premier lab in terms of additive manufacturing. All of those fundamental science tools at ORNL are really the building blocks you need for additive manufacturing to be successful."

According to Love, these technologies may also lead to a fundamental change in the way we approach manufacturing.

"If you think about it, back before the time of Henry Ford every town had everything it needed to produce for itself," he said. "I think we're establishing a new paradigm in manufacturing where customizable fabrication can be achieved locally with high fabrication rates.

"If you look at the BAAM and the things we've printed on one machine, it's mind-boggling. We've printed tooling for aerospace, automotive, appliances, marine applications, and large wind turbine blade molds. In addition, we've printed cars, trucks, boats; it's limitless. One machine and a fairly small area is able to manufacture a broad spectrum of applications."

Even the materials going into the products may be produced locally, noted ORNL materials scientist Soydan Ozcan, who is focused on creating renewable materials that can be grown domestically and used in additive manufacturing (see "Biomaterials for additive manufacturing," p. 12).

"The way we are manufacturing is changing. Additive manufacturing is making it possible to have one machine very close to the feedstock or very close to end users. So can we combine local feedstocks and local manufacturing and create a local job? That's a question we are also asking. This can change the way society sustains itself and creates jobs."

"What we're showing is the killer application for 3D-printing today is printing tools, molds, and dies. Usually these things take months, if not years, and cost hundreds of thousands of dollars. They're one-of-a-kind parts, which is what additive is really good at."

— ORNL Manufacturing Systems Research Group leader **Lonnie Love**

PRINTING BETTER MATERIALS, from page 7

"We no longer can think only about traditional approaches and scan strategies for making additively manufactured components," said Turner, who is principal investigator of ExaAM, the Transforming Additive Manufacturing through Exascale Simulation project. ExaAM is a multilaboratory program led by ORNL focused on linking physical phenomena across widely varying lengths to create predictive models.

computer, as many of the individual data sets are on the order of tens of terabytes.

Turner agreed, noting that researchers must learn much more about the science of solidification and the way microstructures grow within a material. A substantial reason he is leading the project is to prepare these questions for future exascale computers that will be able to tackle a billion billion calculations each second.

Vincent Paquit, data analytics lead for ORNL's Manufacturing Demonstration Facility. Image credit: Carlos Jones, ORNL

"The research at the Manufacturing Demonstration Facility over the past couple of years has shown how complex additive manufacturing processes can be," Turner said. "The ability to change the scan paths, or even use spots rather than lines to control the microstructure, yields almost unlimited possibilities. The power to simulate the result and optimize the outcome will be critical for the success of additive manufacturing technologies."

To take advantage of these computational tools, researchers must incorporate every step in the process, from the intent of a designer to inspection of the finished part.

"We are developing a framework to overlay multiple data modalities from additive manufacturing technologies, including the build intent, the outcome from predictive modeling, in situ process monitoring data, and post-build inspection information," said ORNL imaging scientist Vincent Paquit. "We can then perform data analytics, machine learning and artificial intelligence to understand the intricacies of the process. This can only happen if we use a super-

"At this point there's a significant amount of trial and error, which wastes time and energy," he said. "Ultimately we'd like to be able to describe a part and prescribe the process parameters that would give us the strength and performance properties we want and then go build it—in one try. That's the goal."

As they develop the techniques that will allow them to customize grain patterns, researchers need to evaluate their progress. That's where neutrons come in, specifically ORNL's two neutron science facilities—the Spallation Neutron Source and the High Flux Isotope Reactor.

Not only does the penetrating power of neutrons allow researchers to see deeply within a metal component, but neutrons also reveal the grain patterns that affect a part's strength. This information can be extracted in a fraction of the time required by conventional metallography.

"Neutrons can penetrate a material easily; you don't have to slice or cut it," noted ORNL neutron scientist Ke An. "Neutron diffraction is a powerful way to see polycrystalline structures, giving us information on crystal orientation."

Controlling the quality

of printed parts

by Leo Williams
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Additive manufacturing has many advantages over traditional manufacturing. It creates parts with essentially no waste. It produces complex designs as easily as simple ones. And it can go from design to finished product in a matter of hours rather than weeks or months.

As impressive as it is, however, additive manufacturing does have its challenges, chief among them controlling the material properties within a printed object.

"We wrongly assume that what you print will be identical to what was designed," said Suresh Babu, who holds the Governor's Chair for Advanced Manufacturing at the University of Tennessee and ORNL. "Printing a material involves a very complex temperature profile for the material due to multiple heating, melting, and cooling events that are all interconnected and inherently dependent on one another."

The challenge is that this complex process governs the underlying physics of the material—things such as porosity, defect structure, and nonuniform microstructures—and creates uncertainty over how the part will ultimately perform. This uncertainty means industry must conduct exhaustive testing and inspection that drive up cost and can limit the real-world usefulness of additive manufacturing.

If the business case warrants, process controls can be implemented to certify additively manufactured components, such as for a General Electric–produced fuel-injector tip that improved the fuel efficiency, emissions and reliability of turbine technology critical for aircraft engines. Yet the process is lengthy and expensive.

When the geometry of a printed part changes, the entire certification process must be performed for the new geometry. "In order for additive manufacturing technologies to be widely implemented in industrial applications, we must revolutionize how we think about the certification process," said Vincent Paquit, imaging scientist and data analytics lead for ORNL's Manufacturing Demonstration Facility. "We need to get to where we can certify the process, not individual parts."

"Another major challenge in additive manufacturing is residual stress and distortion," said Ryan Dehoff, leader of the lab's Deposition Science and Technology Group. "These complicated thermal cycles during processing result in a lot of internal residual stress and can vary widely within a part, which ultimately manifests itself in distortion."

Neutron analysis at ORNL's High Flux Isotope Reactor and Spallation Neutron Source are especially good at detecting residual stress and defects within a part. Among other benefits, it can show warping and porosity in a large component without the necessity of cutting that component apart.

Suresh Babu, Governor's Chair for Advanced Manufacturing at the University of Tennessee and ORNL. Image credit: Carlos Jones, ORNL

"The advantage of neutrons is they can go through metals quite easily," said ORNL neutron scientist Hassina Bilheux. "You can see internal structures and features in an additive manufacturing sample. Right now, if you want to do this with X-rays, it's extremely hard. You need to crank up the energy in your X-rays, and by doing that you lose resolution."

To take full advantage of the insights provided by neutrons, researchers must first thoroughly monitor the conditions under which a part is produced. Infrared cameras collect the

See CONTROLLING THE QUALITY OF PRINTED PARTS, page 13

Soydan Ozcan, ORNL materials scientist. Image credit: Carlos Jones, ORNL

Biomaterials for additive manufacturing

by Leo Williams
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A thermoplastic-based composite feedstock known as carbon fiber–ABS is the workhorse of polymer-composite 3D printing at DOE's Manufacturing Demonstration Facility, located at ORNL.

It was the material that created the first 3D-printed car (the Strati), one of the first 3D-printed buildings (the AMIE Demonstration Project), the world's largest solid 3D-printed component (a tool for The Boeing Company), and myriad other parts and objects.

While carbon fiber–ABS is easy to work with and offers great performance, it is a nonrenewable, petroleum-based product. ORNL researchers are working to bring additive manufacturing into the green economy by developing renewable alternatives.

Plant-based fibers have been investigated to improve the properties of biobased polymer resins and make them easier to work with. One of these alternatives uses plant-based polylactic acid reinforced with cellulose nanofibrils from woody plants. Known as CNF-PLA, it has proven to be stronger and is projected to be cheaper than a comparable version of carbon fiber–ABS.

Another alternative formulation of the renewable material includes bamboo as the reinforcing fiber. It was used to print seating for two outdoor pavilions—as well as a large serving stand that supports a big 3D-printed overhead structure—last winter at the DesignMiami architecture exposition in Florida.

See BIOMATERIALS FOR ADDITIVE MANUFACTURING, page 13

BIOMATERIALS FOR ADDITIVE MANUFACTURING, from page 12

According to ORNL materials scientist Soydan Ozcan, the material is very promising and has great potential in many areas that do not require that fibers be long, continuous strings. "This material is also lower cost," Ozcan added, "and it is performing in many ways close to carbon fiber–ABS in mechanical properties."

> *"The way we are manufacturing is changing. Additive manufacturing is making it possible to have one machine close to the feedstock or close to the end users."*
>
> — ORNL materials scientist **Soydan Ozcan**

Ozcan noted that the renewable material supports the environment in at least two ways. First, it has a far lower carbon footprint than petroleum-based options. Second, while the production of carbon fiber and carbon fiber–ABS is energy intensive, far less energy goes into the production of biopolymers and plant-based fibers such as bamboo.

The potential benefits of biomaterials, however, go even further, supporting a larger economy. In a sense, Ozcan said, this mimics the evolution of petroleum-based products over the past century. "When we look at the petroleum industry, it's not just the business of selling gasoline for your car, but it's also about the whole petrochemical industry, benefitting all products, bringing the cost down together.

"We have to create value from byproducts such as polymers and reinforcement materials that can be used to produce a wide range of products using additive and other manufacturing techniques."

Looking forward, the researchers also hope to support American farming by making use of crops such as poplar that can be widely grown domestically, linking agriculture with biofuels and biomaterial products. The new Center for Bioenergy Innovation at ORNL is working on advanced poplar strains that tolerate a wide variety of growing environments.

Agriculture may become even more tightly linked with biofuels and biomaterials products because additive manufacturing can succeed in relatively small manufacturing operations, Ozcan noted.

"The way we are manufacturing is changing," he said. "Additive manufacturing is making it possible to have one machine close to the feedstock or close to the end users.

"Can you create local agricultural businesses in conjunction with manufacturing? Can we plant locally, and can we manufacture locally and create businesses in local areas? Those are some of the questions that we are asking ourselves."

CONTROLLING THE QUALITY OF PRINTED PARTS, from page 11

exact temperature when a beam hits the powder bed, while other instruments monitor the pressure within the print chamber, roughness of the print surface, variations in the power supply and other information.

"We start by collecting as much data as possible to establish a link between process intent and final outcome," Paquit said. "Every additional sensor adds value to the puzzle."

To better help industry understand and utilize additive manufacturing, ORNL has created a portfolio of open-source software tools to help users understand the nuances of the process. These tools can be used to certify that the machine is operating as expected and creating quality material.

In addition, an interdisciplinary team at ORNL is contextualizing data analytics results by combining expertise in materials science, manufacturing, data analytics, sensing, modeling, high-performance computing and neutron science to link the physical phenomena and process outcomes.

"The goal is to examine the compiled data and find the set of events that will induce a certain type of defect, microstructure or property," Paquit said. "At the end of the day, what we want to be able to do is train a machine-learning technique that will automatically capture this information and output it as a quality metric."

> *"We start by collecting as much data as possible to establish a link between process intent and final outcome. Every additional sensor adds value to the puzzle."*
>
> — ORNL data analytics scientist **Vincent Paquit**

As this process moves forward, it may allow printed parts to be used in critical applications, paving the way for in-depth analysis of every printed part that can be put directly into service, components that are "born qualified."

"I can clearly envision critical parts going on a plane, and the government requiring you to keep a record of everything that happened in the print chamber every single time," Paquit said. "The aerospace industry will validate every single object that comes out of a 3D printer. They will not fly anything that's not 100 percent certified for final use.

"Quality control will definitely not go away."

Accelerating biofuels development

A conversation with ORNL's Jerry Tuskan

by Stephanie Seay
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The new DOE Center for Bioenergy Innovation led by ORNL is focused on accelerating the development of specialty plants and microbial systems to support a biobased economy. ORNL Corporate Fellow Jerry Tuskan, CBI's director and chief executive officer, sat down with *ORNL Review* to discuss CBI's initial five-year mission and the legacy of biofuels research at ORNL.

What is CBI's mission?

CBI's mission is to accelerate the development of advanced biofuels for the displacement of transportation fuels such as gasoline. Our goal is to move the conversion of plant biomass into advanced gasoline drop-in substitutes like butyl acetate, or butanol, which have fuel properties similar to those of gasoline. This is different from the mission of the previous ORNL-based BioEnergy Science Center, which focused on ways to improve mostly ethanol production.

Another CBI difference is a concentration on new uses for lignin. Currently, lignin is the leftover portion of biomass used mostly to generate heat and steam to fuel the conversion of carbohydrates into alcohols. But there are potentially higher-value products from lignin. Lignin can be used to create advanced materials, and we have done a lot of work here using lignin to create carbon fiber. We now want to look at converting lignin into chemicals. Rather than using petroleum-based chemical precursors, we hope to create new plant-based precursors.

We will also be focused on sustainability as part of an effort to minimize competition with food crops. In a biobased economy, we will target the use of marginal lands not particularly well suited to agriculture, where you more commonly run into drought. We want to create bioenergy feedstock plants that will use water efficiently. Another element of sustainability is to create crops that are pest and pathogen resistant. If we develop a viable biofuels economy, we're looking at capturing 20 million to 40 million acres of marginal land, which will inevitably attract pests and pathogens.

What techniques will you use to accomplish these goals?

To create better bioenergy crops, we will leverage the genome-wide association study that we developed in poplar trees during BESC. This approach to studying an organism's genome allows us to link traits to the genes that cause variation in biomass quality or quantity. We have numerous examples of how that has worked successfully for ethanol production. We're now bringing

those same approaches to bear on increasing the value of lignin, producing butanol, and promoting sustainability.

On the conversion side, we're moving strongly into the concept of consolidated bioprocessing with cotreatment, that is, deconstructing biomass and fermenting resulting sugars all in one bioreactor. BESC discovered that if you apply minimal milling, or grinding, of plant material during the deconstruction phase, you can release greater than 90 percent of the sugar. As a result, we're developing and refining this process as our sole conversion platform.

Finally, on lignin, we're using a concept called biological funneling, where we take native lignin and use microbial biocatalysts to change it into high-value chemical precursors and feedstocks.

These three techniques encompass the main technical thrust of CBI, namely rapid domestication, or the rational engineering of plants and microbes for desired traits. We're applying techniques to rapidly domesticate our feedstocks (chiefly poplar and switchgrass), engineer microorganisms that perform consolidated bioprocessing, and advance microorganisms that will convert lignin to products.

Why is this mission important?

Much of the fossil fuels we use for transportation are derived from offshore sources that come with associated economic and fuel security tradeoffs. Our mission is important because we can displace some of our reliance on offshore petroleum. It's also important because we believe biofuels are easier on the environment, in terms of both production and consumption. Finally, the renewable energy sector of the economy is growing rapidly. CBI's success can result in more domestic jobs, particularly in rural areas.

Neutrons improve underwater welds

by Jeremy Rumsey
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Massive offshore structures like oil rigs and wind turbines are designed to withstand the myriad punishments oceans mete out. However, over time, just the saltwater itself can significantly decrease the durability of a structure's welds.

Zhenzhen Yu (left) and Michael Joachim Andreassen use neutrons at HFIR's Neutron Residual Stress Mapping Facility to investigate residual stresses expected to occur in the welds of offshore underwater wind turbine foundations. Image credit: Genevieve Martin, ORNL

That's why professors Michael Joachim Andreassen from the Technical University of Denmark and Zhenzhen Yu from the Colorado School of Mines are using neutron analysis at ORNL to validate a more advanced method of welding that involves high-power lasers.

Neutrons have highly penetrating properties—more so than X-rays—and can probe almost any material in a nondestructive fashion. The Neutron Residual Stress Mapping Facility at ORNL's High Flux Isotope Reactor enables researchers to study the quality of their welds at the atomic scale. The team's findings could lead to faster, more cost-effective production methods, as well as significantly stronger, longer-lasting welds.

"We're studying residual stresses in really huge structures," said Andreassen, "especially supersized monopiles—enormous steel cylinders that form the underwater foundations for wind turbines. We want to look at the relationship between residual stress and varying thicknesses in the steel plates used in construction by comparing two different welding methods."

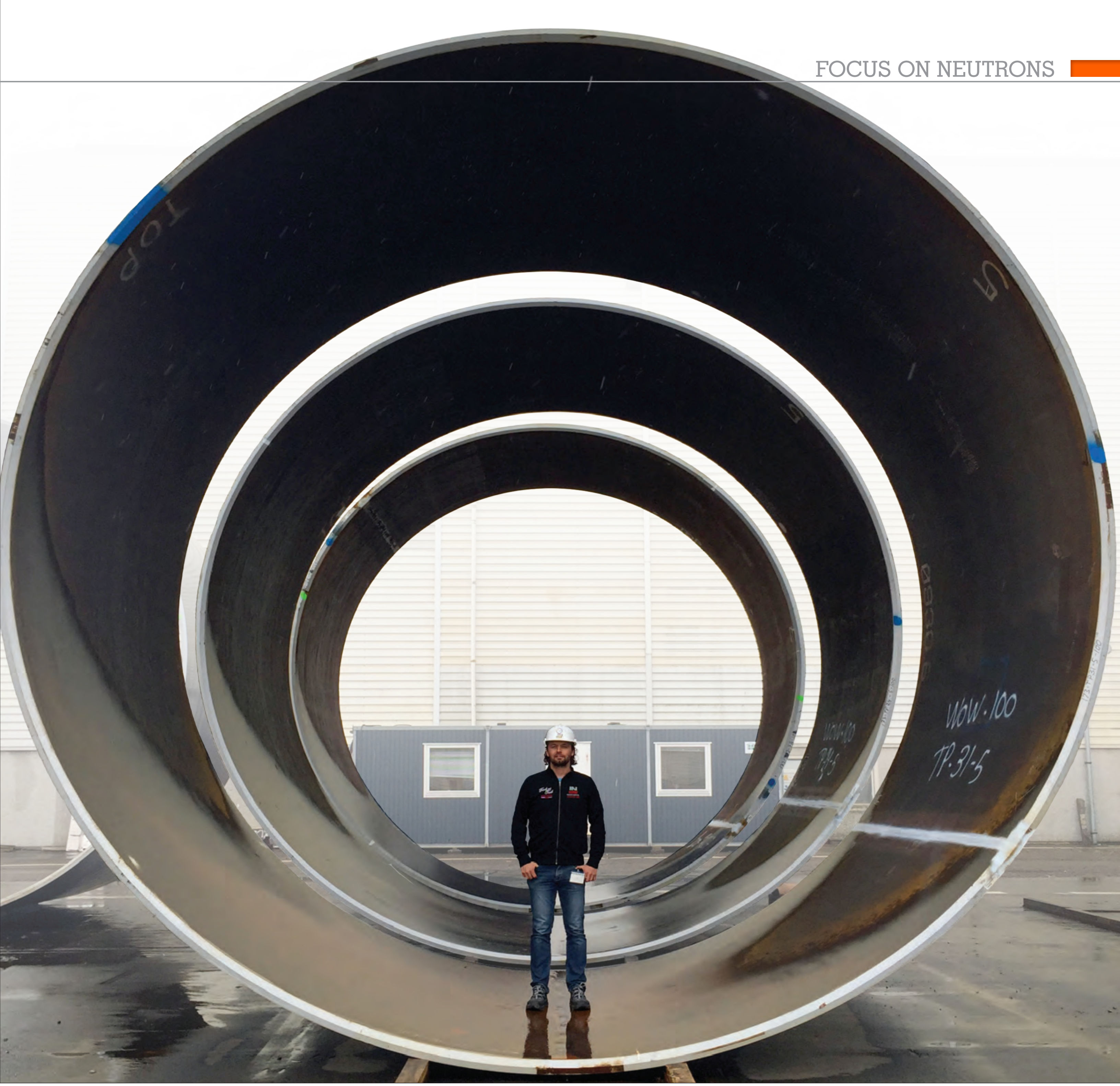
In general, residual stresses are stresses that remain in the weld's structure after applied loads or pressures have been removed. In some cases, residual stresses lead to premature failures like cracks or leaks. They can be caused by several factors, such as fluctuations in temperature, exposure to harmful chemicals, or metal fatigue resulting from repeatedly applied loads.

The steel plates used to build monopiles can be up to 130 millimeters thick, Andreassen said. They are typically welded together using a traditional method called submerged arc welding, where electric arcs are used to melt the joining materials. The weld's molten seam, or weld pool, is continually "submerged," or covered, in a granular flux of various compounds used to support the weld and protect it from atmospheric contaminants.

There are a variety of benefits to submerged arc welding. Among other things, the technique produces fewer impurities, sparks and toxic fumes than similar methods produce. However, said Andreassen, there are significant burdens, too.

"You have to remove a lot of material to do the weld and then add filler material after. It costs a lot to remove and add the materials, and in the end you have a really huge groove with a lot of introduced residual stresses," he explained.

Naturally, the more tensile residual stresses there are, the more susceptible a weld will be to failure.



Michael Joachim Andreassen from the Technical University of Denmark stands in one of the steel sections that are fused together with circumferential welds to build a monopile foundation. Image credit: Louis Andersen, Technical University of Denmark

"The hybrid laser-arc welding technique introduces a more focused heat source that allows us to mitigate residual stress," Yu said. "In the ocean, saltwater eventually creates corrosion, and if you have high degrees of tensile residual stress, the faster corrosion occurs and the greater the likelihood of fractures or cracks propagating through welded regions."

Neutrons provide an extraordinarily detailed picture of how the atoms are behaving deep inside the welds, comparing residual stresses from both the submerged arc and hybrid laser-arc samples. The neutron measurements show any changes in residual stress as Andreassen and Yu increase the steel plate sample sizes from 10 to 20, 40 and finally 60 millimeters thick.

"The reason we like neutrons for this research is because it's the only technique that can penetrate through the steel plates to give us a complete profile of the residual stress," Yu said. "We will use the neutron data and compare it with simulation work from Michael's group that we can apply directly to the actual structure."

Neutron tool

captures catalysis in the act

by Elizabeth Rosenthal
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ORNL scientists and collaborators recently created equipment allowing them to study catalysis in progress at the lab's Spallation Neutron Source.

With the help of colleagues from ORNL and Colorado State University, ORNL's Daniel Olds and Katharine Page developed a U-tube gas flow cell that can study catalysts and demonstrate how they facilitate chemical reactions under realistic operating conditions. Image credit: Genevieve Martin, ORNL

Catalysts are materials that facilitate chemical reactions without being consumed by them, with applications from refining petrochemical products and purifying gases to processing fuel and preparing food.

According to the North American Catalysis Society, catalysts contribute to more than a third of the gross domestic product worldwide and represent a $12 billion market in the United States alone. As a result, understanding the material properties and optimizing the performance of catalysts during industrial processes is a high priority in the scientific community.

Traditional research approaches examine catalysts and other products before or after the catalytic reaction has taken place, but not during the reaction. A team of scientists from ORNL and Colorado State University developed a U-tube gas flow cell capable of studying the atomic structure of these materials in real time. Using neutron scattering techniques, experiments mimic real-world conditions with industrial relevance—like catalytic converters in vehicles—to provide insights into the impermanent relationships between catalysts and reaction products.

"If we want to understand the limits of current technologies and help design new and better materials, we have to understand why they work," said Daniel Olds, a postdoctoral researcher at SNS.

Neutrons can probe light atomic species, such as those commonly found in industrial gas streams, even when they are hidden in a heavy-atom catalyst structure. This sensitivity, combined with the ability to differentiate between isotopes, makes neutrons a valuable resource for studying gas–solid interfaces between a catalyst and a material sample.

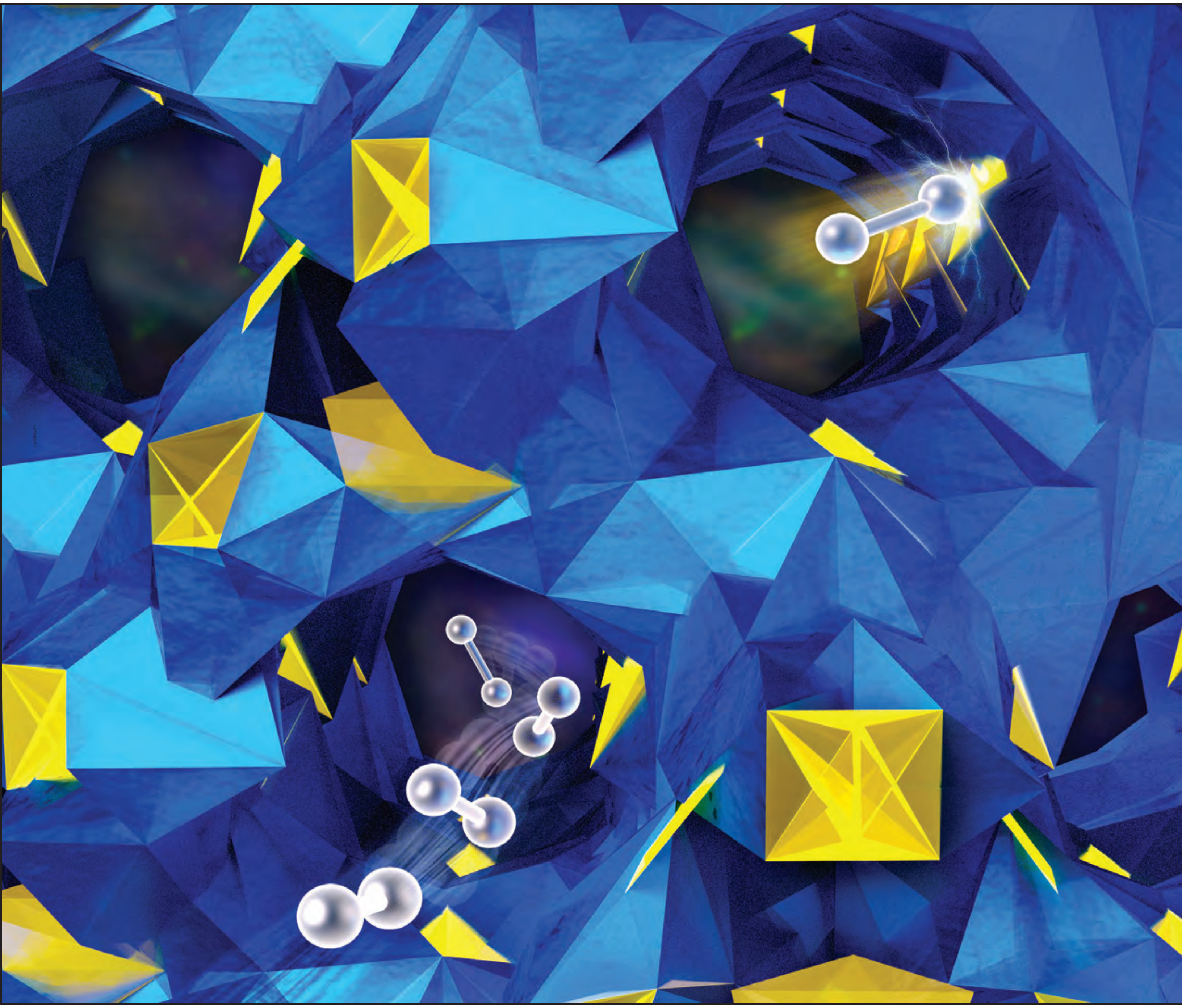
Using the gas flow cell, the team created a sample environment at SNS's NOMAD instrument, where users can harness these abilities to examine catalytic reactions under realistic operating conditions.

"Diffraction techniques can probe changes to the catalyst itself, but the interaction of the catalyst with the entity you're catalyzing is often very difficult to probe," said NOMAD instrument scientist Katharine Page.

Simultaneously using neutron powder diffraction and the steady-state isotope transient kinetic analysis technique, the team studied the interaction of an adsorbing gas with a packed bed reactor of the mineral zeolite-X, a common commercial catalyst.

A high-speed valve in the flow cell allowed switching between different gases so their impacts on the reaction could be observed, while a residual gas analyzer measured gas coming off the sample. Combined with results from the diffraction and transient kinetic analysis methods, this data helped locate areas of interest while filtering out nonessential information.

Alternating between different isotopes of nitrogen, the team used



Depicted as translucent moving diatomic molecules, nitrogen flows through the crystalline framework of the catalyst zeolite, represented by the blue geometric structure. Neutrons can identify the active calcium adsorption sites (illustrated in yellow) found along the largest channels of the structure.
Image credit: Jill Hemman, ORNL

neutron diffraction to identify the atomic-level adsorption sites of the gas in the zeolite molecular framework. The uninterrupted gas flow kept the sample in the steady-state reaction required to perform measurements.

"We were able to see this signal that you would be hard pressed to find any other way, and it was not easy," Olds said.

The researchers described their work in a 2016 study titled "A high precision gas flow cell for performing in situ neutron studies of local atomic structure in catalytic materials," published in the journal *Review of Scientific Instruments*.

"The gas flow cell project generated a whole new class of sample environment capabilities," Page said. "And as we expected, users are already taking advantage of this new resource."

Peatlands hold carbon

even in warming environment

by Stephanie Seay
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Two years into a decade-long field experiment, ORNL scientists and their collaborators have found that ancient carbon buried deep inside northern peatlands is resistant to release even as the soil warms.

ORNL is leading the Department of Energy, Office of Science, project called SPRUCE—for Spruce and Peatlands Responses under Changing Environments—to gauge the ecosystem's sensitivity to future conditions, both plausible and extreme. Peatlands are of particular interest because they hold an estimated third of the world's carbon despite occupying only 1.5 to 3 percent of the Earth's surface.

Because peatlands store so much carbon, the concern is whether they will release significant amounts of carbon dioxide or methane—the latter being a more potent greenhouse gas—under changing conditions.

To undertake the study, ORNL scientists designed 10 open-top enclosures, 12 meters across and 8 meters tall, into which warmed air and elevated CO_2 are injected into the atmosphere and the soil is warmed to a depth of 2 to 3 meters. The enclosures sit atop deep collars isolating the belowground water supply. The full experiments occupy a 7-acre plot in the U.S. Forest Service's Marcell Experimental Forest in northern Minnesota (see Infographic, Page 22).

Scientists from 30 institutions are working with ORNL to explore the peatlands' fundamental response to four different temperature conditions—ranging from 2.25 to 9 degrees Celsius—with and without elevated levels of atmospheric CO_2. In addition, two enclosures serve as controls, with no artificial warming or added CO_2. The system is designed to provide whole ecosystem warming, using both underground heat and atmospheric warming from the elevated CO_2 levels.

"We built a system to study peatlands, from the bottom of the peatland's microbial system to the tops of trees, that gives us a glimpse of what various futures might be like as temperatures increase," said ORNL environmental scientist Paul Hanson, the project's coordinator.

The scientists use automated systems at half-hour intervals to measure environmental characteristics such as soil and atmospheric temperatures, light and moisture levels, wind speed and direction, and levels of CO_2, methane and other gases. They use periodic measurements to study plant growth and survival, microbial community activity and composition, peat decomposition, and ecosystem biogeochemical and hydrologic functions.

"We are running the experiment 365 days a year, 24 hours a day, maintaining constant differential temperature treatments. That is unusual; other experiments having limited infrastructure might only be warmed when the sun's up. We're also doing it in such a way that we retain seasonal temperature patterns," Hanson noted.

As detailed in a recent issue of *Nature Communications*, SPRUCE scientists found only surface peat, less than 30 centimeters deep, to be responding to elevated temperatures, while deeper reserves of ancient peat were unaffected even after being warmed by 9 degrees Celsius in the first 13 months.

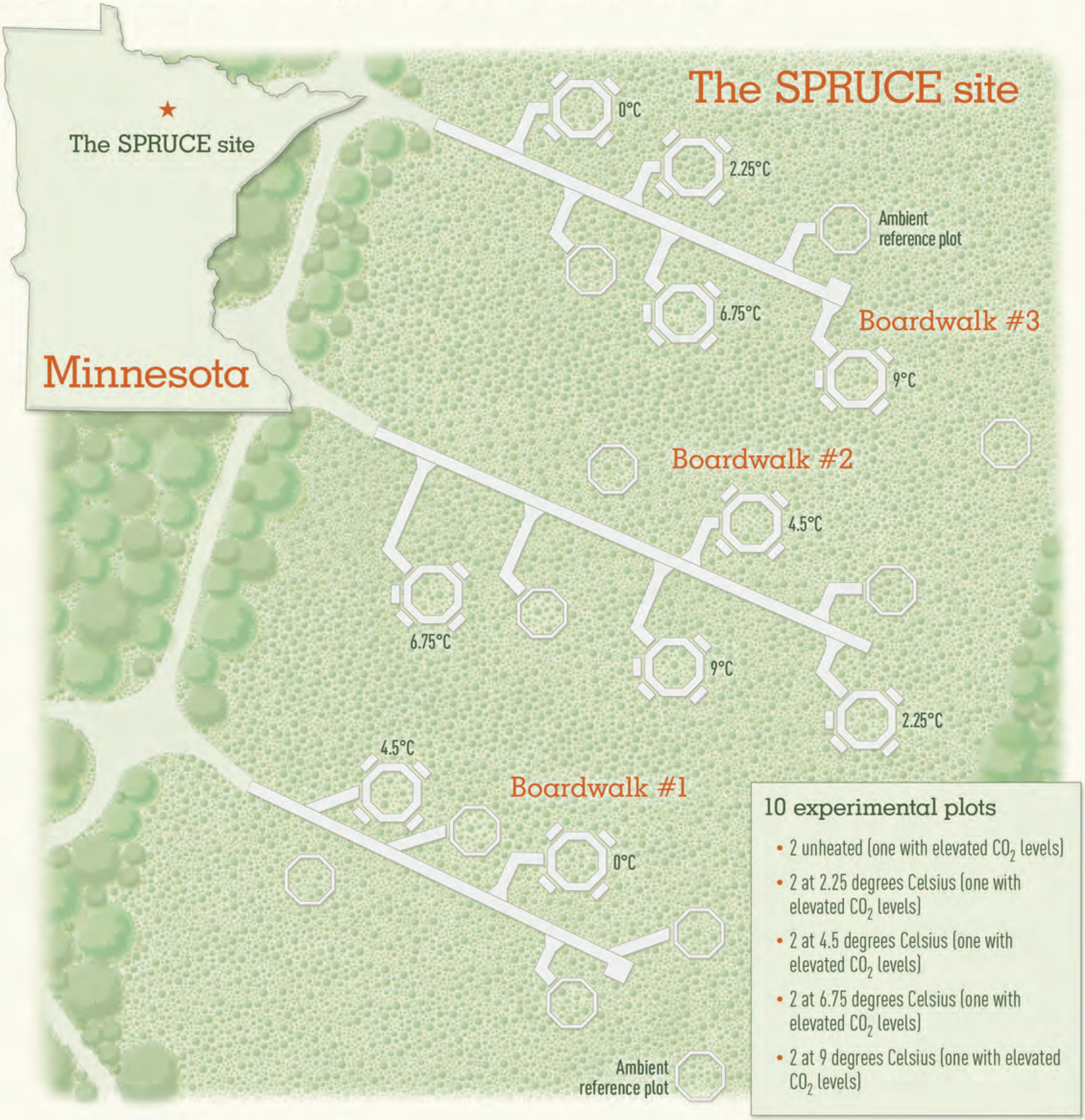
The end of the 2017 growing season marks two years of whole-ecosystem warming, and the deep stores of carbon have maintained insensitivity to changing conditions so far, Hanson said.

"The experiment is giving us exactly what we wanted as a footprint for studying future conditions of this important, understudied ecosystem," Hanson said. "After just a few years, we are able to conclude that the ancient carbon in these peatlands is not highly sensitive to warming in the short term. That's a big deal, because it demands that earth system models capture this new result."

Hanson added that there is a possibility that belowground communities may adjust themselves to the new conditions and change their activity through time, so ORNL scientists will continue to sustain the manipulations and take measurements over a full decade. He also clarified that the findings are specific to the temperate SPRUCE peatland and could be different in other high-carbon ecosystems such as those occupying permafrost areas farther north.

What will happen to peatlands as they warm?

Peatlands occupy from 1.5 to 3 percent of the Earth's surface, yet they hold about a third of the world's carbon. The Spruce and Peatlands Responses under Changing Environments project, better known as SPRUCE, is a 10-year experiment in Minnesota that will help us understand the fundamental response of peatland ecosystems and the organisms within them to warming environments with and without elevated CO_2.



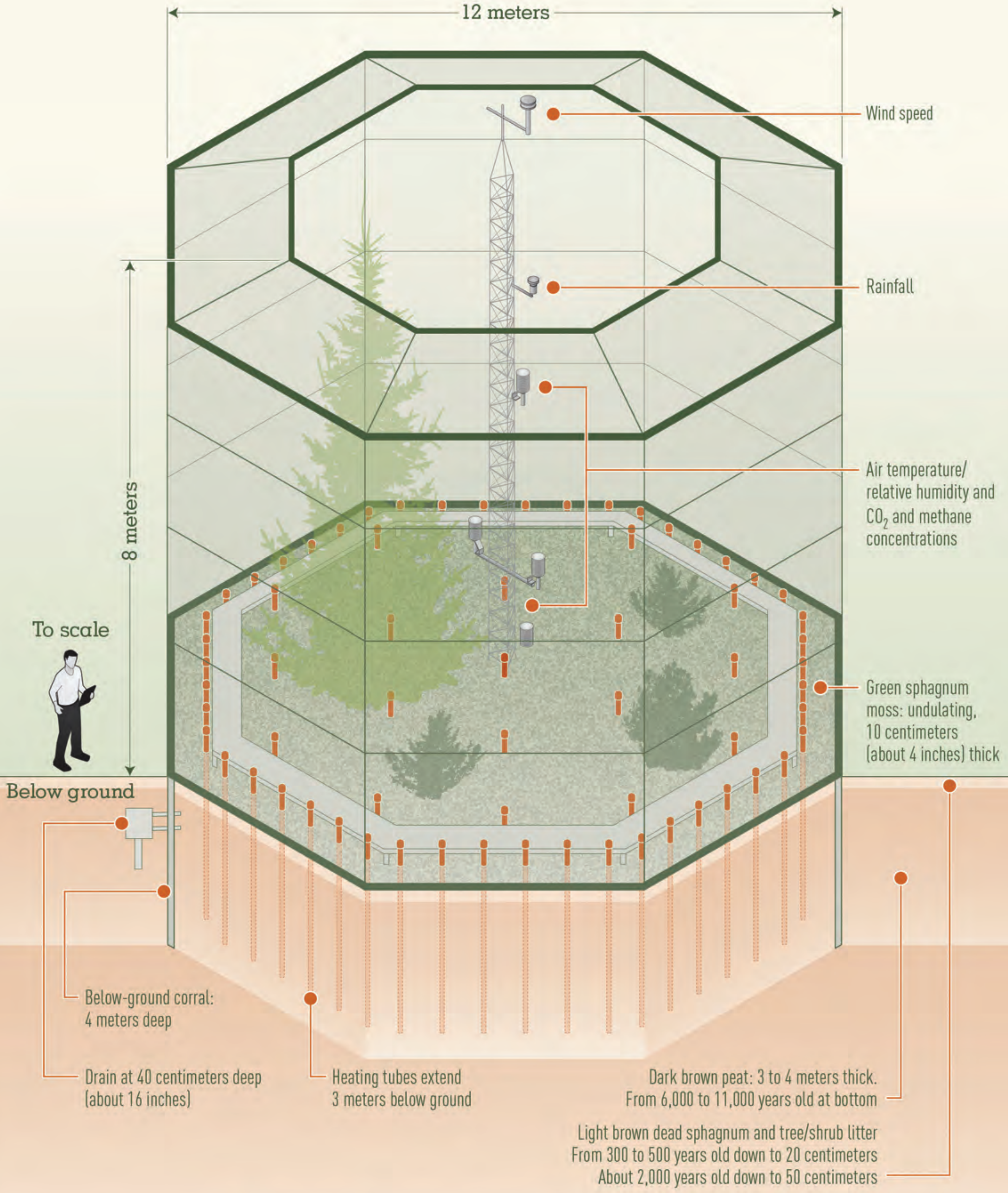


Image credit: Brett Hopwood, ORNL

Typical warmed enclosure

World's smallest neutrino detector confirms prediction from Standard Model

by Dawn Levy
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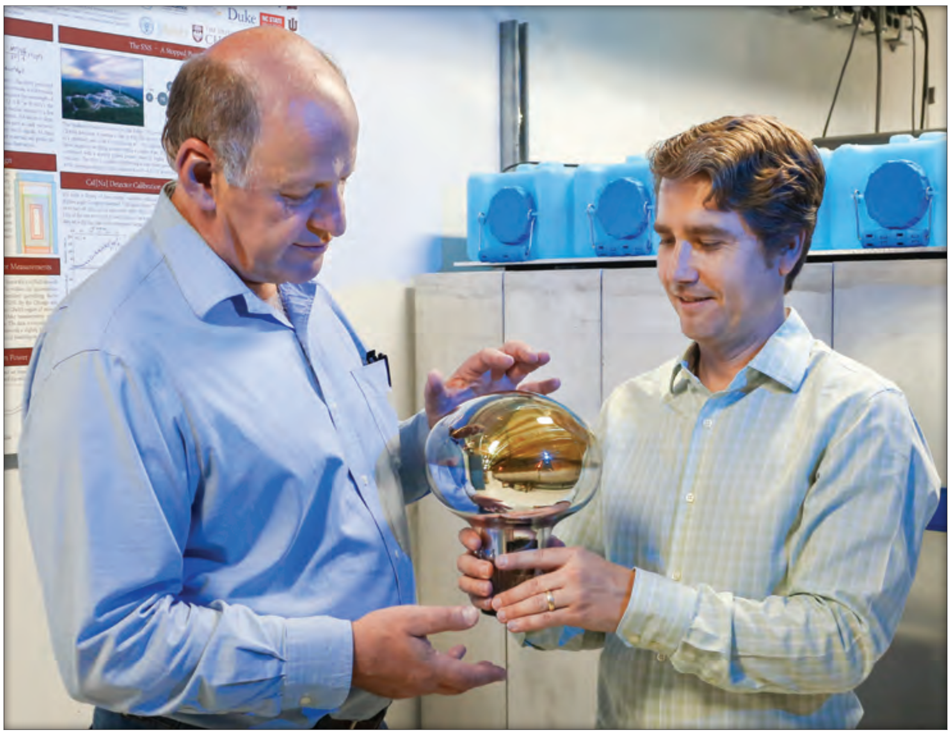
After more than a year of operation at ORNL, the COHERENT experiment, using the world's smallest neutrino detector, succeeded in finding evidence of a process carried out by the elusive, electrically neutral particles, which interact only weakly with matter.

The research, performed at ORNL's Spallation Neutron Source, was published in the journal *Science*, where it landed on the cover. It provides compelling evidence for a neutrino interaction process predicted by theorists 43 years ago, but never seen.

"The one-of-a-kind particle physics experiment at Oak Ridge National Laboratory was the first to measure coherent scattering of low-energy neutrinos off nuclei," said ORNL physicist Jason Newby, technical coordinator and one of 11 ORNL participants in COHERENT, a collaboration of 80 researchers from 19 institutions and four nations.

Neutrinos are notoriously hard to detect. In fact, approximately 100 trillion neutrinos bombard your body each second without notice.

As it produces neutrons for scientific research, SNS also generates a torrent of neutrinos as a byproduct. Placing the detector at SNS a mere 65 feet from the neutrino source vastly improved the chances of interactions and allowed the researchers to decrease the detector's weight to just 32 pounds.



Professor Yuri Efremenko of the University of Tennessee, left, and ORNL's Jason Newby are among 80 participants in COHERENT, a large, collaborative particle physics experiment to record neutrinos at the Spallation Neutron Source. Photomultiplier tubes that look like giant light bulbs are used to detect light from neutrino interactions in detectors. Image credit: Genevieve Martin, ORNL

> *"The energy of the SNS neutrinos is almost perfectly tuned for this experiment—large enough to create a detectable signal, but small enough to take advantage of the coherence condition. The only smoking gun of the interaction is a small amount of energy imparted to a single nucleus."*
>
> — ORNL physicist **Jason Newby**

In comparison, most neutrino detectors weigh thousands of tons. Although they are continuously exposed to solar, terrestrial and atmospheric neutrinos, these detectors need to be massive because their chances of interaction are more than 100 times lower than at SNS.

The scientists are the first to detect and characterize coherent elastic scattering of neutrinos off nuclei. This long-sought confirmation, predicted in the particle physics Standard Model, measures the process with enough precision to establish constraints on alternative theoretical models.

Typically, neutrinos interact with individual protons or neutrons inside a nucleus. But in "coherent" scattering, an approaching neutrino "sees" the entire weak charge of the nucleus and interacts with all of it.

"The energy of the SNS neutrinos is almost perfectly tuned for this experiment—large enough to create a detectable signal, but small enough to take advantage of the coherence condition," Newby said. "The only smoking gun of the interaction is a small amount of energy imparted to a single nucleus."

That signal is as tough to spot as a bowling ball's tiny recoil after a ping-pong ball hits it.

Physicist Juan Collar of the University of Chicago led the design of the detector used at SNS, a cesium iodide scintillator crystal doped with sodium to increase the prominence of light signals from neutrino interactions.

Success depended on finding the right combination of neutrino detector and source. "The detector was designed with SNS in mind," Collar said. "SNS is unique not only as a neutron source, but also as a neutrino source. It will provide us with opportunities for many more exciting sorties into neutrino physics."

Because SNS produces pulsed neutron beams, the neutrinos are also pulsed, enabling easy separation of signal from background. That aspect makes data collection cleaner at SNS than at steady-state neutrino sources such as nuclear reactors.

COHERENT saw three neutrino flavors—muon neutrinos that emerged instantaneously with the neutron beam, and muon antineutrinos and electron neutrinos that came a few microseconds later. "The Standard Model predicts the energy and time signatures we saw," Newby said. "Juan wanted to make sure that he chose a detection mechanism with the timing resolution to distinguish the prompt from delayed signals."

The Sept. 15, 2017, issue of Science. Image credit: Jean Lachat/University of Chicago. Reprinted with permission from AAAS

The calculable fingerprint of neutrino–nucleus interactions predicted by the Standard Model and seen by COHERENT is not just interesting to theorists. In nature, it also dominates neutrino dynamics during neutron star formation and supernovae explosions.

"When a massive star collapses and then explodes, the neutrinos dump vast energy into the stellar envelope," said Duke University physicist Kate Scholberg, COHERENT's spokesperson. "Understanding the process feeds into understanding of how these dramatic events occur."

For more information: https://go.usa.gov/xnx3J

Predicting flood wave behavior with 3D models

by Rachel Harken
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Heavy rainfall can cause rivers and drainage systems to overflow and dams to break, leading to floods that damage property, roads and other infrastructure, and that sometimes take human life.

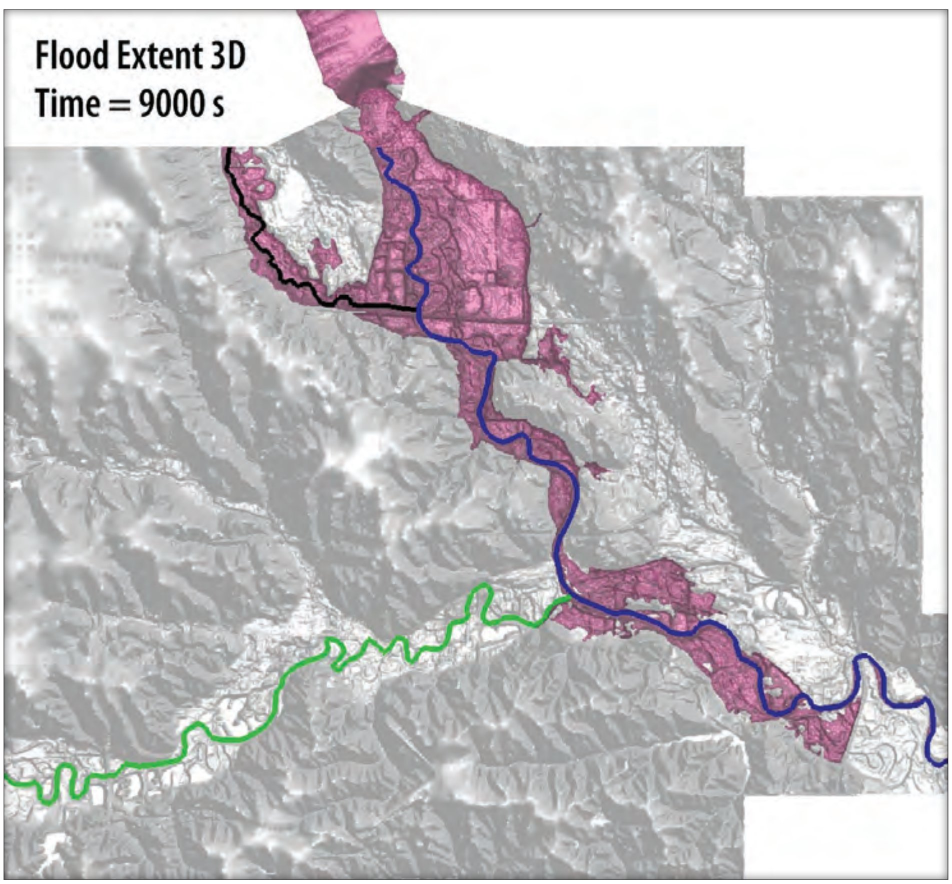
A 2008 storm cost $10 billion across Iowa and led to creation of the Iowa Flood Center at the University of Iowa, the country's first center for advanced flood-related research and education.

Today, simplified 2D flood models are the state of the art for predicting flood wave propagation, or the spread of floods across land. A team at the flood center led by Iowa Professor George Constantinescu is creating 3D nonhydrostatic flood models that don't make simplified assumptions about vertical pressure distribution in flows. Because of this, they can more accurately simulate flood wave propagation and account for the interaction between the flood wave and large obstacles such as dams or floodplain walls.

These 3D models can also be used to assess and improve the predictive capabilities of the 2D models that government agencies and consulting companies use for predicting the spread of floods and associated hazards.

Using ORNL's Titan supercomputer, Constantinescu's team performed one of the first highly resolved, 3D, volume-of-fluid Reynolds-averaged Navier–Stokes simulations of a dam break in a natural environment. RANS is a widely used method for modeling turbulent flows, while the volume-of-fluid method in the team's software allowed the researchers to track the position of the water's free surface—the areas where water meets the air. This combination of modeling tools enabled the team to map precise water levels for actual floods over time.

The team's 3D simulations showed that commonly used 2D models may inaccurately predict some aspects of flooding, such as the timespan over which dangerous flood levels last at certain locations and the amount of surface area flooded.



Visualization of a flood wave propagation simulation for the Saylorville Dam in Iowa at 9,000 seconds. The blue lines indicate the main channel of the Des Moines River, while the black and green lines indicate the positions of the two main tributaries: Beaver Creek and Raccoon River. Image credit: George Constantinescu, University of Iowa

The Coralville Dam on Coralville Lake overflowed into its spillway during the Iowa flood of 2008. The flood cost Iowa $10 billion due to the overflowing of the Iowa and Cedar Rivers. Image credit: U.S. Army Corps of Engineers

Simulation results also demonstrated that 2D models may underestimate the speed at which floods spread and overestimate the time it takes for flood waves to reach their highest point.

"We need to know what's going to happen for situations in which a dam breaks," Constantinescu said. "We need to know who's going to be affected, how much time they will have to evacuate, and what else might happen to the environment as a result."

Because 2D models make simplified assumptions about some aspects of the flow, they can't account for changes in it, such as when the flood wave moves around large obstacles, rapidly changes direction, or fully immerses bridge decks.

Using a fully nonhydrostatic 3D RANS solver, the team performed the first simulations of the hypothetical failure of two Iowa dams: the Coralville Dam in Iowa City and the Saylorville Dam in Des Moines. The researchers also computed the same dam break test cases using a standard 2D model commonly used by the flood center. When they compared the 2D results against those of the 3D simulations, they found that the 2D model underestimated how quickly the flood wave moved across land and overestimated the time it takes for flood waves to reach their highest point.

"By performing these 3D simulations, we provided a huge data set that can be used to improve the accuracy of existing 2D and 1D flood models," Constantinescu said. "We can also examine the effectiveness of deploying flood protection structures for different flooding scenarios." The team ultimately showed that high-performance computing can answer engineering questions related to the consequences of structural failure of dams and related hazards."

Assembling life's molecular motor

by Jonathan Hines
hinesjd@ornl.gov

Despite the grand diversity among living organisms, the molecule used to store and transmit energy within aerobic, or oxygen-using, cells is, remarkably, the same. From bacteria to fungi, plants and animals, adenosine triphosphate, or ATP, serves as the universal energy currency of life.

ATP isn't just produced and consumed by the cell. It's also recycled, relying on a highly efficient molecular motor called ATP synthase to do the job.

As part of a project dedicated to modeling how single-celled purple bacteria turn light into food, a team of computational scientists from the University of Illinois at Urbana-Champaign used ORNL's Titan supercomputer to simulate a complete ATP synthase in all-atom detail. The work builds on the project's first phase—simulation of a 100-million-atom photosynthetic organelle called a chromatophore—and gives scientists an unprecedented glimpse into a biological machine whose energy efficiency far surpasses that of any artificial system.

"Nature has designed the chromatophore in such a way that it can generate enough ATPs for these bacteria to survive in low-light environments such as the bottom of ponds and lakes," said Abhishek Singharoy, an assistant professor at Arizona State University and coprincipal investigator of the project. "Our work captured this energy conversion process in all-atom detail and allowed us to predict its efficiency."

Often referred to as the power plant of the cell, ATP synthase is a complex enzyme that speeds up the synthesis of its molecular precursors, adenosine diphosphate and phosphate. Embedded within the chromatophore's inner and outer membrane, the enzymatic motor consists of three major parts—an ion-powered rotor, a central stalk and a protein ring.

> *"You could potentially genetically modify a chromatophore or change its concentration of proteins. These predictions promise to bring forth new developments in artificial photosynthesis."*
> — Arizona State University Assistant Professor **Abhishek Singharoy**

Similar to a waterwheel that's turned by the force of a flowing stream, the ATP synthase rotor harnesses the electrochemically spurred movement of ions, such as protons or sodium, from high concentration to low concentration across the membrane. The resulting mechanical energy transfers to the central stalk, which assists the protein ring in synthesizing ATP.

Remarkably, the process works just as well in reverse. When too many ions build up on the outer side of the chromatophore, the ATP synthase protein ring will break down ATP into adenosine diphosphate, a process called hydrolysis, and ions will flow back to the inner side.

"Normally you would expect a lot of energy loss during this process, like in any man-made motor, but it turns out ATP synthase has very little waste," Singharoy said.

Using Titan, the team identified previously undocumented swiveling motions in the protein ring that help explain the molecular motor's efficiency. Similarly, the team's simulations captured the rubber-band-like elasticity of the enzyme's central stalk. Singharoy's team estimated that when paired with the protein ring, the stalk absorbs about 75 percent of the energy released during hydrolysis.

Additionally, simulations of the protein ring by itself revealed a unit that can function independently, a finding reported in experiments but not in computational detail.

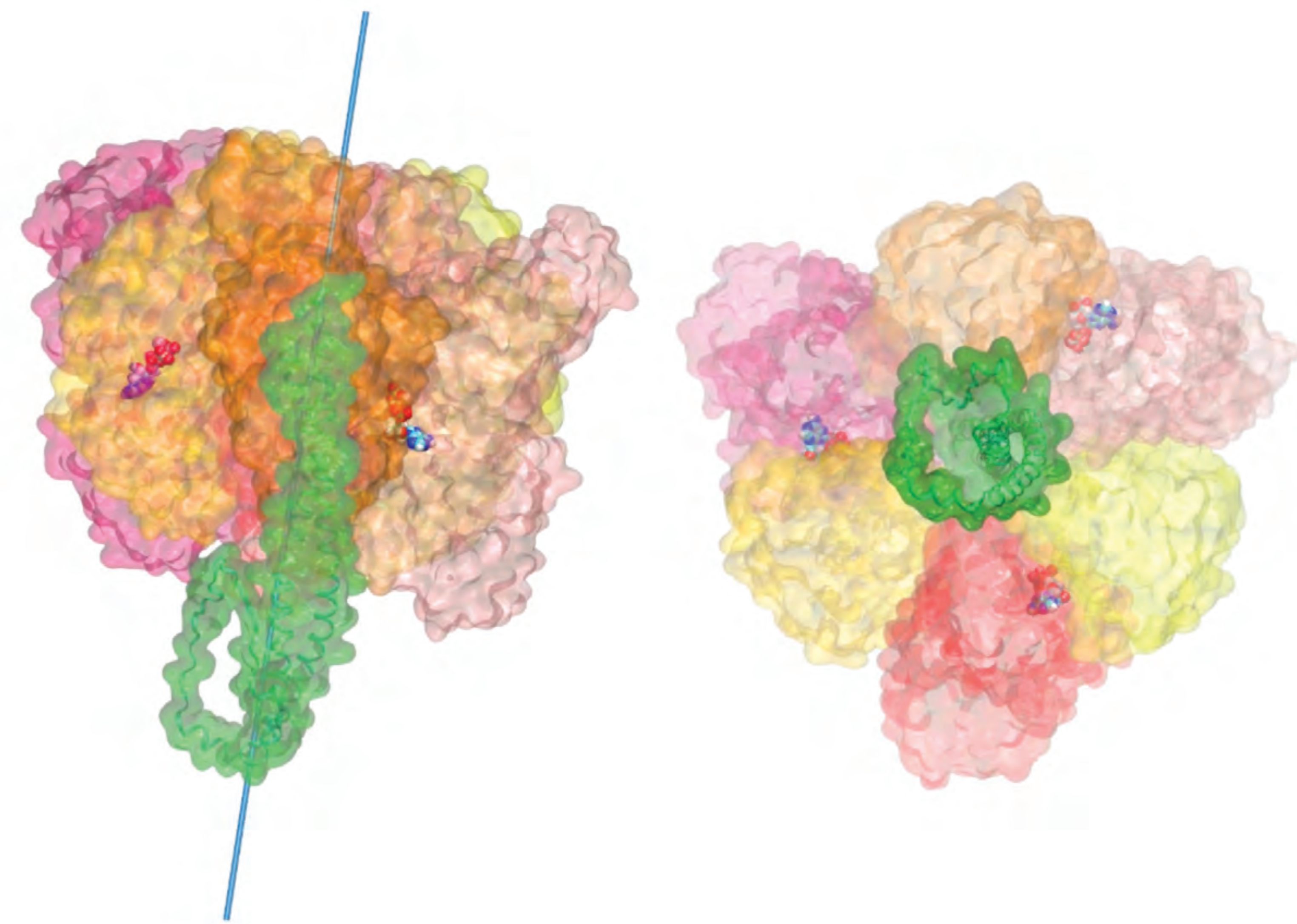
After simulating its complete ATP synthase model, the UIUC team went a step further, incorporating the enzyme into its previously constructed chromatophore model. With this virtual biological solar panel, the team measured each step of the energy conversion process—from light harvesting, to electron and proton transfer, to ATP synthesis.

Nature's chromatophore is designed for low-light intensity, absorbing only between 3 and 5 percent of sunlight on a typical day. The team found this absorption rate translates to around 300 ATPs per second, which is the amount a bacterium needs to stay alive.

Now the team wanted to see if it could improve upon natures design. Assuming the same amount of light intensity, the team designed an artificial chromatophore with a decidedly unnatural protein composition, boosting the presence of two types of specialized proteins. Analysis of the new design predicted a tripling of the photosynthetic system's ATP production, opening up the possibility for the chromatophore's human-guided optimization.

"You could potentially genetically modify a chromatophore or change its concentration of proteins," Singharoy said. "These predictions promise to bring forth new developments in artificial photosynthesis."

For more information: https://go.usa.gov/xRA2Y



ATP hydrolysis drives the central stalk in the V-type ATP synthase of the bacteria Enterococcus hirae.
Image credit: Barry Israelewitz, University of Illinois at Urbana-Champaign

How are elements made?

A conversation with physicist Kelly Chipps

As a young girl Kelly Chipps believed she would become a field biologist. Then, in her junior year of high school, she studied physics with a teacher so in love with the subject that Chipps fell in love with it, too. She dropped biology in her senior year, opting to take a more advanced, calculus-based physics course and has never looked back.

Chipps is one of four young researchers from ORNL to receive a 2017 Early Career Research Program award from DOE's Office of Science. She studies rare nuclei typically found only within exploding stars. She and her colleagues use beams of these nuclei produced at radioactive ion beam facilities. One such facility is DOE's Facility for Rare Isotope Beams, currently under construction at Michigan State University.

FRIB is the focus of Chipps' 2017 Early Career Research Program proposal, titled "Next-Generation Particle Spectroscopy at FRIB: A Gas Jet Target for Solenoidal Spectrometers." In this project she will work to overcome challenges in designing targets for nuclear reaction studies planned at the facility.

Chipps holds a bachelor's degree in engineering physics and a Ph.D. in applied physics from the Colorado School of Mines and has been an ORNL Liane B. Russell Fellow since spring 2015. We talked with her about her work and about what drew her to science. This is an edited transcript.

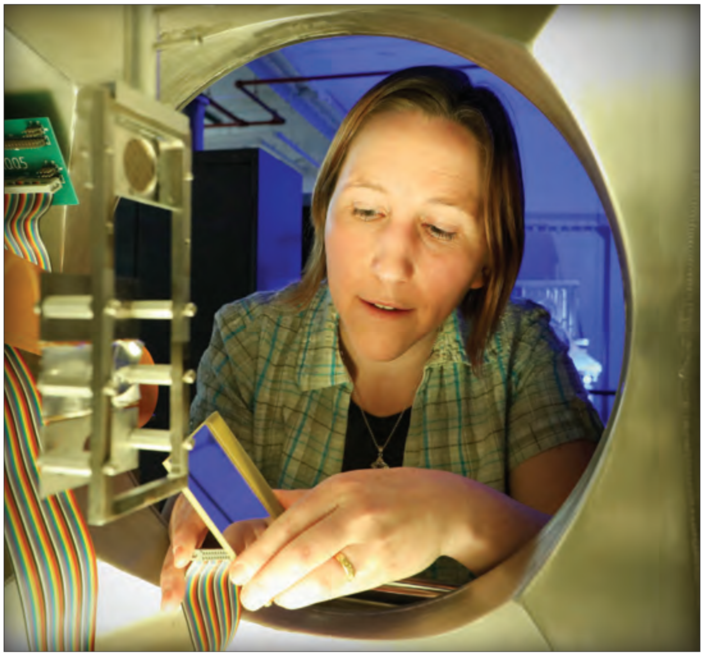
1. What do we learn from radioactive ion beam facilities?

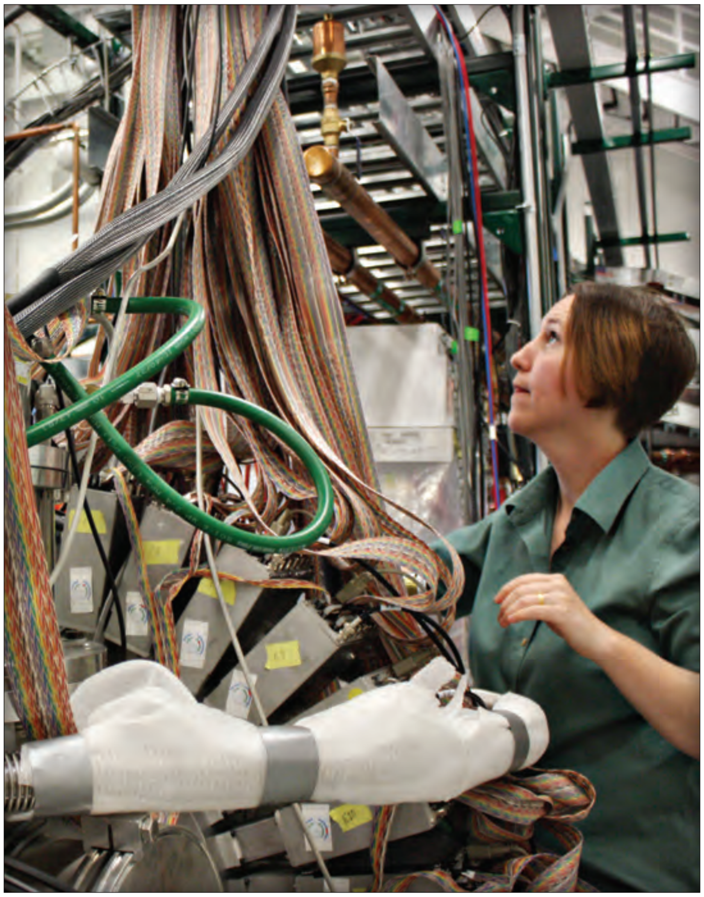
One of the outstanding questions in nuclear physics today is the origin of the elements. We have to understand the abundance patterns that we observe in the universe, and to do that we have to understand nuclear reactions that are taking place on stable and unstable nuclei. In explosive astrophysical events like supernovae, these unstable nuclei are being produced in tremendous numbers. And those are actually affecting the stable nuclei that we see on earth.

So we want to be able to study unstable nuclei, which means we have to produce them somehow in the laboratory. This is where radioactive ion beam facilities come in. A radioactive ion beam facility produces these exotic unstable nuclei and quickly delivers them to our experimental instruments, where we're able to study them.

2. What challenges are you working to overcome at FRIB?

There are three main ingredients to doing a nuclear reaction study. First is the radioactive ion beam. Second is the suite of detectors that we use to observe the reaction products. And third is the target, which is the material we use to induce the nuclear reaction of interest. In astrophysical events like





supernovae, you have a lot of hydrogen and helium, and we're having a lot of nuclear reactions taking place on those elements. So we want to produce a target of those gases.

Previously I worked to develop a supersonic gas jet target to improve how we're able to study radioactive ion beam measurements. What I'd like to ask now is: Can we take that optimized target and combine it with other state-of-the-art devices to further improve these nuclear reaction studies? This Early Career award is going to provide me the opportunity to see if we can combine a gas jet with a solenoidal magnetic field to improve the resolution and the signal to noise that we get in measurements of this type.

3. Why is this work important?

Let's take an example. In a supernova explosion, a lot of the synthesis of the elements we see passes through a particular unstable isotope: nickel-56. Nickel-56 is produced in abundance in supernovae, and yet we don't actually know very much about it experimentally. I'd like to take advantage of these advances in instrumentation to study the properties of nickel-56 and better understand to what extent it affects the supernova explosion. This will allow us to understand how that explosion is producing the elements that we see around us.

4. What made you choose a career in science?

I like to think of myself as a pretty even left brain/right brain kind of person, so when I got to the end of high school, I was faced with the decision of which of my many interests to pursue. I figured that it would be easier to be a scientist with a music hobby than a musician with a science hobby, so here I am.

Replicating the sun:

A conversation with fusion scientist David Green

David Green learned an important lesson about hard work as he pursued a bachelor's degree at the University of Newcastle in Australia. Namely, if he put in the effort to understand a difficult subject, that subject became less difficult and was sometimes even fun.

The subject at hand was physics, and Green was deciding whether he wanted to turn it into a career. The eventual answer was "yes," and Green went on to earn his Ph.D. from the University of Newcastle and later landed at ORNL as a staff scientist.

His research focuses on developing the understanding required to enable fusion reactors, facilities that will generate electricity by heating a plasma to many times the temperature of the sun. Specifically, he uses computer simulation to study the magnetic confinement of fusion plasmas.

Green is one of four ORNL recipients of Early Career Research Program awards from DOE's Office of Science. His award-winning proposal was titled "Scale-Bridging Simulation of Magnetically Confined Fusion Plasmas." We asked him about his proposal and his choice of a career in science. This is an edited transcript.

1. Why do you simulate the magnetic confinement of fusion plasmas?

In magnetically confined fusion, we're really trying to take the process that drives the sun and replicate it inside a laboratory vessel. As you can imagine, the environment in there is pretty extreme; just sticking a probe in to measure what's going on doesn't always work out. So we have a whole field of diagnosticians coming up with clever ways to figure out what is going on inside a fusion device.

Even with all that, we don't have a complete picture of what's happening in there. So that's where computer simulation comes in. If we have a computer model—a set of equations that describe what happens—and we solve those equations, then we have all of the information within the assumptions of the model and the uncertainties of that calculation.

We also have something happening in parallel—this increasing computational power that's available—here we have massive supercomputers, but I'm sure everybody's familiar with computing power continuing to go up. What that translates to for fusion and computational physics in general is removing more and more of the assumptions you have in your model, so the computer model gets closer and closer to reality. So the simulations are providing a lot of information that you might not be able to get at experimentally, which is why we simulate the fusion environment. And I think simulation now has become one of the key thrusts that are required to advance fusion.

2. What do you hope to achieve with your Early Career award project?

The Early Career award is focused on solving one aspect of the computer simulation problem. A fusion plasma is what we call a multiscale system. It has spatial scales from the micron or smaller level up to a several-cubic-meter level. Those physics scales can interact with each other. The spatial part of that—small and large scales—is something we've been able to solve with computer simulation for a while. You simply parallelize the problem. You take a large computer, and you say one node of that computer works on one piece of the problem and another node works on another piece, and if you get a big enough computer, you can parallelize your way to a solution.

But a fusion plasma also has multiple timescales present. What that means is you have some really fast timescales—nanoseconds, microseconds—impacting things that happen at the observable timescales. We can't just parallelize our way out of that like we can with the spatial problem. If you want to predict what happens at some future time, you needed to know what happened in the past. So it tends to be a serial process.

The Early Career project is looking at applying some new applied math techniques that allow us to incorporate the physics of the fast timescale into simulations of the observable timescales.

3. Why is this research important?

Fusion devices cost a lot to build. We're still in the experimental stage, with multiple millions if not billion-dollar experiments; they take years to decades to build, depending on the scale. And with these large supercomputers we have here, there's an allure of using a large computer to simulate the whole device, and then you might be able to look at alternate configurations.

So trying to confine the plasma, we use a magnetic field or a magnetic bottle of a certain shape—you might want to investigate certain shapes. To do that experimentally would be cost-prohibitive. But doing that with a computer, if you had simulation capability, that would be something that you could do, hopefully in a cost-effective manner.

4. What attracted you to a career in science?

I like solving problems in general, the harder the better. It really wasn't until the end of my undergraduate studies in physics that I realized that if you put in some effort to solve what may have come across originally as something that was just unsolvable, when you actually do spend the time to learn and propose solutions, irrespective of what the problem is, I get a great deal of satisfaction in solving those sorts of things.

What keeps me in science is the same thing. Working at a national lab, you have experts in just about everything. Any question you want to ask, there's someone around who will know more about it than you will, so the scale of problems we can solve here is pretty fantastic. So for someone who enjoys solving problems, this is a good place to be.

Understanding atomic structure and function:

A conversation with condensed matter physicist Zac Ward

What does condensed matter physics have in common with hitchhiking around the world? For ORNL's Zac Ward, the answers would include "new experiences" and "uncomfortable challenges."

Ward discovered physics after earning a bachelor's degree in English literature, teaching a year in Japan, and doing a lot of traveling. He went back to school, picking up a bachelor's degree in physics from the University of Missouri and a Ph.D. in physics from the University of Tennessee. He arrived at ORNL in 2009 as a Eugene Wigner Fellow.

Ward won a 2017 Early Career Research Program award from DOE's Office of Science for his proposal "Designing Metastability: Coercing Materials to Phase Boundaries." We talked with him about the project and what drew him to a career in science. This is an edited transcript.

1. What draws you to condensed matter physics?

Experimental condensed matter is a fun area of physics to work in. My typical day includes working at vacuum pressures lower than near Earth orbit, shooting things with lasers and X-ray beams, and working at temperatures just above absolute zero. If I have an idea, but there isn't currently a way to measure that idea, I get to design and build something that can do it. Then, collecting the data and being the first person to have seen a particular behavior which gives a new insight into how the world works is great.

Being at ORNL is especially nice. If you have an idea that requires expertise that you don't have, you can just walk down the corridor, knock on a door, and find somebody that is a leading expert in whatever that may be. So we can flesh out what we need to do to solve whatever the question is.

2. Tell us about your project.

The way that materials behave—Are they magnetic? Are they resistive? Are they structurally strong?—can be simply thought of as a response to what the electrons in a particular material are doing. The electrons are part of the atoms. Controlling the atoms' arrangement to one another changes where the electrons reside and how they interact with one another. If we can control the atomic structure, we can then manipulate what the electrons are doing. By studying the relationship between structure and function, we can then gain a deeper understanding of the electronic correlations that drive complex materials.

My project aims to understand how electrons behave and how they talk to each other in functional materials where the electrons are strongly correlated with one another. We have recently discovered a way to control structural symmetry in these materials using noble ion implantation. This method allows us to arrange the atoms in ways that nature wouldn't normally permit. This should allow new insights into how these materials generate functionally important properties while giving us a means to control them in a simple way. This can then lead to new types of sensing, energy conversion, or computing applications.

3. Why is this research important?

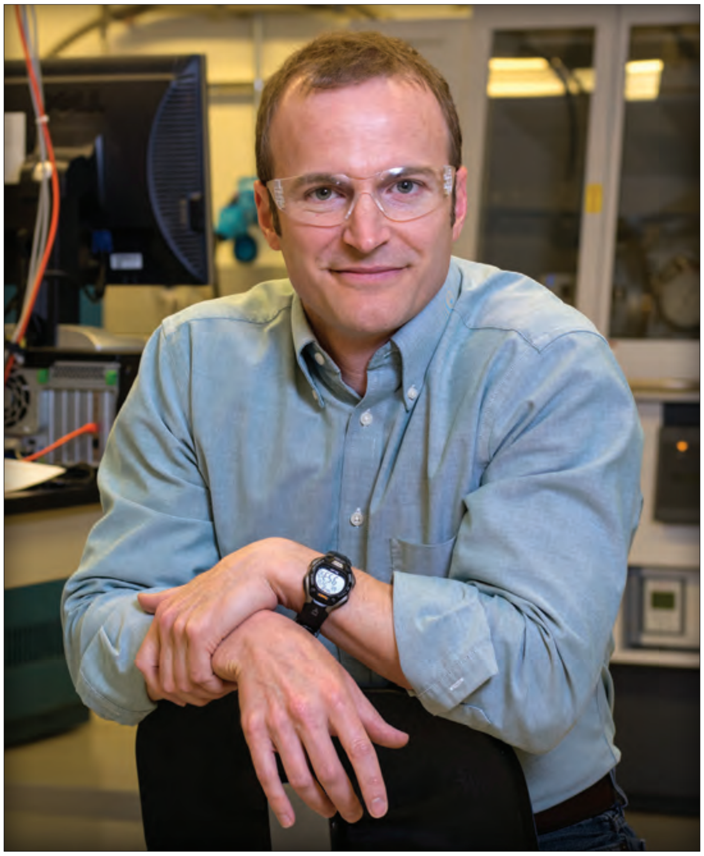
It's fundamental science. We don't know exactly what's going to come from it, other than we will know more about how things work after doing the research. The promise of learning something new is the important part for me. It would be great if I could tell you that the work's ultimate importance is that it will spawn a new industry, cut our country's energy consumption by 80 percent, and cure aging. But I can't.

Fundamental science is the base over which all of our technologies grow. So that's what this project is. It's a way of going in and fertilizing the ground, and hopefully something useful grows out of that. The importance is just learning new properties and learning how things work, and then from that something great may come. But there's no way to tell what that is yet. What I can tell you is that there is a fundamental project being funded right now that will spawn the next billion dollar industry. Maybe it's this one. Maybe it's a different one.

4. What attracted you to a career in science?

I spent quite a bit of time traveling and wandering around before getting into physics. What I realized is, as far as traveling goes, everything's been discovered. So you can go out and put yourself in uncomfortable situations, and learn something about yourself, but if you want to be the first person to go somewhere in the world, it's pretty much impossible now.

So this is one thing that physics did. I found that you can go into your own lab, have an idea about something, and be the first one to see a property and be the first one to do something and share that with other people. That's what really drove me toward this career.



Understanding how organisms work together:

A conversation with biologist David Weston

David Weston has been drawn to the natural world since he was a child exploring a small forest near his home.

Turning that fascination into a science career, he has examined topics such as plant genomics and the relationship between plants and the organisms in their environment. Weston has bachelor's and master's degrees in plant biology from Cornell University and a Ph.D. in biology from Clemson University. He worked at ORNL as a postdoc before joining the lab's research staff in 2009.

Weston won a 2017 Early Career Research Program award from DOE's Office of Science for his proposal "Determining the Genetic and Environmental Factors Underlying Mutualism Within a Plant–Microbiome System Driving Nutrient Acquisition and Exchange." We talked with him about the project and about what drew him to a career in science. This is an edited transcript.

1. What will you be studying in this project?

I'll be studying, at a very fundamental level, symbiosis, the question of how two organisms with very different physiologies—very different genetic backgrounds—interact in a way in which both benefit.

The system we're using is a small plant. It's called sphagnum peat moss. The living part is only a few centimeters high. It doesn't even have any roots. But yet it has a lot of open cells that allow bacteria to colonize, and these bacteria colonize often in a symbiotic fashion, meaning they'll take nitrogen from the atmosphere and provide it to the plant. In return, the plant provides sugars back to these bacteria, and together they seem to grow in a beneficial manner.

2. How do you plan to conduct this research?

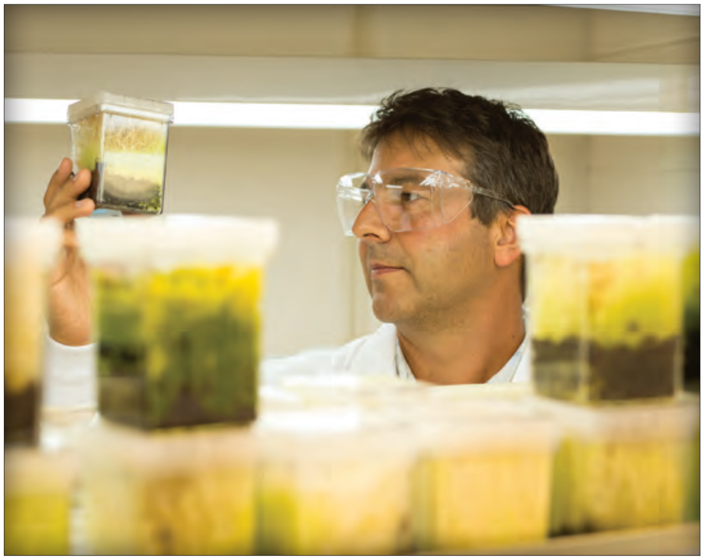
The research is going to take place in two separate areas. In the first area we're going to use a system called synthetic communities. Here we have created a population of moss plants that all have their genomes sequenced.

So we have a bunch of plants that are different genetically. We also have a bunch of microbes and nitrogen-fixing bacteria that are very different. And then we're going to put these plants and microbes together. In these synthetic communities we're going to ask questions regarding what the underlying genetic and environmental basis is for these organisms to operate together. But I think just as importantly, we're interested in how you can change this so that the organisms break apart. Are there certain combinations that are harder to break apart than others? If so, why?

What we hope to get from that synthetic community are these rules or principles by which the symbiosis operates. And then we want to see if we can observe those rules, or the behavior of those rules, under natural field settings. So we have field sites that we will be investigating, as well.

3. Why is this work important?

I'm lucky. I'm working in a system which has impact at an ecosystem, landscape and even global scale. This is nice, because as a scientist you can really get into the weeds of discovery and forget about what the real implications of your research are. Just finding something new is interesting, but in this case we have impact.



In particular, the moss we're looking at and the microbes that we're investigating reside in peat bogs or peatlands. And peat bogs in particular are only about 3 percent of the entire global land area, but they contain upwards of 25 percent of all the stored soil carbon. In these particular ecosystems, what happens is this plant material dies, and it goes into the ecosystem, where it stays in a recalcitrant form for many thousands of years. So it tends to create a large carbon sink.

Because sphagnum peat mosses are dominant members in many peat bog ecosystems, how they operate really dictates in large part how these ecosystems function. The idea is if these parts decline, it may change how these ecosystems function. What we worry about, of course, is that these large carbon sinks may eventually become a carbon source to the atmosphere.

4. What attracted you to a career in science?

That path has taken a couple of routes. From a really early age, I took to natural history. Being out in nature was always a great thing. And then, like many Americans, I had family members, especially a grandmother and aunt, who had a strong tie to gardening.

So on one hand I had this tie to nature from a natural sense as well as from an agricultural sense, but then on the other hand, I went to college during the time of the Human Genome Project, and there you're unlocking the discovery of biology through the genetic code of an organism.

Really what I ended up doing was putting these two systems together. So a lot of what I do is considered ecological genetics, or genomics, where we're tying these two disciplines together.

William D. Phillips is co-recipient of the 1997 Nobel Prize in physics, given for the development of methods to cool and trap atoms with laser light.

He works at the National Institute of Standards and Technology as leader of the Laser Cooling and Trapping Group within the institute's Quantum Measurement Division. The group pursues research in a variety of areas including laser cooling and trapping, Bose-Einstein condensation, atom optics, collisions of cold atoms and quantum information processing.

Phillips received a bachelor's degree in physics from Juniata College in Pennsylvania and a Ph.D. from the Massachusetts Institute of Technology. He is a member of the American Physical Society and the National Academy of Sciences.

Phillips delivered the Eugene P. Wigner Distinguished Lecture August 9, 2017, on the topic "At the Crossroads of Atomic and Solid-State Physics: Ultracold Atoms as a New Condensed Matter System." This is an edited transcript of our conversation following his lecture.

Distinguished

William D. Phillips

1. You shared a Nobel Prize in 1997 for developing the means to cool gases to a millionth of a degree above absolute zero using laser light. Why was this breakthrough important?

There are a number of reasons why it has become important to laser-cool atoms, but at the beginning we wanted to make better measurements on the atoms. I'm at an institute—the National Institute of Standards and Technology—that's all about measurement. Temperature is about motion. When something is hotter, it means the atoms and molecules making up that thing are moving around fast. When something is colder, it means those atoms and molecules are moving more slowly. If you want to make measurements on those atoms and molecules, it's a whole lot better if they're moving more slowly. The big motivation for us was to make better atomic clocks. The best clocks that there are, are clocks whose tickers are atoms because all atoms of the same kind tick at exactly the same rate, as opposed to manufactured tickers like pendula or quartz crystals, which all tick at slightly different rates. But when atoms are moving really fast, it's not so easy to measure their ticking rate, so our idea was to cool them down, make them more slow.

2. What new basic science discoveries/phenomena have been enabled by the study of ultracold atoms and materials?

One thing we learned in the process of cooling atoms was that the cooling process was not what we had thought. It was remarkable because it represented a violation of Murphy's law, which tells you that anything that can go wrong, will go wrong. Well, in this case we got lucky; laser cooling works better than it was supposed to, and as a result we were able to get our atoms much, much colder than the original theory told us was possible. So our original idea about how laser cooling worked was wrong; it was both more complicated and worked better as a result, which is another violation of Murphy's law because usually when something gets more complicated, it's not as good. Since then we have used laser-cooled atoms to do all kinds of new physics that we hadn't anticipated would be important. One thing we didn't anticipate was that we could use our laser-cooled atoms as a way of making a kind of toy model of solids. In this toy model we use interfering laser beams—laser beams that overlap. They form what we call a standing wave, where the distance between bright regions and dark regions is a fraction of the wavelength of light. Atoms can be trapped in those—what we call nodes and antinodes of the standing wave of the laser beam—and we make a kind of a toy model of a solid where you have a crystal lattice with electrons that can move from one site in the crystal lattice to another. We can use it to study the behavior in a simplified form of electrons moving in a solid.

Lecturer

3. What applications are made available by the study of ultracold atoms?

As a result of having ultracold atoms, we have been able to, just as we had hoped, revolutionize the way in which atomic clocks work. Today essentially every big industrialized country keeps time using laser-cooled atomic clocks. In the United States the time is kept for civilian purposes by NIST, my organization, and for military purposes by the U.S. Naval Observatory. Both of those institutions use laser-cooled atomic clocks as the basis for their time standards. In fact, at the Navy the people running the atomic clocks were postdocs at my laboratory and took the skills they learned about laser-cooling atoms to the Navy and made clocks. But if you go to places like England or France or Germany or China or Japan, in all of these places laser-cooled clocks are keeping time for their country. And all of those places report their information to a central organization in France and keep time for the entire world.

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

For me, coming to Oak Ridge has importance both from a personal and from a professional point of view. Oak Ridge has always been, from my youth, kind of a legendary place. The story of the Manhattan Project and Oak Ridge's role in making fissionable material was part of the story of physics that I read about when I was a child. When I was doing science projects, I remember writing a letter and just addressing it to Oak Ridge National Lab, and somehow or other it got to some scientist who knew something about what I was asking and wrote back a very kind letter explaining some things to me. So my relationship with Oak Ridge goes back in a very positive way, a very warm way, to my childhood.

When I was an undergraduate, I spent a semester at Argonne National Laboratory, which was one of the first places where I was able to engage in research essentially full time and work side by side with other researchers who were doing research as their full-time occupation. It was one of the things that cemented in my mind the idea that this is what I wanted to do with my life.

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.

Martin Karplus is co-recipient of the 2013 Nobel Prize in Chemistry, awarded for the development of multiscale models for complex chemical systems.

A native of Austria, Karplus received a bachelor's degree from Harvard College and a Ph.D. from Caltech before holding faculty positions at the University of Illinois, Columbia University and Harvard University. He is the Theodore William Richards Professor of Chemistry, Emeritus, at Harvard and director of the CNRS/Strasbourg University Biophysical Chemistry Laboratory.

Over the years, Karplus has conducted research in many areas of computational and theoretical chemistry and biochemistry and has presented his results in over 800 journal articles and book chapters, as well as two books. His work since the 1970s has focused mainly on the use of theory and high-performance computers to understand biomolecular structure, dynamics and function.

Karplus delivered the Eugene P. Wigner Distinguished Lecture November 7, 2017, on the topic "What Does the Future Hold?" This is an edited transcript of our conversation following his lecture.

Distinguished

Martin Karplus

1. You were using high-performance computing to solve questions in chemistry as early as the 1950s. How has supercomputing contributed to your work and the discoveries you've made over the years?

It's obvious that what was a supercomputer in the 1950s—with 3 megaflops [3 million calculations per second, or 9 billion times slower than ORNL's current Titan system] or even less—was limiting what we could do in terms of studying complex systems in biology, proteins and such, which is my primary interest. And, as the computers have become faster and faster following Moore's law, we have been able to do more and more things and been able to look at problems that in the 1950s we knew were there, but there was no way of doing them with the computing power that was available.

2. How have the attitudes of experimentalists and theorists toward numerical science evolved in the intervening decades?

It depends of course in what area you are. In physics, theory and numerical methods have been accepted for a much longer time than in chemistry, and again from chemistry to biology. As I said in my lecture, in the first studies we did of how proteins' internal motions occur, the chemists—I am a chemist officially, though I've been working in biological areas for much of my life—the chemists said we can't even look at the very simplest molecules and understand what's going on. To look at a protein makes no sense. And the biologists said, even if we could do it, it wouldn't be of any interest.

Since then things have evolved, and I think probably a very important element has been that there was a Nobel Prize in this area, so people said, well, if there's a Nobel Prize, it must be good for something. And I think in the last 10 years or so, there's been a real revolution in terms of the acceptance of computing results by experimentalists.

3. In the 1980s you were involved in the first work combining high-performance computing simulations with neutron scattering to understand motions in proteins. What role does simulation play in interpreting experiments on biological molecules?

Actually, it's not quite true. I was involved indirectly. [University of Tennessee–ORNL Governor's Chair for Molecular Biophysics] Jeremy Smith, who is on the staff here, has been trying to use neutron scattering to look at the motion of biomolecules, and he worked with me as a postdoctoral fellow and brought this project of neutron scattering to Harvard.

Lecturer

Interpretation of experimental results based on computations, it's a routine part of trying to understand what is going on in biology. One of the points is that crystallographers may be able to determine the structures of a protein under one condition, and another condition, and they are different. So they determine these two end points. But what one needs is computations to interpolate between them. And that's being accepted now.

Experimentalists are, in fact, beginning to use the techniques that we developed. We have a program, CHARMM [for Chemistry at Harvard Macromolecular Mechanics], which is widely used, and the experimentalists are now doing their own calculations rather than waiting for us to do them in many cases.

I might mention that we were looking for a name for our program and a student, Bob Bruccoleri, suggested the name HARMM—for Harvard Macromolecular Mechanics—and I said that didn't really sound very good. So I added the "C" for chemistry at Harvard. But now I sometimes wonder whether having kept the old name wouldn't have been a good idea, because it would warn people that you can't just run the program and use the results without realizing what the limitations are of the computations that you're doing.

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

The people here will have to decide whether or not it was important. I'm a great admirer of Wigner and felt that having the opportunity to expose the idea of what we will be able to do in the future with computational methods as supercomputers become faster and faster would be a worthwhile thing to do. My lecture was titled "What Does the Future Hold?" And, as I realized, the whole 25th anniversary meeting [celebrating the Oak Ridge Leadership Computing Facility] was really directed toward not the past so much as trying to understand what one would be able to do in the future. So, I think my take on when we will be able to do what studies in what year, this prediction which I did in my talk, made a very worthwhile contribution to this celebration of supercomputers here.

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.

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 staff members, and put them to work 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.

Bhavna Sharma

Postdoc, Environmental Sciences Division
Ph.D., Biosystems Engineering, Oklahoma State University
Hometown: Himachal Pradesh, India

What are you working on at ORNL?

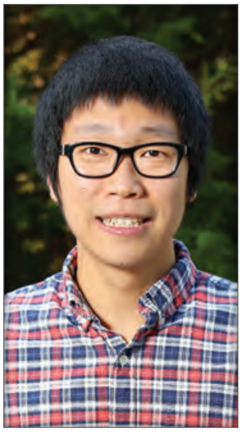
Much of my work in the Feedstock Modeling and Logistics Group is focused on developing and applying simulation and spatial models for biomass supply chain systems for production of biofuels and bioproducts. I currently evaluate risk and logistical resources required for an alternate biomass supply chain system configuration.

What would you like to do in your career?

In the near future, I would like to continue to develop modeling frameworks to address challenges associated with the biomass supply chain. Ultimately, I hope to lead a research program with the integration of mathematical, simulation and spatial models to address challenges in the environmental and energy sciences.

Why did you choose a career in science?

I am an inquisitive person by nature. In my early years science was the only place where I could find answers to my endless queries about how and why things work the way they do. Today my work allows me to find answers to challenging problems and feed my inquisitive mind.



Xiahan Sang

Postdoc, Center for Nanophase Materials Sciences
Ph.D., Materials Science, University of Pittsburgh
Hometown: Shishou, China

What are you working on at ORNL?

My research focuses on characterizing the atomic structure and defect evolution in 2D materials at elevated temperatures using in situ scanning transmission electron microscopy. Insight from these studies is crucial in order to link atomic-scale structure to how materials function.

What would you like to do in your career?

I would like to advance the field of scanning transmission electron microscopy by developing novel approaches to probe the structure and chemistry of materials at high spatial and temporal resolution under controlled in situ conditions.

Why did you choose a career in science?

Science offers so many challenges that give me the opportunity to discover new ways to solve problems. I will never get bored because there are always new things to be discovered in science.

Deborah Weighill

Graduate student, Biosciences Division
Ph.D. student, Energy Science and Engineering, University of Tennessee (Bredesen Center)
Hometown: Paarl, South Africa

What are you working on at ORNL?

I analyze omics data derived from *Populus trichocarpa*, a biofuels feedstock. We develop new approaches for the concurrent analysis of omics data to provide fundamental knowledge about how the components of the biological system interact and to facilitate the generation of new hypotheses around genes and functions of interest.

What would you like to do in your career?

I love to see abstract mathematical concepts find meaning in real-world problems. I would like to continue to work as a computational biologist, finding ways to apply mathematical and computational methods to biological data and contribute to the solutions of important problems.

Why did you choose a career in science?

The precision and elegance of mathematics, as well as the complexities of biological systems, have always intrigued me. Being able to follow those two interests in combination made science an easy choice.

Scott Greenwood

Postdoc, Reactor and Nuclear Systems Division
Ph.D., Nuclear Engineering, University of Wisconsin
Hometown: Parker, Colorado

What are you working on at ORNL?

From advanced molten salt reactors to traditional light water reactors, there exists an untapped opportunity to couple reactor technologies with additional systems such as energy storage and industrial processes. I investigate the integration of these unique hybrid energy systems to enable more economical and environmentally conscious solutions for the future.

What would you like to do in your career?

A common refrain in the nuclear world is that we need to "build something." The same applies to my career. I want to significantly contribute to a serious effort to explore and apply advanced technologies, experimentally and computationally, in energy or elsewhere, that have a substantive impact on our society.

Why did you choose a career in science?

To me, one purpose of this life is to learn. A scientific career provides the skills necessary to actively pursue knowledge and independently evaluate it. Knowledge is power; it enriches all aspects of my life, including making me a better chef and farmer!

Adeola Adediran

Graduate student, Energy and Transportation Science Division
Ph.D. student, Energy Science and Engineering, University of Tennessee (Bredesen Center)
Hometown: Lagos, Nigeria

What are you working on at ORNL?

I work with the Manufacturing Systems Research Group on large-scale metal additive manufacturing through laser metal deposition, with a focus on the aerospace industry. The goal of my research is to develop fully autonomous process controls for detection and correction of manufacturing defects to ensure component integrity and minimize failure risks.

What would you like to do in your career?

I would like to remain in the research and development space and continue to explore ways of optimizing industrial processes through automation and robotics. I also plan to re-establish outreach programs and robot assembly/programming lessons at the high school level (launched in Nigeria) to encourage young girls to embrace STEM [science, technology, engineering and mathematics].

Why did you choose a career in science?

I have always been curious about the way things—particularly machines—work, how self-driven mechanical systems interact to produce motion. My educational and work choices have been molded by my desire to learn about, utilize and contribute as much as I can to the world of machines.

David Walter

Graduate student, Physics Division
Ph.D. student, Experimental Nuclear Physics, Rutgers University
Hometown: Greeley, Colorado

What are you working on at ORNL?

My research group uses accelerated beams of exotic isotopes to study how protons and neutrons organize themselves in neutron-rich nuclei. We develop detectors and design experiments to measure the nuclear reactions that created elements through the rapid neutron capture process theorized to occur in supernovae and neutron star mergers.

What would you like to do in your career?

I would like to contribute toward developing new types of detectors and techniques in nuclear science. I hope to extend my research and experience to address questions in other areas such as reactor and medical applications.

Why did you choose a career in science?

I chose my path in science in order to be at the forefront of discovering the fascinating inner workings of our universe. I enjoy learning about nature and the fundamental laws that are common to everything.

The workers behind the science

by Tim Gawne
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It takes more than scientists to run a scientific institution, especially one like ORNL that operates reactors, accelerators and other highly specialized facilities.

Machinists, electricians, welders, mechanics and other craft and trade workers have been an indispensable part of the lab since Day One. They arrived among the first workers doing site preparation in 1942, many stayed, and some were among the world's most talented individuals in their disciplines. It is not unusual to find their grandchildren and great-grandchildren working at the lab now.

Like all men and women who came to the newly created Oak Ridge in World War II, tradespeople had to make sacrifices. One was that they could not organize a union. The mere existence of Oak Ridge was a heavily guarded secret, and one worker had very little idea what others were doing. In such an environment, the Army decided that labor organizing would simply involve too much sharing of information.

A "gentleman's agreement" deferred organization until after the war, but for a time workers still were prevented from general canvassing because of potential security breaches. It was nearly a year after the war before laborers were allowed to canvass and eventually vote to organize what was then known as X-10.

Photos and oral histories give the impression that trade workers were a tight bunch from the beginning. One local celebrity was a sheet metal worker nicknamed "Mink," who was short in stature, meek in appearance, and the reigning checker champion of Roane County.

During lunch he would take on all comers, sometimes conducting two games at once in the sheet metal shop. Section heads, supervisors and managers all met their demise at the checkerboard of the unassuming Mink.

Scientists may have been X-10's rock stars, but they understood how much they needed the lab's skilled workers.

ORNL's neutron science pioneers were no exception. When Ernie Wollan's physics section was transferred in 1944 from the University of Chicago down here to "Dogpatch"—an epithet for the East Tennessee site—he was working on an idea: to stream neutrons from the lab's Graphite Reactor using a crystal to select desired wavelengths, a technique called crystal diffraction.

Clifford Shull (1946)

With the help of "the shop," he was able to modify a two-circle X-ray diffractometer and fabricate a sample holder and a cadmium collimator, which was used to narrow the neutron beam. Using what Wollan called a "very simple and useful tool," he and his team observed and recorded (with a pen and paper) the first evidence of success. Without skilled welders and machinists on hand, this achievement would have been impossible.

The neutron pioneers continued their close relationship with the shop, with a machinist at one point fabricating a mahogany tobacco pipe for Wollan's collaborator, future Nobelist Clifford Shull. The pipe included a hand-fluted aluminum square channel, with taps added to affix the bowl and mouthpiece.

The pipe sits in a locked cabinet, awaiting its final resting place.

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