OAK RIDGE NATIONAL LABORATORY

Review

Nuclear is here:

OAK RIDGE National Laboratory

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On the Cover

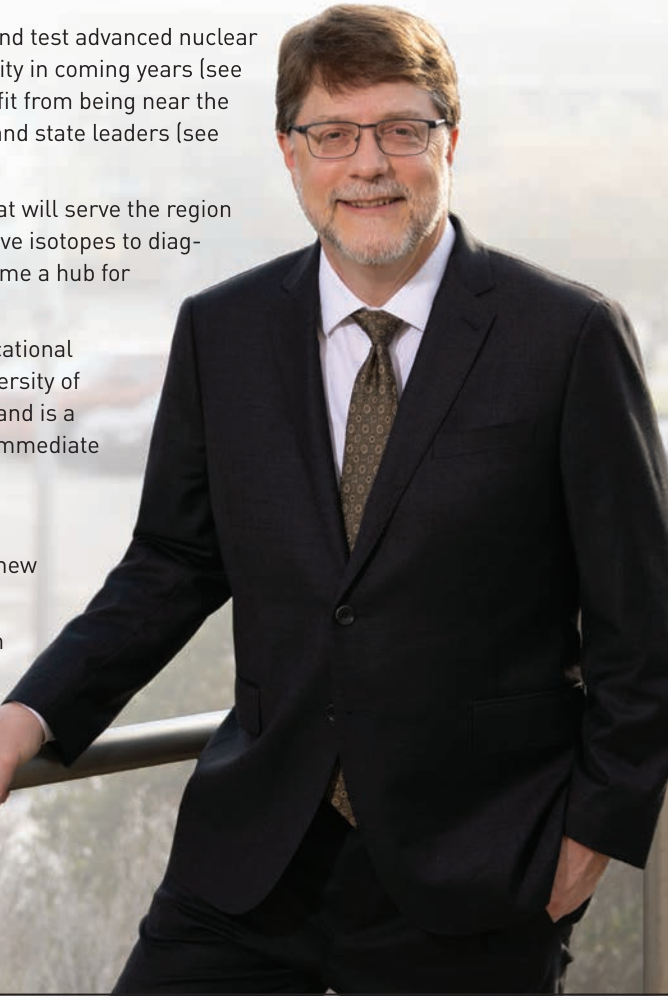
Image credit: Laddy Fields, ORNL

Tennessee hosts a resurgent nuclear industry

Oak Ridge and East Tennessee pioneered nuclear energy, from the earliest technology that harnessed the atom to its broad application for the advancement of science, society and security. It is not surprising, then, to see a surge of nuclear-related businesses moving into the region, and this issue of ORNL Review takes a look at the rapid growth that builds on our historic foundation.

The city of Oak Ridge and Oak Ridge National Laboratory were, of course, created by America's wartime race to produce the world's first nuclear weapons.

In the intervening eight decades, the lab has been at the forefront of peaceful nuclear research, designing reactors whose energy powers our electrical grid, producing isotopes that fight cancer and enable critical industrial processes, and conducting neutron-scattering research that answers big science questions and spurs innovations in industry, medicine and energy.



In recent years, new companies have located in East Tennessee to create and test advanced nuclear technologies that will provide safer, more affordable, more reliable electricity in coming years (see "Tennessee's growing nuclear industry," page 10). These businesses benefit from being near the lab, but they also have support from business leaders, local communities and state leaders (see "Nuclear industry gets a boost from Tennessee government," page 16).

ORNL is a major player in the production of medical isotopes, a position that will serve the region well as dramatic advances come to nuclear medicine, which uses radioactive isotopes to diagnose and treat cancers and other diseases (see "East Tennessee may become a hub for nuclear medicine," page 17).

To support these growing sectors, ORNL is also actively engaged with educational partners in preparing a well-trained workforce, including not only the University of Tennessee — which has a nationally ranked nuclear engineering program and is a partner in operating ORNL — but with community colleges that can meet immediate demand, too (see "Paving paths for a new nuclear workforce," page 20).

The Review goes digital

This is the final print issue for *ORNL Review*. Starting this fall, we'll have a new newsletter that will be distributed via email and found on social media.

The digital version will keep sharing ORNL's most compelling stories, from deep-dives that illustrate the lab's most world-changing initiatives, to early career researchers who will lead ORNL and other institutions years into the future, to history that shows what a unique place ORNL has always been.

With the new format, we will be able to present lab news not only in text and images but with videos, animations, graphics, conversations and a range of digital storytelling techniques.

I hope you enjoy this issue of *ORNL Review*, and I especially hope you subscribe to the digital version to see what we have in store.

Stephen Streiffer
Laboratory Director

ORNL scientists unveil secrets of promethium

Oak Ridge National Laboratory scientists have uncovered the properties of a rare earth element that was first discovered 80 years ago at the lab, opening a new pathway for the exploration of elements critical in modern technology, from medicine to space travel.

Promethium was discovered in 1945 at Clinton Laboratories, now ORNL, and continues to be produced at the lab in minute quantities. Some of its properties have remained elusive despite the rare earth element's use in medical studies and long-lived nuclear batteries. It is named after the mythological Titan who delivered fire to humans and whose name symbolizes human striving.

"The whole idea was to explore this very rare element to gain new knowledge," said Alex Ivanov, an ORNL scientist who co-led the research. "Once we realized it was discovered at this national lab and the place where we work, we felt an obligation to conduct this research to uphold the ORNL legacy."

The ORNL-led team of scientists prepared a chemical complex of promethium, which enabled its characterization in solution for the first time. They exposed the secrets of this extremely rare lanthanide, whose atomic number is 61, in a series of meticulous experiments.

Their landmark study, published in the journal Nature, marks a significant advance in rare earth research and might rewrite chemistry textbooks. — *Lawrence Bernard and Leo Williams*

For more: bit.ly/4bW6tEh

ORNL's groundbreaking promethium research was led by, from left, Alex Ivanov, Santa Jansone-Popova and Ilja Popovs of ORNL. Image credit: Carlos Jones, ORNL

Flooding model created to help urban planners

To better predict long-term flooding risk, ORNL scientists have developed a 3D modeling framework that captures the complex dynamics of water as it flows across the landscape. The framework seeks to provide valuable insights into which communities are most vulnerable as the climate changes and was developed for a project that's assessing climate risk and mitigation pathways for an urban area along the Southeast Texas coast.

The modeling framework offers a powerful tool for urban planning by providing robust estimates of both frequent and rare floods. By modeling the physical processes that transform rainfall into runoff, the framework accounts for factors such as land cover, soil properties and slope of the land. These elements, incorporated alongside population density, provide a unique perspective on flood risk across vast areas such as river basins. This comprehensive approach is detailed in a study published in the *Journal of Hydrology*.

The modeling capability was developed for the Southeast Texas Urban Integrated Field Laboratory, a DOE project using multidisciplinary science to inform pathways for climate resilience in the Beaumont-Port Arthur, Texas, region. The area is home to the nation's largest oil refinery and is a major industrial center for the United States. Its proximity to the Gulf Coast makes the region vulnerable to flooding

Scientists, from left, Ethan Coon and Phong Le of ORNL, Gabriel Perez, currently of Oklahoma State University, and Saubhagya Rathore of ORNL gather in the ORNL Everest visualization lab to discuss flood-prone areas. Image credit: Carlos Jones, ORNL and land subsidence — the gradual sinking of the ground over time — with additional stressors from population density and pollution presenting multiple challenges to local decision-makers. — *Stephanie Seay*

For more: bit.ly/3WErbUA

Neutron analysis boosts solid-state cooling materials

An ORNL-led research team has bridged a knowledge gap in atomic-scale heat motion, an advance that promises to boost solid-state cooling technology.

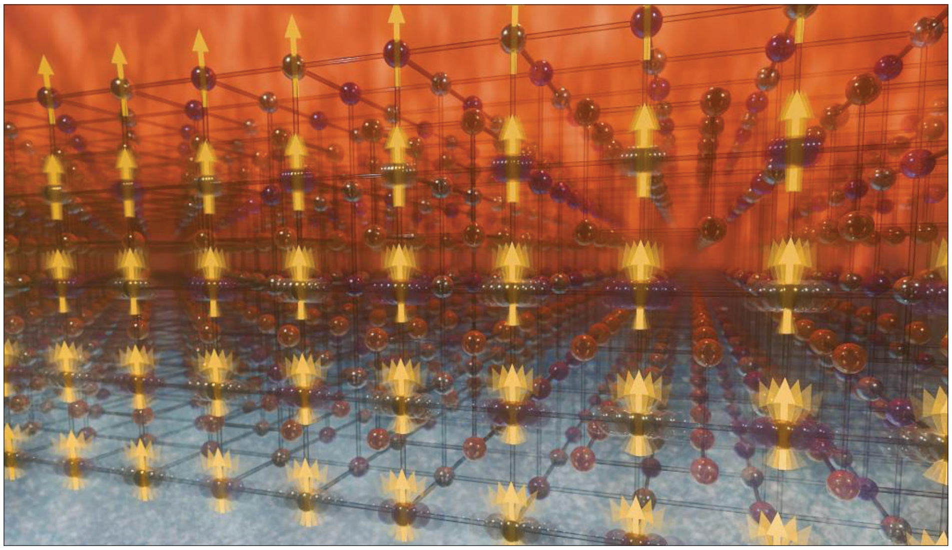
An environmentally friendly innovation, solid-state cooling could efficiently chill many products in daily life, from food to vehicles to electronics, without traditional refrigerant liquids and gases or moving parts. It would operate via a quiet, compact and lightweight system that allows precise temperature control.

Although the discovery of improved materials and the invention of higher-quality devices are already promoting the growth of this new cooling method, a deeper understanding of material enhancements is essential. The research team used a suite of neutron-scattering instruments to examine at the atomic scale a material that scientists consider to be an optimal candidate for use in solid-state cooling.

Frontier. Image credit: Carlos Jones, ORNL

The material, a nickel-cobalt-manganese-indium magnetic shape-memory alloy, can be deformed and then returned to its original shape by driving it through a phase transition either by increasing temperature or by applying a magnetic field. When subjected to a magnetic field, the material undergoes a magnetic and structural phase transition during which it absorbs and releases heat, a behavior known as the magnetocaloric effect. In solid-state cooling applications, the effect is harnessed to provide refrigeration. — *Scott Gibson*

For more: bit.ly/3zSChwg



Strong coupling between localized atomic vibrations and spin fluctuations increases the absorption and release of heat, shown from the bottom to the top, in a magnetic shape-memory alloy. Image credit: Phoenix Pleasant, ORNL

Vendor sought for next supercomputer at ORNL

The Department of Energy has released a request for proposals to advance its leadership in high-performance computing, inviting vendors to submit their plans for a successor to ORNL's Frontier, currently the world's fastest supercomputer.

The future system, to be called Discovery, will be designed to offer new computational capabilities beyond Frontier's 1.206 exaflops — or 1.2 quintillion calculations a second — on the High-Performance Linpack benchmark. The target for Discovery's delivery to the Oak Ridge Leadership Computing Facility is 2027 or early 2028.

The request for proposals for Discovery sets a wide range of goals for the next-generation system, such as advanced artificial intelligence and machine learning capabilities, improved energy efficiency, full-system modeling and simulation, and seamless interoperability with other DOE facilities through the Integrated Research Infrastructure initiative, which seeks to combine research tools and scientific facilities.

Unlike with previous systems, the request does not cite a specific speedup goal over its predecessor, but the facility expects Discovery to deliver three to five times more computational throughput for benchmarks and scientific applications than Frontier.

"This project is exciting because we will be building something even more capable than Frontier, with technologies that will push the edge of what's possible," said ORNL's Matt Sieger, the facility's project director for Discovery. — *Coury Turczyn*

For more: bit.ly/3y3n5fv

Hardy transistor material boosts reactor safety

The safety and efficiency of a large, complex nuclear reactor can be enhanced by hardware as simple as a tiny sensor that monitors a cooling system. That's why ORNL researchers are working to make those basic sensors more accurate by pairing them with electronics that can withstand the intense radiation inside a reactor.

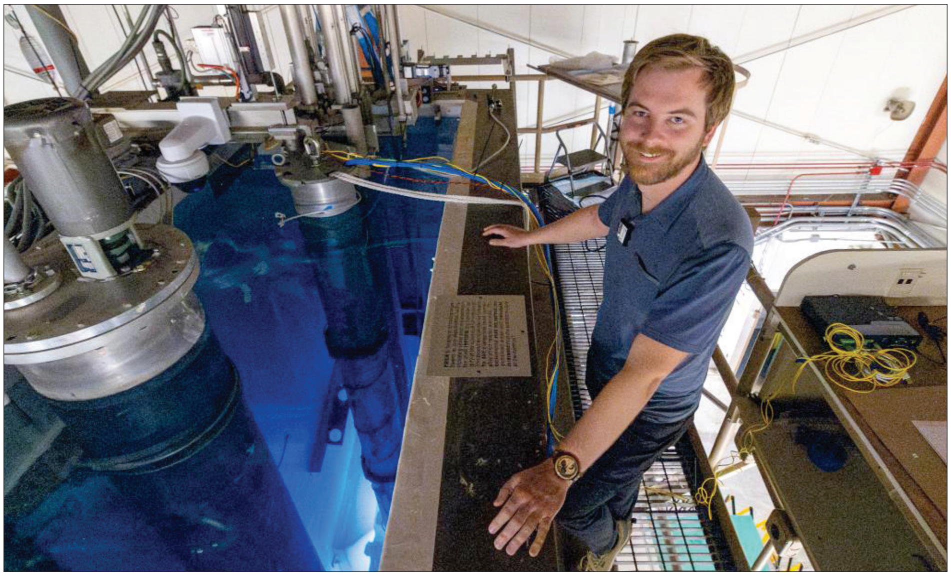
The ORNL research team recently met with unexpectedly high success using a gallium nitride semiconductor for sensor electronics. A transistor made with the material maintained operations near the core of a nuclear reactor operated by research partner The Ohio State University.

Gallium nitride, a wide-bandgap semiconductor, had previously been tested against the ionizing radiation encountered when rockets hurtle through space. Devices with wide-bandgap semiconductors can operate at much higher frequencies, temperatures and irradiation rates. But gallium nitride had not faced the even more intense radiation of neutron bombardment. "We are showing it is great for this neutron environment," said lead researcher Kyle Reed, a member of ORNL's Sensors and Electronics group.

That could offer a big boost for equipment monitoring in nuclear facilities. The information gathered by sensors provides early warnings about wear and tear on equipment, allowing timely maintenance to avoid broader equipment failures that cause reactor downtime. Currently, this sensing data is processed from a distance, through yards of cable connected to electronics with silicon-based transistors.

"Our work makes measuring the conditions inside an operating nuclear reactor more robust and accurate," Reed said. "When you have lengthy cables, you end up with a lot of noise, which can interfere with the accuracy of the sensor information. By placing electronics closer to a sensor, you increase its accuracy and precision." — *S. Heather Duncan*

For more: bit.ly/4c92YKQ



ORNL's Kyle Reed led a team testing an ORNL-made, hardy new type of transistor in the reactor pool at The Ohio State University Nuclear Reactor laboratory. Image credit: Michael Huson, The Ohio State University

Study shows how plants fare in extreme heat

Local decision-makers looking for ways to reduce the impact of heat waves on their communities have a valuable new capability at their disposal: a new study on vegetation resilience.

ORNL scientists have completed a study of how well vegetation survived extreme heat in both urban and rural communities across the country in recent years. The analysis informs pathways for climate mitigation, including ways to reduce the effect of urban heat islands.

Vegetation such as trees provides a valuable cooling effect, shading surfaces and deflecting solar radiation while releasing moisture into the atmosphere through evapotranspiration — the process in which plants absorb water through their roots and release it as water vapor through their leaves.

The study, published in the journal PNAS Nexus, is the first nationwide accounting of vegetation resilience that takes into account the influence of human-built infrastructure. Using machine learning methods, ORNL researchers examined about two decades' worth of satellite and other data covering 85 large cities and surrounding rural areas. The team found that impervious surfaces such as roads and other infrastructure, moisture conditions and type of land cover affect vegetation resilience. They also evaluated how vegetation is impacted by the intensity, duration and timing of heat waves.

The data provides crucial insights into how ecosystems can be guarded against climate change, including pathways to counteract the influence of urban heat islands and to improve the stewardship of natural resource areas, said Jiafu Mao, ORNL Earth system modeling scientist and the project's lead. — *Stephanie Seay*

For more: bit.ly/3LIZbcb

Researchers demonstrate 270-kw wireless charger

ORNL researchers have successfully demonstrated the first 270-kW wireless power transfer to a light-duty electric vehicle. The demonstration used a Porsche Taycan and was conducted in collaboration with Volkswagen Group of America using the ORNL-developed polyphase wireless charging system.

The achievement surpasses ORNL's recent 100-kW wireless charging demonstration and is another breakthrough for fast wireless charging.

"In (recent) months, the ORNL vehicle power electronics and electric drives research teams have set impressive world records for wireless charging," said Lee Slezak, DOE's Vehicle Technologies Office technology manager for grid and charging infrastructures. "These achievements will further speed up the adoption of electric vehicles in the U.S."

As a light-duty passenger vehicle, the Porsche Taycan would be difficult to equip using conventional large, heavy wireless power transfer systems. The vehicle can't support the charging hardware due to space, weight and volume limitations. Existing wireless charging systems for light-duty vehicles are currently under development for up to 11-kW power levels with up to 92% efficiency. Current industry standards cover up to 20-kW power levels.

The ORNL-invented system that transferred power to the Porsche uses lightweight polyphase electromagnetic coupling coils with a diameter just over 19 inches, allowing for higher power density in the smallest coil possible. This process is similar to the wireless charging of small consumer devices, but the unique geometry and design of the polyphase coils enable the transfer of extremely high power levels using rotating magnetic fields generated by the coil phase windings to boost the power. The charging system was seamlessly integrated into the undercarriage of the vehicle. — *Jennifer Burke*

For more: bit.ly/3Sn1lBS

ORNL researchers collaborated with Volkswagen Group of America to demonstrate wireless 270-kW power transfer to a Porsche Taycan. Image credit: Carlos Jones, ORNL

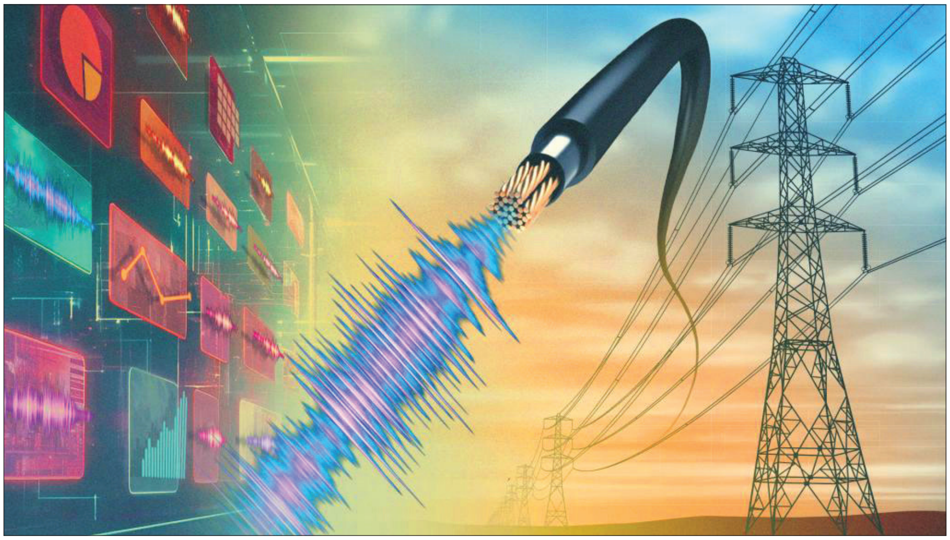
Waveform library shows electric grid behaviors

ORNL researchers have opened a new virtual library where visitors can check out waveforms instead of books.

The Grid Event Signature Library is an open-access online collection of datasets containing waveforms, which are visual representations of behaviors of the electric grid. Utilities and research institutions contributed anonymized data including voltage, current and frequency information collected by operating equipment. So far, more than 350 users worldwide have utilized the library, which provides vital understanding of an increasingly complex grid.

"Researchers can search different variables, like the type of sensor or a description of the event — for example, a waveform that represents a blown transformer and its effect on transmission line voltage," said ORNL's Aaron Wilson, who manages the tool.

A recent paper described the datasets and their applications. Machine learning can be trained to recognize waveforms that provide an early warning of equipment malfunction, enabling power system operators to prevent blackouts, wildfires and damage to the power grid. — *S. Heather Duncan*



The Grid Signature Event Library energizes utility and researcher understanding of grid behavior by providing access to datasets of waveforms from grid operations. Image credit: Adam Malin, ORNL

AI method identifies ecofriendly solvents

ORNL scientists have developed a method leveraging artificial intelligence to accelerate the identification of environmentally friendly solvents for industrial carbon capture, biomass processing, rechargeable batteries and other applications.

The research targets a class of solvents known for being nontoxic, biodegradable, highly stable, cost-effective and reusable.

The scientists developed a method to predict solvent viscosity — a key property impacting performance for industrial applications. The team compiled nearly 5,000 data points on 672 solvents, evaluated quantum chemical features that guide solvent molecular interactions, and deployed an algorithm called categorical boosting to quickly analyze the data and determine the best candidates.

"We reduced computational time and complexity with our approach, while still incorporating all possible molecular interactions," said ORNL's Mohan Mood.

ORNL's Michelle Kidder said, "Interpretable machine learning helps us to design solvents with desired properties for carbon capture by reducing experimental time and cost in the laboratory." — *Stephanie Seay*

Electron-beam 3D printer produces tungsten parts

ORNL researchers have used additive manufacturing to produce the first defect-free complex tungsten parts for use in extreme environments. The accomplishment could have positive implications for clean-energy technologies such as fusion energy.

Tungsten has the highest melting point of any metal, making it ideal for fusion reactors, where plasma temperatures exceed 180 million degrees Fahrenheit. In comparison, the sun's center is about 27 million degrees Fahrenheit.

In its pure form, tungsten is brittle at room temperature and easily shatters. To counter this, ORNL researchers developed an electron-beam 3D-printer to deposit tungsten, layer by layer, into precise three-dimensional shapes. This technology uses a magnetically directed stream of particles in a high-vacuum enclosure to melt and bind metal powder into a solid-metal object. The vacuum environment reduces foreign material contamination and residual stress formation.

ORNL researchers used electron-beam additive manufacturing to 3D-print the first complex, defect-free tungsten parts with complex geometries. Image credit: Michaela Bluedorn, ORNL

"Electron-beam additive manufacturing is promising for the processing of complex tungsten geometries," said ORNL's Michael Kirka. "This is an important step for expanding the use of temperature-resistant metals in energy resources that will support a sustainable, carbon-free future."— *Greg Cunningham*

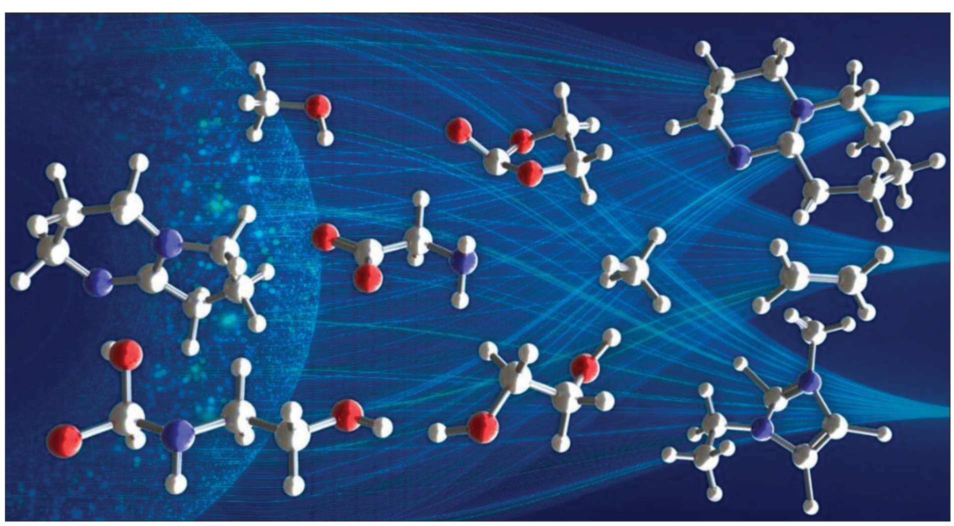
Rotating sample holder boosts neutron research

Scientists from the University of California, Davis, and ORNL have developed a sample holder that tumbles powdered photochemical materials within a neutron beamline. The rotating holder exposes more of the material to light for increased photoactivation and better photochemistry data.

Conventional sample holders were unable to rotate, or tumble, powdered samples, which meant light could only reach and activate molecules on the sample's surface, reducing the amount and quality of data that could be captured.

The new sample holder has already enabled the first neutron scattering observations of an optically excited photon splitting into two particles — a process that could lead to increased solar energy conversion efficiency in photovoltaic devices, such as solar cells or solar panels, and industrial processes.

"Our neutron scattering measurements were performed at cryogenic temperatures — typically below minus 150 degrees Celsius (minus 238 degrees Fahrenheit) — within a rotating mechanical chamber inside a modified sample stick," said lead author Daniel Vong, formerly with UC-Davis. "This sample environment offers expanded neutron research capabilities for studying photovoltaics, photosynthesis, photoactive cata-



ORNL researchers are using artificial intelligence to speed the identification of environmentally friendly solvents for industrial applications. Image credit: Andy Sproles, ORNL lysts and other photochemical processes and materials."

A photochemical reaction is a chemical reaction triggered when light energy is absorbed by a substance's molecules.

"The collaboration was a win-win, demonstrating how university and ORNL scientists can work together successfully," said Adam Moule, corresponding author on the two papers and professor of chemical engineering at UC-Davis. "It was a great opportunity for one of our researchers to intern at ORNL, learning from an expert instrument scientist and having access to the resources needed to build such an innovative sample holder." — *Paul Boisvert*

New techniques identify uranium, fluorine mixture

Combining two techniques, analytical chemists at ORNL became the first to detect fluorine and different isotopes of uranium in a single particle at the same time.

Because fluorine is essential for converting uranium into a form suitable for enrichment, spotting both elements together may help inspectors of the International Atomic Energy Agency determine the intended use of a nuclear material.

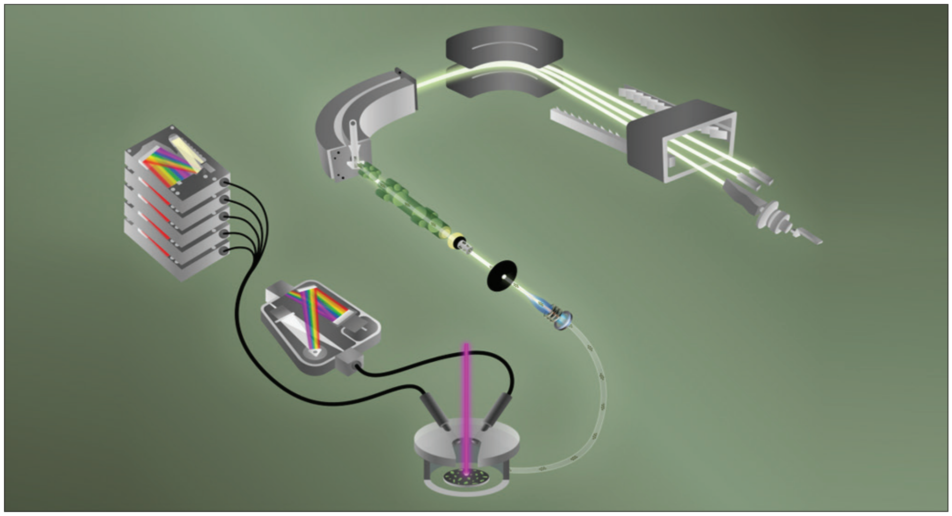
The findings, published in the Journal of the American Chemical Society, push the limit of how fast single particles can be characterized in terms of their chemical, elemental and isotopic compositions. Critical for understanding chemical processes and dating materials, isotopes are different forms of a chemical element having the same number of protons but a different number of neutrons.

"Determining isotopic ratios on single particles takes a lot of time," said ORNL's Benjamin Manard, who led the study. "Rapid particle analysis for fluorine and uranium isotopic determination is what we've enabled."

The first technique is laser-induced breakdown spectroscopy, or LIBS. It quickly spots the element fluorine with great sensitivity.

"LIBS vaporizes a sample, like a uranyl fluoride particle, breaking it down and forming a plasma, or cloud of excited ions. As the plasma cools, light is emitted," said ORNL's Hunter Andrews, the study's LIBS task lead. Spectroscopy then measures the light to characterize elements in the plasma.

Simultaneously, helium gas sweeps atoms of the plasma into a mass spectrometer, where isotopes of uranium are characterized via the second technique, called laser ablation multicollector inductively coupled plasma mass spectrometry, or ICP-MS. Inductively coupled means radio-frequency energy heats the plasma. It reaches 8,000 kelvins — hotter than the surface of the sun. — *Dawn Levy*



ORNL's tandem technologies detect fluorine and isotopes of uranium at the same time to discern the fingerprint of a nuclear material. Image credit: Benjamin Manard and Jacquelyn DeMink, ORNL

Energy use estimated for buildings in 2100

ORNL researchers have developed free datasets to estimate how much energy any building in the contiguous U.S. will use in 2100. These datasets provide planners a way to anticipate future energy needs as the climate changes.

Considering only existing buildings, the team analyzed energy use and weather records dating back to 1980, identifying which months displayed the most typical weather patterns. They combined that data with future projections by the Intergovernmental Panel for Climate Change, including four possible levels of atmospheric warming

ORNL has created publicly available datasets projecting energy use for all U.S. buildings through 2100 under different climate change scenarios. Image credit: Andy Sproles, ORNL and four policy outcomes incorporating variables such as population and economic growth. The county-specific weather data, enhanced by a free visualization tool, can predict a building's energy use down to the day and hour.

ORNL project lead Joshua New said the data, made publicly available a few months ago, is already being utilized more than expected. Power companies are using it to project future electricity demand, cities are developing climate-friendly building codes and architects are designing sustainable buildings. — *S. Heather Duncan*

For more: bit.ly/4fjNExv

Program helps businesses develop grid innovations

A new technical collaboration program at ORNL will help businesses develop and launch electric grid innovations. Sponsored by the Transformer Resilience and Advanced Components program in DOE's Office of Electricity, the initiative will provide companies with access to national laboratory resources, enabling them to capture market opportunities.

Even startup and small businesses can now easily submit proposals for cost-shared research in ORNL's Grid Research Integration and Deployment Center, or GRID-C. Located at ORNL's Hardin Valley campus in Knoxville, Tennessee, GRID-C takes grid advances from conception to deployment by industry.

The GRID-C technical collaboration program will provide access to more than a dozen labs and test beds for research in power and energy systems, vehicle and buildings science, power electronics, energy storage, sensors and controls, data science, modeling, and cybersecurity. Related facilities on ORNL's nearby main campus also provide a platform to develop and test new conductor and transmission technologies.

GRID-C researchers previously partnered with large companies through individual agreements. But the technical collaboration program streamlines the process, making it newly accessible to partners with varying levels of resources and for seed projects with a tightly targeted research scope.

"This opens the door for small businesses to come in and use our amazing infrastructure to improve grid systems that will benefit everyone while bringing additional American jobs," said Madhu Chinthavali, ORNL Electrical Systems Integration program director.

ORNL offers expertise in design, development, prototyping and evaluation of grid hardware, software, architecture and modeling.

Companies eligible to participate in the GRID-C collaboration program must have or develop a focus on advanced components and power stages, advanced converter systems or resource integration and management systems for commercial applications in the U.S. — *S. Heather Duncan*

For more: bit.ly/4eyqrHk

Through a new technical collaboration program, companies will be able to propose research projects that utilize the labs and expertise in ORNL's Grid Research Integration and Deployment Center. Image credit: Carlos Jones, ORNL

ORNL's John Field provided expertise on sustainable biomass feedstock potential for a new report focused on the role of the bioeconomy in U.S. decarbonization strategies. Image credit: Carlos Jones, ORNL

US has biomass to meet sustainable aviation goals

The United States has enough biomass potential to produce 35 billion gallons per year of aviation biofuel by 2050, a new report confirms.

ORNL's John Field provided biomass feedstock production expertise to the report, which focused on the role of the bioeconomy in U.S. decarbonization strategies. It was produced by DOE's DECARB program.

The report examined the role of biomass in reducing greenhouse gas emissions across the economy, including opportunities to reach negative emissions. It includes data from the ORNL-led 2016 Billion-Ton Report, which identified potential biomass from agricultural and forestry residues, wastes and bioenergy crops.

The latest 2023 *Billion-Ton Report* identifies up to 1.7 billion tons per year of potential biomass, including winter oilseed crops for jet biofuels.

Carbon-negative bioenergy is expected to be essential to a net-zero emissions economy and could account for 4% to 11% of the nation's total energy mix by 2050, according to the DECARB report. — *Stephanie Seay*

Nuclear is here ... and here and here

East Tennessee hosts a nuclear resurgence

by Leo Williams
williamsjl2@ornl.gov

In fall 2020, California-based Kairos Power announced plans to build an advanced nuclear demonstration reactor within the site of the former K-25 uranium enrichment plant in Oak Ridge.

It was a good location for the company. The decommissioned K-25, now named Heritage Center Industrial Park, came with impressive infrastructure, including ample electricity from the Tennessee Valley Authority, abundant water from the nearby Clinch River, and more than 11 miles of rail line connected directly to the Norfolk Southern system. Interstate 40 was less than five miles away.

Perhaps more importantly, the location gave Kairos' scientists and engineers close access to an unmatched pool of nuclear expertise. ORNL, which helped start the nuclear age more than 80 years ago and remains at the forefront of nuclear research, is all of five miles away. The University of Tennessee, Knoxville, which hosts a prestigious nuclear engineering department dating back to 1957, is just 30 miles down the road. And the federally owned TVA, which has operated nuclear power plants since 1974, is developing its own next-generation nuclear reactor about three miles away.

In particular, though, the company wanted to be near a national lab, according to its co-founder Mike Laufer.

"The big decision for us was where we were going to put the Hermes reactor," he said. "For that, we pretty quickly narrowed down that we had a strong preference to be in close proximity to a national laboratory, with capabilities that could augment our own infrastructure."

Hermes will be a 35-megawatt molten salt-cooled reactor that uses a new kind of uranium fuel called TRISO — short for tristructural isotropic particle fuel. The billiard ball-sized TRISO pebbles will consist of uranium, carbon and oxygen particles surrounded by carbon- and ceramic-based materials designed to prevent the release of radioactive fission products. The reactor will not produce electricity; rather, it will demonstrate the company's technology before Kairos moves on to building much larger commercial reactors.

A torrent of new businesses

When Kairos made that announcement in 2020, it was among the first of many new East Tennessee businesses looking to join a resurgent nuclear industry. Other nuclear newcomers include:

- TRISO fuel manufacturer Ultra Safe Nuclear Corp., which announced in March 2022 that it would build its Pilot Fuel Manufacturing facility at Heritage Center.

We believe it has the potential to be the largest nuclear hub in the U.S., if not the world.

— East Tennessee Economic Council President and CEO **Tracy Boatner**

- Type One Energy Group, which announced in February 2024 that it would build a prototype fusion device called Infinity One at the site of TVA's retired Bull Run Fossil Plant just outside the Oak Ridge city limits in Anderson County.

ORNL played a key role in these three announcements, owing to its role in the development of particle fuels and fusion energy. TRISO-X, for example, developed the prototype for its fuel fabrication facility at ORNL.

Then in September 2024, Orano USA announced Oak Ridge as the site of a new multibillion-dollar uranium enrichment facility, the single largest investment in Tennessee history. Orano's 750,000-square-foot plant will be built on a 920-acre site transferred to the company by DOE. It's expected to create more than 300 jobs.

According to the East Tennessee Economic Council, there are more than 200 nuclear-focused companies doing business in Tennessee at more than 350 locations. More than 150 of those companies are doing business in and around Oak Ridge and Knoxville.

The number is rising steadily, according to the council's president and CEO, Tracy Boatner.

"We get calls regularly," Boatner said. "I know the Chamber, ORNL, TVA and the state Economic Development Department do. Even UCOR said recently that they get calls probably on a weekly basis from companies that are interested in moving here."

The Oak Ridge Chamber manages economic development inquiries for the city of Oak Ridge. Chamber President and CEO Christine Michaels echoed Boatner's experience.

"Last week it was every day," she said earlier this year. "And they were not all the same company. Right now we have probably half a dozen very active prospects and others that are in various stages of exploration for sites."

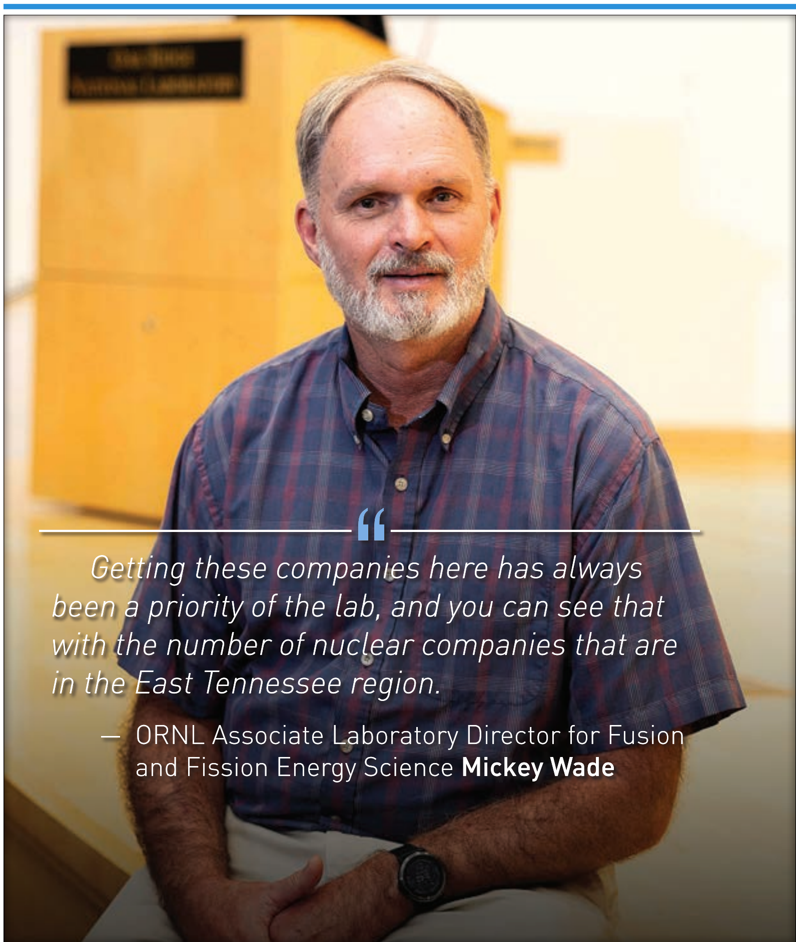
ORNL catalyzes growth

According to Mickey Wade, ORNL's associate laboratory director for the Fusion and Fission Energy and Science Directorate, the lab is actively involved in promoting the region's nuclear industry and consulting with nuclear businesses that move into the area.

"Getting these companies here has always been a priority of the lab," he said, "and you can see that with the number of nuclear companies that are in the East Tennessee region.

Wade said both larger and smaller businesses are critical to the success of the region's nuclear ecosystem. He said Kairos, with its embrace of molten salt technology, and Type One Energy, which is developing advanced fusion technology, are of particular interest to the lab.

"These are examples in fission and fusion that we feel are very important for us to be connected with because they are sea



changes about how you do nuclear energy in the future. These are approaches that we feel like the lab is very well suited to be engaged with."

Wade said that while large facilities are important to the lab, a robust ecosystem of smaller support businesses in the supply chain is also critical.

"Ultimately in an industry, it is about the end product, and the companies that really make it happen are those that are on the leading end of the supply chain."

Wade said the lab is especially on the lookout for businesses in the supply chain that have the technical and business know-how to succeed.

"Those companies really need the national labs to get them over the hump with regard to their idea," he said, "and we need them because they're telling us what's important, what science and technologies we need to develop to enable the U.S. industry in the future."

A natural home for nuclear businesses

East Tennessee offers a particularly attractive business environment for a nuclear renaissance. Not only does it already boast a wealth of nuclear expertise, but the K-25 cleanup provided 2,000 acres of industrial property with existing infrastructure, with another 440 acres of developable land available at the recently created Horizon Center.

According to Boatner, the decades-long cleanup at Heritage Center, proximity to ORNL, and TVA's effort to locate small modular reactors along the Clinch River helped focus attention on the area, as did the state's creation of a $50 million Nuclear Fund in 2023 to support the nuclear industry (see "Nuclear industry gets a boost from Tennessee government," page 16).

"The catalyst for the growth of nuclear here in Oak Ridge has been the interest in TVA and the fact that that UCOR and the Department of Energy Environmental Management program have cleaned up the former K-25 Site," she said. "Governor Lee's $50 million investment to recruit nuclear companies has also significantly amplified Tennessee's appeal as a prime location."

In addition, she noted, Oak Ridgers are especially welcoming to nuclear businesses. Kairos co-founder Laufer agreed.

"I would say the community in Oak Ridge has been incredibly welcoming," he said. "Our expectations were high, but everything has been met and exceeded in terms of the engagement and not just the acceptance but a lot of the excitement that we have seen from the local community."

Good for the region

That openness will almost certainly boost the regional and state economies, say local officials.

Their assessment is supported by a report released by the Southeast Nuclear Advisory Council and conducted by E4 Carolinas in February 2024. The report looked at the nuclear industry's economic impact in five states: Tennessee, North Carolina, South Carolina, Virginia and Georgia. It concluded that nuclear businesses and their suppliers in Tennessee employ more than 29,000 people who bring in $2.5 billion in salary. The economic output of these businesses and their employees totals nearly $8 billion.

Greg Boerschig

Add in the effect of this spending on local economies — the meals, movies, vehicles and so on that these employees spend their money on — and the total comes to more than 40,000 Tennessee employees making $3.2 billion and generating nearly $10 billion in economic output. Tax revenue from all this spending comes to $1 billion.

The report also notes that jobs created by the nuclear industry pay substantially more than most other jobs. Average pay across the region for nuclear workers averaged nearly $90,000, which is nearly two-thirds more than the average job.

First there was TVA

Boatner said community efforts to promote the industry grew naturally out of TVA's interest in building two or more small modular reactors at the Clinch River location.

Small modular reactors are a relatively new idea in the nuclear world. Besides their size — the reactors under consideration are designed to produce about 300 megawatts of electricity, less than a third that of TVA's other reactors — what distinguishes them is their standardized designs.

In the past, nuclear power plants varied substantially in design, making each unique and making it difficult to achieve the cost and safety benefits that come with standardization.

"If you go back to the current commercial nuclear industry, virtually every plant is different," said TVA's Greg Boerschig, vice president of the Clinch River Project. "The equipment is different, much of the engineering is different, and that adds a lot of expense."

"The more of the plant that you can maintain standard — parts, engineering, structures — that brings the cost down."

While the concept of these small reactors is relatively new, the technology being considered by TVA — boiling water reactors — has been around for decades. Indeed, the utility's 50-year-old Browns Ferry plant in Alabama is powered by three boiling water reactors.

Jeff Smith — who served as interim ORNL director after 21 years as the lab's chief operating officer and who also served on the TVA board — said TVA is wise to pursue a proven technology, noting that cost is especially important to the utility.

"The Tennessee Valley Authority Act of 1933 says that TVA is obligated to provide power as low as reasonably achievable in terms of rates. When I sat on the TVA Board, that's something you thought about every time you got together.

"So, the TVA approach is, we're going to use an existing design that's been proven. We're going to use existing fuel that's already licensed. And we're going to concentrate on controlling costs by going at it with a small design, a smaller plant."

If the project succeeds, he said, that success could accelerate the industry regionwide.

"If they can get that done, that creates a tremendous center of gravity around new nuclear that I think will bring additional companies and economic activity to the state of Tennessee and East Tennessee in particular."

> *If you go back to the current commercial nuclear industry, virtually every plant is different. The equipment is different, much of the engineering is different, and that adds a lot of expense.*
>
> — TVA vice president of the Clinch River Project **Greg Boerschig**

The project, which is still in the planning phase, has a way to go, Boerschig said. The Nuclear Regulatory Commission granted TVA an early site permit in late 2019, and in 2022 the TVA board OK'd up to $200 million for evaluation of the technology and establishment of a New Nuclear Program. TVA will likely submit a construction permit to the NRC in early to mid-2025.

"It's about a three-year review process," Boerschig said. "The board would have to approve going to the project phase. During the project phase the NRC would review our construction permit, and we would complete the standard and site-specific design and prepare for construction.

"Another possibility is to remain in the planning phase for the NRC construction permit application review and standard-design completion, then seek project approval for site-specific engineering and preconstruction work. We would have to go to the board again for construction phase approval with our final cost and schedule estimates for the first plant, demonstrate all our planning is rigorous and complete, discuss the economic viability of building multiple reactors, and seek TVA board approval to begin construction."

Over the entire process, he said, it will be a decade or more before reactors would be generating electricity at the site.

Bringing fusion to East Tennessee

Type One Energy is the third entity developing a new platform in the region. But unlike the Kairos and TVA projects, Infinity One will be a fusion device, fusing the nuclei of atoms together rather than splitting them apart.

Infinity One will be located 20 miles east of TVA's Clinch River location and will occupy a portion of the utility's coal-burning Bull Run Fossil Plant, which was retired at the end of 2023.

Like the Kairos project, it will not produce electricity. Rather, it will be a prototype stellarator, a device that uses external magnets to confine a hydrogen plasma in the shape of a twisted donut or a bicycle tire. Stellarators were conceived more than 70 years ago, and the first dates back to 1953.

The project was announced in February 2024 by the company and Governor Lee. Besides locating the reactor itself, Type One moved its headquarters to Oak Ridge.

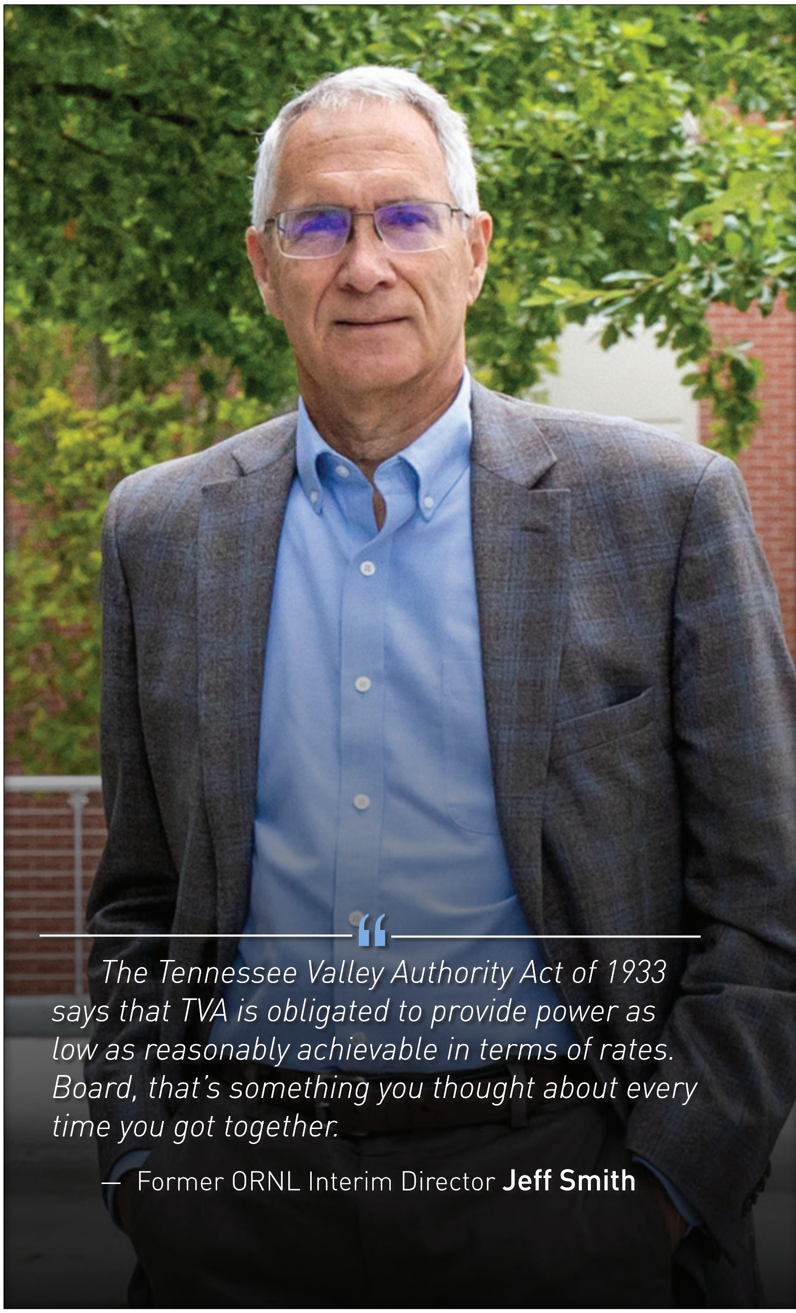
According to Matt Miles, the company's senior vice president for marketing and external affairs, the company found the area attractive both because of a highly trained workforce — which he attributes to ORNL and the nearby Y-12 National Security Complex — and because of the support Type One has found from the lab, TVA, the state and DOE. He also pointed to the fusion expertise found in the region, especially at ORNL, which hosts both a Fusion Energy Division and the U.S. headquarters for the international ITER fusion device being built in France.

Miles noted that the company has deep relationships with ORNL. Company co-founder and chief science officer John Canik spent nearly 16 years at the lab, and Bradley Nelson, its vice president of engineering, was chief engineer for US ITER.

The technology has leaped forward in recent years, Miles said, pointing to more recent stellarators in Germany and at the University of Wisconsin, Madison. He pointed also to a 2022 experiment at the National Ignition Facility at Lawrence Livermore National Laboratory in which a fusion reaction created more energy than required for the laser light that induced it.

"With the advances in additive manufacturing techniques and the advances that we now have in high-performance computing, it allows us to model things to a degree of fidelity that we couldn't before," he said. "The success of the HSX optimized stellarator [at UW] and then the W7X [in Germany], the ability of the NIF machine to get a burning plasma — not once, not twice, but now three times out in California — this gives us a degree of confidence that says the foundational science is proven for fusion."

Because TVA is a federal entity, he said, the site will have to be reviewed under the National Environmental Policy Act. If all goes well, the company hopes to start construction in 2025 and begin operating Infinity One in 2028.



The Tennessee Valley Authority Act of 1933 says that TVA is obligated to provide power as low as reasonably achievable in terms of rates. Board, that's something you thought about every time you got together.

— Former ORNL Interim Director **Jeff Smith**

Looking to the future

Given the region's strengths — and assuming the nuclear industry continues to gain traction — it's likely that many more businesses will find their way to the Oak Ridge area and Tennessee. And if state and regional leaders have their way, the state will become a national focal point for nuclear technology and business.

"We believe it has the potential to be the largest nuclear hub in the U.S., if not the world," said the East Tennessee Economic Council's Boatner.

Nuclear industry gets a boost

from Tennessee government

by Leo Williams
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Tennessee's growing nuclear industry has a committed booster in the state's government.

Leaders in the state capital, Nashville, agree with local boosters in Oak Ridge and East Tennessee that the state has what it takes to become a national center for nuclear power, nuclear medicine and other nuclear technologies, with major players and a robust support ecosystem.

> *We see this real opportunity, especially in the Oak Ridge area — as well as other areas of the state — to be the home for so much of the new nuclear technology.*
>
> — Tennessee Chief Operating Officer **Brandon Gibson**

"We see this real opportunity, especially in the Oak Ridge area — as well as other areas of the state — to be the home for so much of the new nuclear technology," said the state's chief operating officer, Brandon Gibson. "We've got a trained workforce. We have citizens who know and understand the nuclear space. And then we have the crown jewel, which is Oak Ridge National Lab."

To take advantage of this opportunity, Governor Bill Lee appointed a Nuclear Energy Advisory Council and partnered with the Legislature to create a $50 million Nuclear Fund.

The fund — besides offering help to businesses that have located in the state — is a signal to others that they will find a friendly environment in Tennessee.

"The state competes with a number of other states to get industry to move to Tennessee," Gibson said. "And oftentimes that involves economic development incentives of one kind or another. Those incentives can be used for a lot of different things. Sometimes it's site preparation work. Sometimes it's construction or other issues."

Brandon Gibson

The fund's first recipient was Type One Energy, which is building a prototype fusion device near Oak Ridge in Anderson County. The company and Lee announced the project in February 2024.

Lee appointed the 22-member Tennessee Nuclear Energy Advisory Council in July 2023, with members representing a wide range of stakeholders, including state environmental and emergency management leaders, federal and local governments, and existing industry players. Jeff Smith, the lab's former interim director, was appointed to represent ORNL.

"The beauty of having a rich history in Tennessee is that we've got a lot of really smart people who understand the nuclear industry and what our potential is," Gibson said. "The governor has always said that government alone is not the answer to our greatest challenges, but it's the people of Tennessee who really hold the answers to our greatest challenges."

The group was asked to produce two reports, one interim, one final. The interim report, delivered in December 2023, recommended two broad strategies: first, to advance new nuclear projects, in particular the small modular reactor being developed by the Tennessee Valley Authority at a site on the Clinch River, and second, to build the workforce and supply chain for the nuclear industry.

The group's final report is due at the end of October 2024.

East Tennessee may become a hub for nuclear medicine

by Leo Williams
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When people a decade from now face a cancer diagnosis, they may well turn to East Tennessee for help.

The region is well-positioned to become a focus for nuclear medicine, or radiopharmaceuticals, which use radioactive isotopes to diagnose and treat cancer and other diseases. East Tennessee boasts two major research institutions in this field — ORNL and the University of Tennessee.

While radioisotopes have been used in medicine for decades — ORNL first shipped a medical isotope, carbon-14, to a St. Louis hospital in 1946 — the field is in its early stages in some respects.

"We are at the beginning of what will be a wave of radiopharmaceutical implementation for cancer," said Sandra Davern, head of ORNL's Radioisotope Research and Development Section. "So radiopharmaceuticals are really only starting to be used to treat cancer."

State leaders would like to see the region become a national center for developing new and better treatments and conducting the clinical trials needed to bring these advances to patients. For that to happen, though, much work lies ahead, including, critically, the development of a robust workforce of physicians, physicists, radiopharmacists and technicians.

The benefits of nuclear medicine

Medical isotopes serve at least two purposes. The first is diagnostic: An isotope is attached to a molecule that seeks cancer or other disease for visualization. The radiation emitted by that radioisotope allows the disease to be pinpointed by technology such as a PET-CT scan. (PET scan technology was developed by an Oak Ridge company, EG&G ORTEC, in the 1970s and commercialized in the 1980s by spin-off CTI Molecular Imaging, which was based in Knoxville and is now owned by Siemens.)

The second purpose is therapeutic: In this case, instead of just observing cancer cells, the isotopes' job is to seek and destroy them.

Currently, radioisotopes are used much more widely to diagnose disease than to treat it, simply because that technology is farther along.

"The nuclear medicine world in East Tennessee is small but growing," Davern said. "We have a lot related to imaging disease and making diagnoses."

Dustin Osborne, director of the Molecular Imaging and Translational Research Program within UT's Graduate School of Medicine, agreed.

"We've seen massive growth in our PET-CT usage in the hospital, and regionally you find that same sort of growth."

On the therapeutic side, Osborne said, UT Medical Center uses two approved radiopharmaceuticals, both with the radioisotope lutetium-177. One, called Pluvicto, treats prostate cancer. The other, called Lutathera, treats neuroendocrine tumors such as those found in the pancreas.

"We're treating prostate and neuroendocrine tumor patients here," he said, "but you're also seeing this growth now from Vanderbilt [Vanderbilt University Medical Center in Middle Tennessee] to a group in the Tri-Cities area [in the northeastern corner of the state] that are delivering this therapy. So it's growing in the state and growing in this area."

So far, he said, these therapies can be both more effective than chemotherapy and have less severe side effects. He pointed to the neuroendocrine therapy Lutathera as an example.

"Nearly 80 percent of the patients in clinical trials saw a 30 percent decreased size of the disease in their body," he said, "which is a massive difference. In chemotherapy, if we get 20 percent efficacy on something, that's good.

"And the side effects for chemo are far, far worse than what we see with radionuclide therapy, where so far the only patient complaints have been fatigue two or three days after the procedure, and sometimes a little bit of nausea."

Benefits to the community

A growing nuclear medicine industry in Tennessee will not only benefit the economy, it will also be a boon to people in the region who need treatment and access to clinical trials.

Davern noted that cancer rates are relatively high in the Southeast and Appalachia, especially among low-income residents. Generally, these are also people who lack the means to travel across the country for treatment.

We are at the beginning of what will be a wave of radiopharmaceutical implementation for cancer.

— ORNL Radioisotope Research and Development Section Head **Sandra Davern**

"If you do an analysis of death rates from cancer, and you compare that to income for these people, you see that over the whole of the U.S., it is often the poorest people who have the highest cancer death rates.

"And so if we can have the infrastructure to support this imaging and this therapy in Tennessee, we can benefit these communities who likely don't get to travel."

ORNL research

Davern and Osborne agree that many more promising therapies are on the horizon. To get there, though, researchers have some technical challenges to solve.

One is to develop more and more effective cages — called chelators — for attaching radioisotopes to the locator molecules. To that end, Davern heads a Laboratory Directed Research and Development initiative at ORNL called Accelerating Radiotherapeutics through Advanced Molecular Constructs, or ARM.

"With the technology that's out there," she said, "you need to heat the reactions pretty intensely to be able to get the radionuclide to go into that cage, and that would destroy any kind of biological molecule like an antibody. So we're looking at ways to do this in more physiologically relevant conditions so that you don't destroy these more sensitive targeting molecules."

The project is also looking closely at other promising isotopes, including actinium-225. ORNL is currently the principal supplier of this isotope for medical research. Other medical radioisotopes produced at the lab using the High Flux Isotope Reactor include actinium-227, which is the critical raw material for the radium-223 that goes into Bayer's prostate cancer drug Xofigo.

"Actinium-225 is what we think will be next in line for regulatory approvals," Davern said, "due to how they're moving through clinical trials. Right now we produce most of the actinium-225 available for these clinical trials."

Nuclear medicine needs workers

Davern is also an anchor researcher for a workforce-focused initiative from the University of Tennessee-Oak Ridge Innovation Institute.

> *The fact that these [therapies] are so effective with less side effects than our current standards of care — what a great combination.*
>
> — University of Tennessee Graduate School of Medicine Molecular Imaging and Translational Research Program Director **Dustin Osborne**

"What we're trying to do with the convergent research initiative is to help build across the whole state — from Memphis to Knoxville and Oak Ridge — a capability that builds up both the education and the workforce to be engaged in developing that next important radiopharmaceutical," she said.

"So we can do the R&D, but we're also thinking about that next generation of worker and researcher who will be necessary to attract new industry to the state."

Davern noted that the workforce needs of the nuclear medicine industry mesh with those of the nuclear power industry, especially for people who work directly with radioactive isotopes.

"We have similar workforce and education needs as people in the nuclear energy industry to work on the radioisotope production side, both in nuclear engineering and in the technician side for working with radioactive materials and the support side for keeping track of nuclear materials," she said.

Many more workers will also be needed in hospitals, Osborne said.

"Not only do we have a shortage of technologists to run the machines and shortages of physicists like me to do the dosimetry calculations and set up the scan protocols, we have shortages also of radiopharmacists, who are the ones who can release the drugs for us to use in the first place."

The future of nuclear medicine in East Tennessee

If the field delivers on the promise it is showing, those needs will only multiply. Davern believes East Tennessee can take advantage of the coming boom in nuclear medicine, but it will take hard work.

Dustin Osborne

"We have all the pieces and parts to be an ecosystem for this development," she said, "but it's how to make them all connect. The whole Tennessee corridor has really interesting capabilities, because we can have medicine linking with research linking with the national lab and going from biology all the way through to radioisotope production."

Osborne noted that the more these therapies succeed, the more people will insist on having access to them.

"The fact that these are so effective with less side effects than our current standards of care — what a great combination, if we can be more effective and less impactful on the patient's quality of life.

"To say that I'm excited about where we're going is still a massive understatement."

Paving paths

for a new nuclear workforce


Clarice Phelps

By Natori Mason
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If East Tennessee's nuclear industry is to grow, it must rely on a robust local workforce.

To prepare students to enter that workforce, local community colleges are offering nuclear-focused classes under their associate degree programs. Students who enroll in the courses will learn fundamentals of the nuclear industry — such as equipment usage and waste management — and gain hands-on experience that is usually only acquired on the job.

> *I was a former technician, so I know the importance of technicians to the ORNL workforce. They are a huge part of researchers and principal investigators being able to get their work done.*
>
> — ORNL engineer **Clarice Phelps**

Pellissippi State Community College signed an agreement with ORNL in June 2023 to offer a chemical radiation technology pathway. Core classes in this program include analytical chemistry, radiochemistry and hazardous waste control. Two of these classes — radiochemistry and hazardous waste control — are taught by ORNL staff members.

The chemical radiation technology pathway connects students to ORNL facility tours, internship programs and potential employment opportunities. Students who complete a two-year degree and a summer internship will be well-positioned to enter the workforce at ORNL or another national lab or through industry-adjacent careers.

ORNL engineer Clarice Phelps developed this pathway to offer underrepresented communities an accessible entry point to careers in science, technology, engineering and mathematics, specifically careers in the nuclear field. She serves as an adjunct professor teaching Pellissippi State's radiochemistry class.

"I wanted to focus on getting people the background knowledge, so they could apply for those entry-level technician positions," Phelps said. "I was a former technician, so I know the importance of technicians to the ORNL workforce. They are a huge part of researchers and principal investigators being able to get their work done."

Phelps said education provides numerous opportunities for students to flourish. She hopes eventually to create similar community college programs that cover other important areas in STEM.

"We're helping to advance the general education of the area, creating new jobs and contributing to building generational wealth for these families," she said.

Roane State Community College is responding to the nuclear workforce need with a nuclear technology program led by the college's Joe Stainback IV. The curriculum combines existing chemical engineering and environmental health classes with three new nuclear-focused classes: nuclear science and radiochemistry, nuclear systems and operations, and radiation detection measurements. Additionally, Stainback is working with industry to bring on course instructors and secure internships for students in the program.

The industry has a need, and the students have a want. You want to match those two. The aperture of nuclear technologies is quite large, so it depends on what the student's goals are and spending time with them to help match that up.

— Roane State Community College nuclear technology program led **Joe Stainback IV**

Students enrolled in the program will be able to earn either a two-year degree or a certificate through a condensed course. Stainback said the certificate track would be beneficial to engineers who are not in the nuclear field but wish to learn about the basics of nuclear history and safety.

"The industry has a need, and the students have a want. You want to match those two," Stainback said. "The aperture of nuclear technologies is quite large, so it depends on what the student's goals are and spending time with them to help match that up."

In 2023, Roane State received $100,000 from ORNL's managing contractor, UT-Battelle, and a $1.4 million grant from the Department of Labor to help launch the program. In 2024, the college has received three grants supporting the program, including $546,000 from the National Science Foundation, $462,000 from the Tennessee Nuclear Energy Fund and $450,000 from the Governor's Investment in Vocational Education grant program.

The first cohort of the nuclear technology program has enrolled, with its nuclear-focused classes beginning in 2025.

Joe Stainback IV. Image Courtesy Roane State Community College

Early career researchers win big

by Natori Mason
ornlreview@ornl.gov

For more than a decade, DOE's Office of Science has motivated and supported young scientists through its Early Career Research Program. Recently, five ORNL scientists were selected to receive an award for their innovative proposals. Additionally, they will receive $500,000 per year over the next five years to cover salary and research expenses.

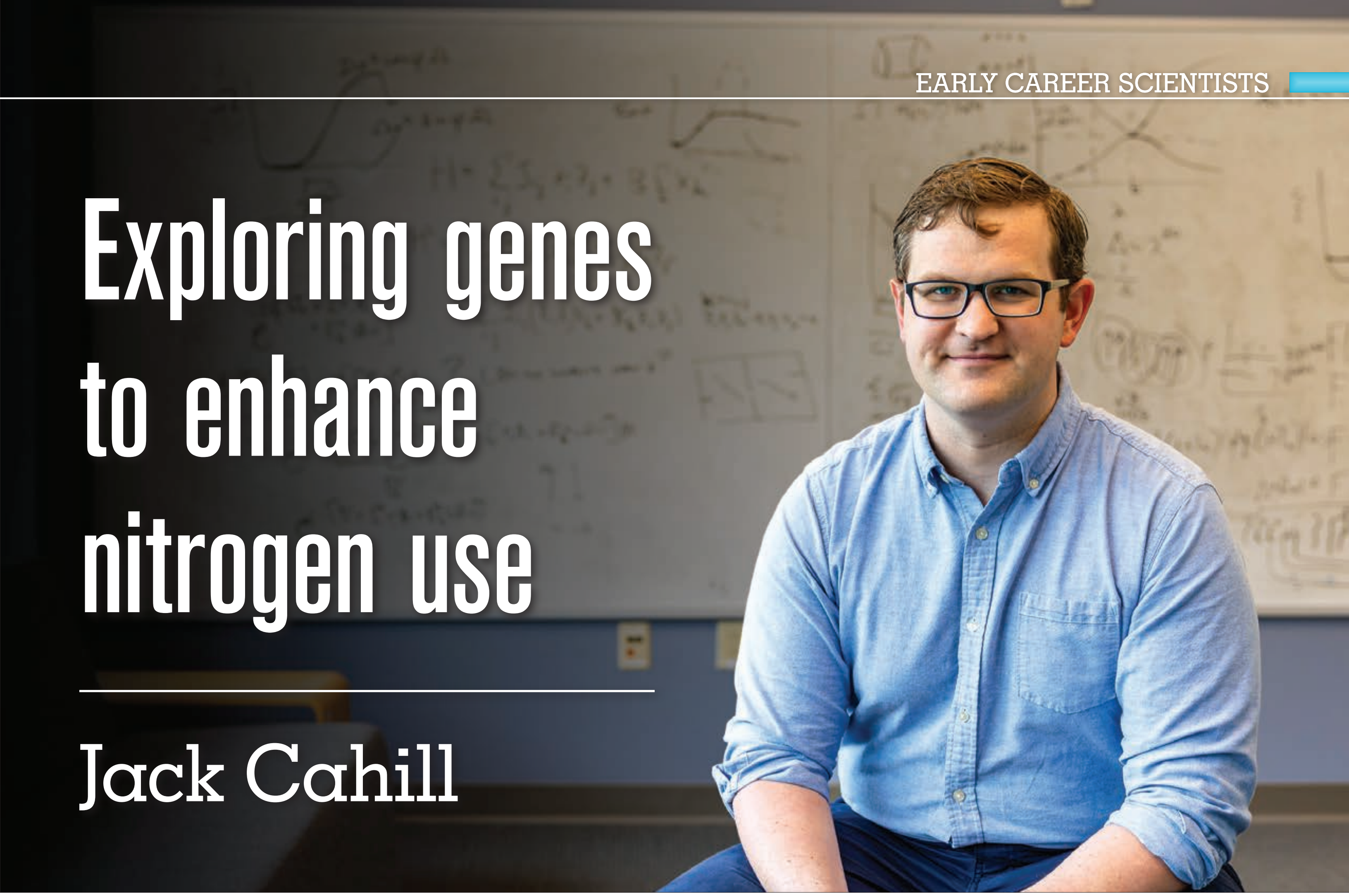
"To ensure the national labs deliver on their important missions, we must support our scientists. DOE's Early Career Research Program is an essential element in doing that," ORNL Director Stephen Streiffer said. "I'm excited for those chosen from ORNL, who I know will build upon this foundational opportunity to expand scientific impact."

ORNL award recipients:

- **Matthew Brahlek**, an R&D staff scientist in the Materials Science and Technology Division, was selected by the Basic Energy Sciences program for his proposal "Epitaxially Imposed Control of Chiral Transport Phenomena."
- **Jack Cahill**, an R&D associate scientist in the Biosciences Division, was selected by the Biological and Environmental Research Program for his proposal "Elucidation and Validation of Genes Associated with Biological Nitrification Inhibition in Populus."
- **Eugene Dumitrescu**, a staff research scientist in the Computational Science and Engineering Division, was selected by the Advanced Scientific Computing Research program for his proposal "MLRep4QC3: Multi-Linear Representations for Quantum Characterization, Control, and Computation."
- **Takaaki Koyanagi**, an R&D staff scientist in the Materials Science and Technology Division, was selected by the Fusion Energy Sciences Program for his proposal "Mechanistic framework for additive manufacturing of highly radiation-resistant SiC components."
- **Dan Lu**, a senior staff scientist in the Computational Sciences and Engineering Division, was selected by the Biological and Environmental Research program for her proposal "Integrating Machine Learning Models into E3SM for Understanding Coastal Compound Flooding."

On the following pages, learn more about these talented researchers and their proposals.

From left to right, Matthew Brahlek, Eugene Dumitrescu, Dan Lu, Takaaki Koyanagi and Jack Cahill. Image credit: Carlos Jones, ORNL



Exploring genes to enhance nitrogen use

Jack Cahill

by Natori Mason
ornlreview@ornl.gov

Nitrification, the conversion of ammonia to nitrates, is necessary for plant growth and development. However, this process is inefficient, as nitrate yields are low and reaction rates depend heavily on factors such as soil moisture, temperature and pH levels.

Fertilizer is often used to address this inefficiency, yet it proves ineffective and costly, as most of the nitrogen in fertilizer is unused by crops. In addition, nitrate runoff can infiltrate and contaminate aquifers.

Jack Cahill's proposal, "Elucidation and Validation of Genes Associated with Biological Nitrification Inhibition in Populus," aims to discover plant mechanisms that will increase nitrogen use efficiency.

"If we understand the genetic basis for why certain plants can manipulate their nitrogen use efficiency, we can potentially manipulate the genes of other plant systems," Cahill said, "meaning we don't have to put as much fertilizer into the ground, which costs less, saves a lot of energy and can help the environment."

Populus trees like aspen, cottonwood and poplars have potential for sequestering carbon, making them attractive candidates for research. Carbon sequestration is the process in which carbon dioxide is removed from the atmosphere and stored in a carbon pool, such as plant roots or soil. Populus trees grow rapidly, around 6 feet per year, enabling them to absorb large quantities of carbon dioxide from the air.

In addition, Cahill has participated in several technology developments that increase the speed, scale and quality of sampling. One example is the Rapid Droplet Sampling Interface, which uses nanoliter-sized droplets of a sample and can analyze up to five samples per second.

"These high-throughput techniques have become an enabling capability. For us to understand what genes are involved in these nitrification processes, we need to be able to measure a lot of plants, a thousand or more. That becomes hard to accomplish with conventional technologies," Cahill added.

Cahill's interest in environmental research began during his graduate studies at the University of California, San Diego. His focus was atmospheric chemistry, specifically how particles become pollution and affect climate. Collaborating with environmental studies professors fueled his ambition to make a significant impact through his work.

Outside the lab, Cahill enjoys woodworking and hiking, activities that reflect his hands-on approach to nature.

"I'm very much a hands-on person and enjoy building, and woodworking is one of those things where you can create anything with wood," he said. "I use a lot of those skills to develop more sophisticated techniques like that at ORNL."

Coastal flooding is personal for climate modeler

Dan Lu

by Natori Mason
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Dan Lu, a senior staff scientist in ORNL's Computational Sciences and Engineering Division, has been deeply fond of water since she was a child. She grew up in a small town in Jiangxi, China, surrounded by the Yangtze River, that regularly faces severe weather and coastal flooding.

"My hometown is facing flooding issues almost every year, so I always think about how we can mitigate these hazards," Lu said. "That's why I pursued my bachelor studies in water resources engineering, then moved to a Ph.D. in computational hydrology."

Lu's Early Career Research award project, "Integrating Machine Learning Models into E3SM for Understanding Coastal Compound Flooding," aims to develop a physics and data-driven modeling system to simulate and evaluate compound flooding, which occurs when two or more flooding sources, such as open oceans and watersheds, interact.

"About 700 million people globally are living along coastal regions. That number is estimated to reach 1 billion by 2050," Lu said. "We want to understand the environmental and societal impacts and importance; that's why our case study is set in coastal urban areas."

Lu will utilize data from coastal regions gathered via sensors, observatories and radars from multiple environmental agencies, such as the National Oceanic and Atmospheric Administration, U.S. Geological Survey and DOE. This data contains critical information on flood drivers, processes and river network geometry and their influences on coastal flooding.

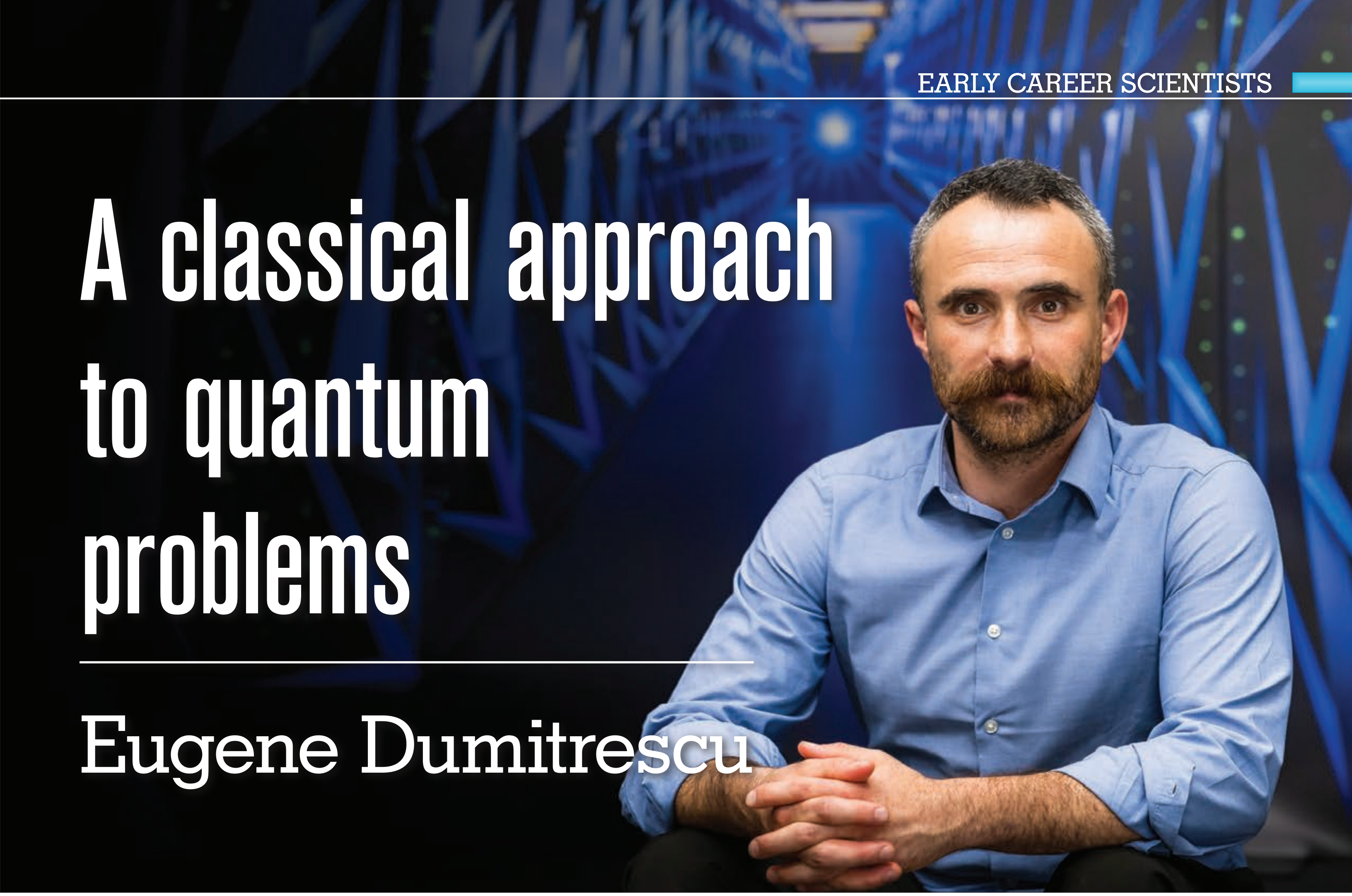
E3SM integrates models of the atmosphere, land, river, ocean, sea ice and land ice. MOSART, or Model for Scale Adaptive River Transport, has been coupled with the program for coastal flood simulation, yet there are several limitations using these models individually.

MOSART uses one-way coupling to measure the motion of fluid flow affected by structural deformation and vice versa. However, this method cannot capture the interactive cause of flooding, resulting in an underestimation of flood risks.

"To fill the knowledge and modeling gaps and leverage a large amount of diverse data, this project will use machine learning methods to extract knowledge from prior data to advance process understanding and build a mesh-free, data-informed river model to improve flood simulations," Lu said. "On the other hand, the E3SM framework can simulate the regional and global water cycle, providing a platform to investigate feedback and interactions of the compound flooding processes under climate change."

A classical approach to quantum problems

Eugene Dumitrescu



by Natori Mason
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Quantum computing is a rapidly developing field that promises breakthroughs in materials science, high-energy physics, and encryption. However, quantum computing has a way to go before it reaches this potential.

Quantum computers rely not on bits — the 1's and 0's that encode information in a classical computer — but on qubits, information units that can have a wider range of values. Though these qubits are potentially very powerful, they are also very fragile and are prone to noise, leading to loss of information.

Eugene Dumitrescu, a staff research scientist in ORNL's Computational Science and Engineering Division, believes classical computers can do a much better job of analyzing quantum systems.

As an example, Dumitrescu compared the acoustic waves of a musical note to a wavefunction in quantum physics, which describes a particle's quantum state.

"We've been studying music longer than we have been studying quantum science, able to express things more beautifully," he said. "With dissipative quantum systems, that's an instrument we haven't learned yet."

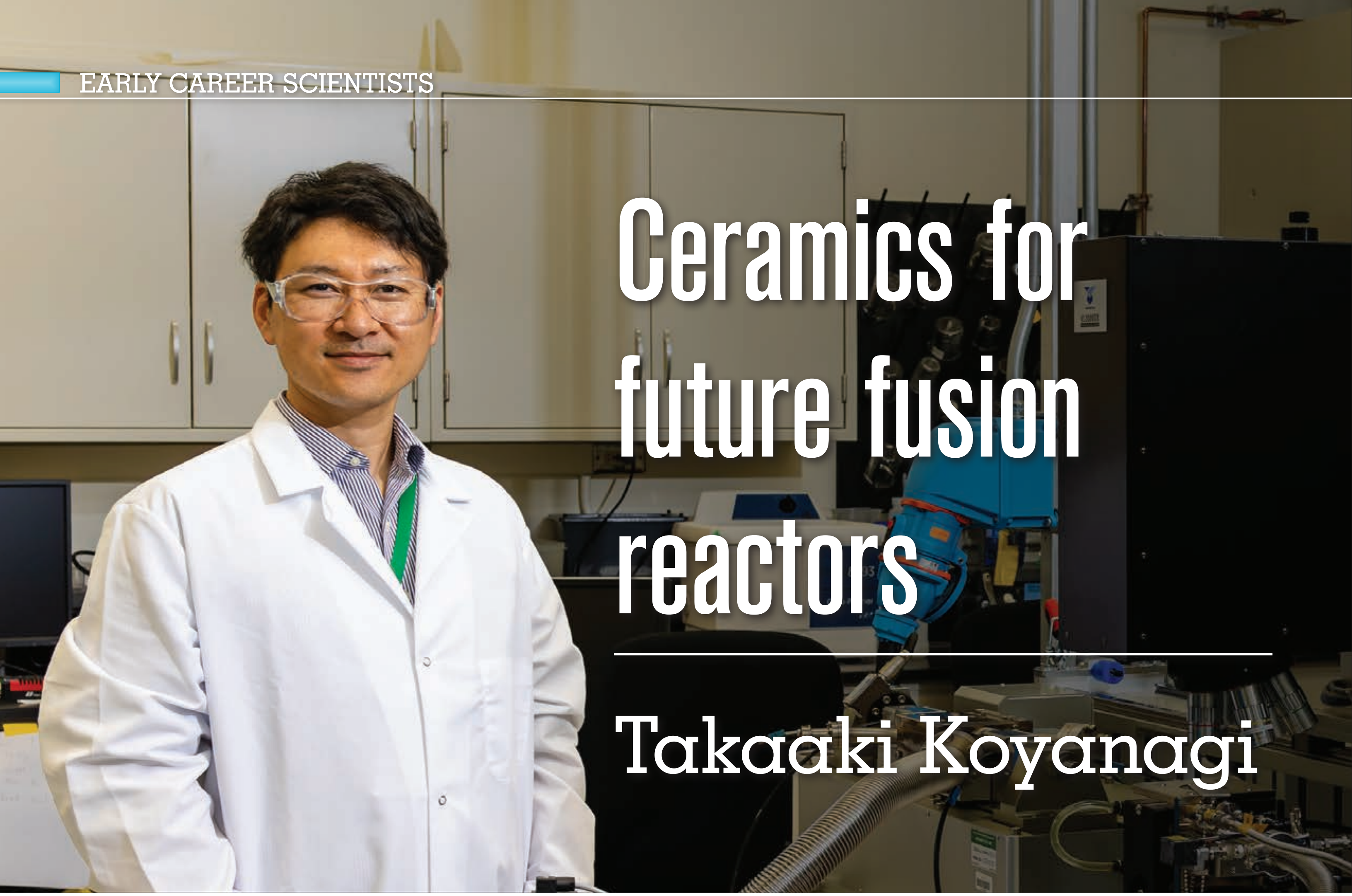
Dumitrescu's Early Career Research proposal, "MLRep4QC3: Multi-Linear Representations for Quantum Characterization, Control, and Computation," focuses on creating a linear algebraic package composed of algorithms that effectively represent quantum states on a classical computer.

"It's important to simulate and push the limits to understand what classical computers can do in the first place," he said. "We suspect they cannot simulate a full universal quantum computer, but it will be possible to simulate pieces of a computation or device."

The project will use tensor networks, models formed by multilinear objects like vectors and matrices, to simulate perfect quantum computers. By combining simulation capabilities with algorithm design, Dumitrescu aims to create a benchmark suite for classical computers, showcasing their ability to model quantum phenomena effectively.

When asked about ORNL's quantum computing capabilities and if the lab has a quantum computer, Dumitrescu adds that the lab not only has a quantum computer, but a state-of-the-art machine. Surprisingly, he's not referring to a superconducting experiment or even a supercomputer.

"People will ask me what qualities make it the best, if it is trapped-ions, superconducting or cold atoms, but that's not the case. The best is our classical computers, laptops and PCs, if used correctly," he said. "My goal is to unleash this latent potential, and I believe Oak Ridge is the natural place for that."



Ceramics for future fusion reactors

Takaaki Koyanagi

Takaaki Koyanagi, an R&D staff scientist in ORNL's Materials Science and Technology Division, discovered materials science and ceramics composition while playing tennis.

"I played tennis from junior year in high school into college," Koyanagi said. "During that time I saw the advancement of the tennis racket; it became lighter and stronger, and that's based on the advancement of carbon fiber composite materials."

While Koyanagi continues to contemplate advances in materials science, his current focus lies in developing ceramic materials for nuclear energy. The objective of his research proposal, "Mechanistic framework for additive manufacturing of highly radiation-resistant SiC components," is to advance fusion research by developing 3D-printed ceramic compositions for fusion reactor cores.

Fusion reactors, powered by the same process that fuels the sun, reach extreme temperatures, demanding components that meet rigorous requirements for resistance to heat and high-energy particle irradiation. Developing technologies to produce materials meeting these criteria can mitigate degradation and enhance long-term reliability.

Currently, alloys are the main materials proposed for fusion reactor core structures because of the maturity of the technology, yet ceramic materials like silicon carbide are proving to be a more attractive option. Their high heat resistance opens the way for high-energy conversion efficiency. Moreover, silicon carbide can reduce the production of large quantities of highly radioactive waste during reactor operation.

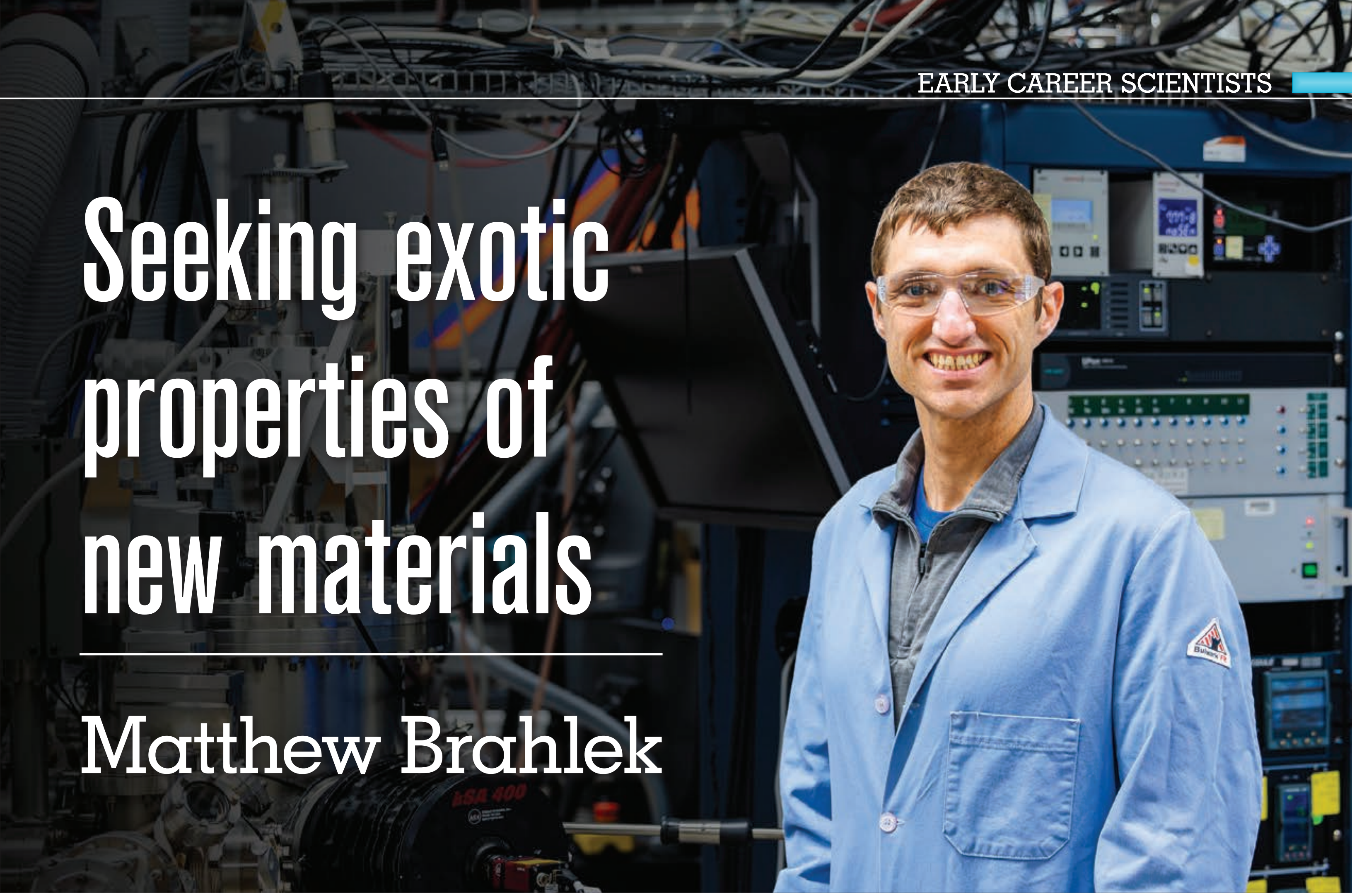
"If you want a structure that can withstand these temperatures or pushes the limit of a material, ceramics have played that role," Koyanagi said.

Koyanagi focuses on additive manufacturing because it allows designers to create complex shapes. Although ceramics have potential, they are very hard and brittle; thus they are difficult to shape into complex geometries using conventional techniques. Additive manufacturing, a way to overcome this limitation, uses a 3D printer that lays down the material in a continuous pattern, building the structure layer by layer.

Additive manufacturing is becoming a more common process for creating structural pieces, whether they are used for scientific instruments or everyday items. After seeing such promise for laboratory-scale productions, Koyanagi believes the next step will be to start scaling for industry-level production.

Fascinated by the role of ceramics, both in scientific developments and everyday life, Koyanagi notes another way this material is changing the game.

"These days, ceramic-based materials are used in aircraft engines and gas turbines," he said. "It's been interesting seeing the technology evolve from my childhood to now, and I'm hoping to add my contributions as well."



Seeking exotic properties of new materials

Matthew Brahlek

Matthew Brahlek, an R&D staff scientist in ORNL's Materials Science and Technology Division, has always been fascinated with how technology works.

"To get at the most fundamental aspects, the most basic understanding of how things work is what drove me from engineering into physics," Brahlek said.

Brahlek's Early Career Research proposal, "Epitaxially Imposed Control of Chiral Transport Phenomena," focuses on the synthetization and control of new materials for applications in quantum technologies. These systems are created through a process called epitaxy, where crystals are grown or deposited in thin layers, with the materials being built up one layer of atoms at a time.

"If you have a large chunk of a material, it behaves very differently than if you have an atomic layer, or are at an atomically sharp interface," Brahlek said. "So being able to control materials at this level is a critical component for applying them to actual technologies."

Brahlek sees his current work as an extension of his childhood tinkering.

"One of the things I really like about ORNL is we have lots of equipment," he said. "Our lab is well equipped with the instruments that enable us to tackle hard problems and address challenging questions. Having an idea of what you want to create, gathering all the pieces together and making it work is one of the things I take the most joy from."

Today's semiconductors are enabled by fundamental research done half a century ago. At the time, the focus was on the properties of silicon and germanium semiconductors and, ultimately, how to control the flow of electricity through the materials.

"These semiconductors have dominated the industry for several reasons," Brahlek said. "They possess the right electronic properties, they can be made sufficiently clean with few defects, and pristine interfaces can easily be created. These two latter points are made possible by the simple chemical and crystalline properties."

Current materials research is pushing toward new materials with exotic properties, and understanding how to create these more complex materials is the critical first step. Brahlek is working to tackle these questions, which will enable researchers to bridge basic research with new applications in electronic and quantum devices.

Dedicating time each day to think about and pursue new ideas is a concept that Brahlek has practiced from a young age. This mindset is ultimately what pushed him in the direction to pursue a career in science. As Brahlek continues his research journey, he manifests goals of finding new problems to solve and growth in project leadership.

Neutrons score

electrochemical win for carbon-neutral ammonia

by Sumner Brown Gibbs
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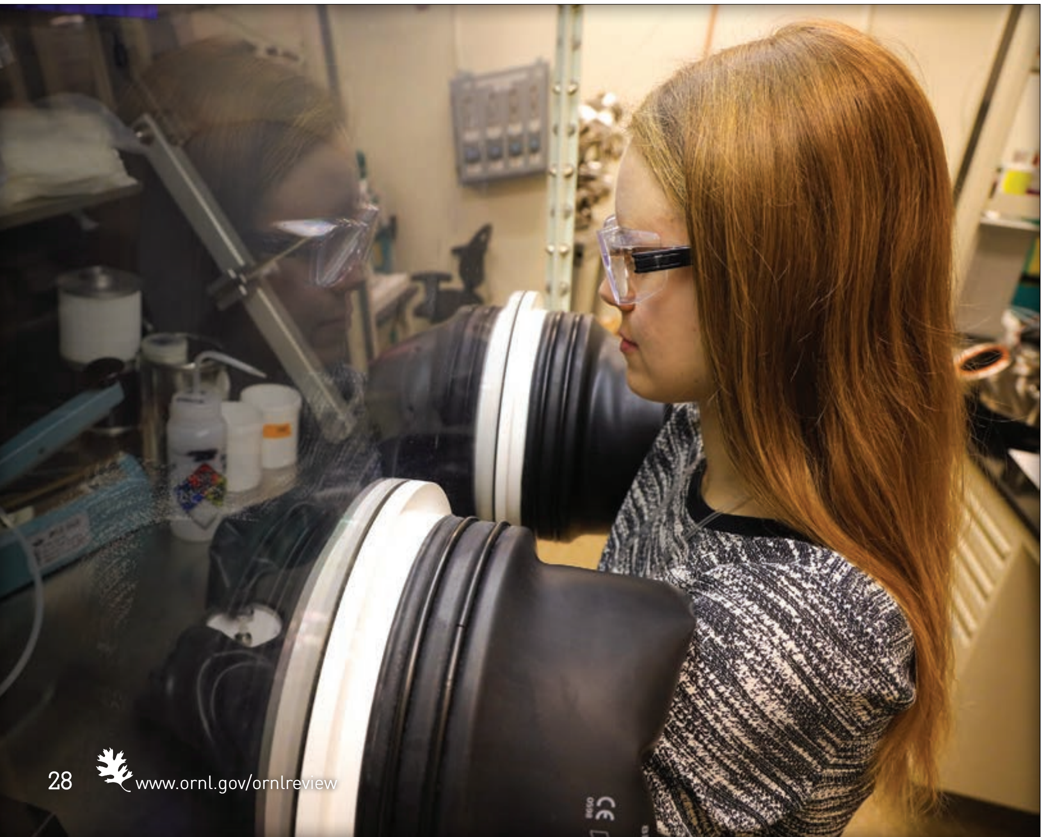
Scientists from Stanford University and ORNL are turning air into fertilizer without leaving a carbon footprint. Their discovery could deliver a much-needed solution to help meet worldwide carbon-neutral goals by 2050.

Published in the Royal Society of Chemistry's *Energy & Environmental Science*, the team's study describes a sustainable electrochemical — rather than chemical — process for producing ammonia, a key ingredient for nitrogen fertilizer. In essence, the researchers used neutron scattering to understand how cycling an electric current during the conversion of nitrogen to ammonia increases the amount of ammonia produced. The study also produced a new technique for neutron scattering at ORNL's Spallation Neutron Source that captures greater detail much like watching a movie frame by frame.



This electrochemical process could enable farmers to convert nitrogen, the most abundant element in our atmosphere, into ammonia-based fertilizers without emitting carbon dioxide.

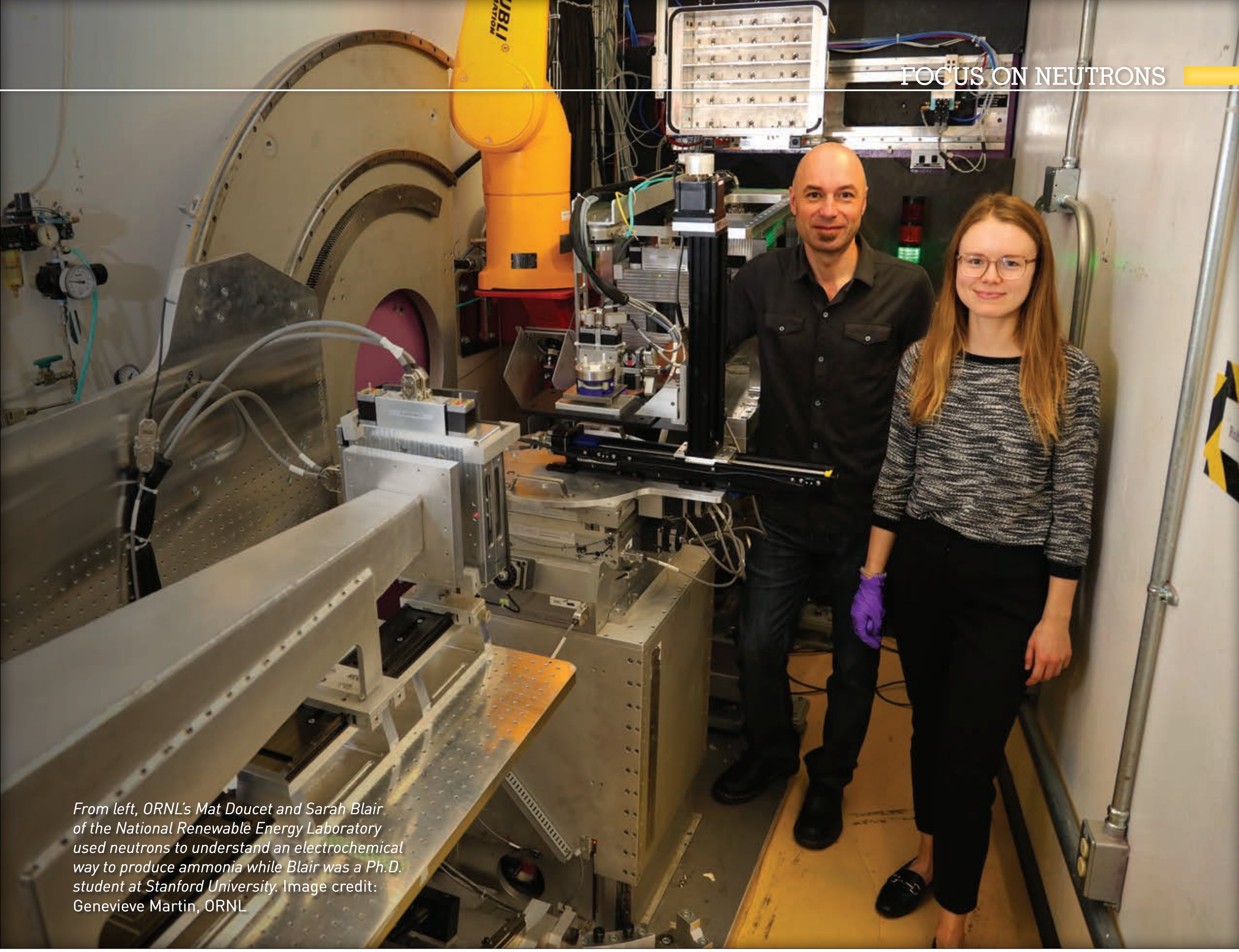
"Ammonia is critical to food supplies for most of the world's population," said Sarah Blair, a postdoctoral researcher at the National Renewable Energy Laboratory who led the study as a doctoral candidate at Stanford's Center for Interface Science and Catalysis. "As the world population continues to grow, we need sustainable ways to produce fertilizers — especially as warming intensifies."

Industrial fertilizers allow farmers to grow more food on less land. Yet the primary method to create industrial ammonia for more than a century, the Haber-Bosch process, accounts for nearly 2 percent of all carbon dioxide emissions because of the fossil fuels it requires. Two percent might not sound like a lot, but carbon dioxide is being released into the atmosphere faster than the planet can absorb it, making every effort count toward reducing that number. The Haber-Bosch process produces about 500 million tons of carbon dioxide each year, which would require the equivalent of almost all of the federal lands in the U.S. to absorb and store.

Insights from the study could also help scientists understand other processes for making carbon-neutral ammonia for other applications. These could include recycling or recapturing fertilizer runoff before it enters water streams and producing ammonia at seaports for fueling ships. Global shipping produces another 3 percent of the world's carbon dioxide emissions, and fossil fuel combustion accounts for the largest source of carbon dioxide from human activity.

"You can't improve the design of something if you don't know how it's already working," Blair said. "Neutrons

Sarah Blair used a glovebox in the experiments, which required close collaboration and careful design by Mat Doucet so the project could make the most of limited beam time. Image credit: Genevieve Martin, ORNL



From left, ORNL's Mat Doucet and Sarah Blair of the National Renewable Energy Laboratory used neutrons to understand an electrochemical way to produce ammonia while Blair was a Ph.D. student at Stanford University. Image credit: Genevieve Martin, ORNL

help science evolve by shedding light at the atomic level on systems that are impossible to study otherwise."

This study not only produced valuable insights for carbon-neutral ammonia but also contributes to producing better batteries. The work of Blair and Mat Doucet, a senior neutron scattering scientist at ORNL, marks the first use of neutron-based techniques to observe the formation of a solid electrolyte interface layer during this type of electrochemical conversion.

The new neutron scattering technique that emerged from the study, time-resolved reflectometry, allows scientists to slice neutron data into increments of a few seconds. Essentially, this provides an ability to observe multiple time scales during these types of experiments.

> *Ammonia is critical to food supplies for most of the world's population. As the world population continues to grow, we need sustainable ways to produce fertilizers — especially as warming intensifies.*
>
> — ORNL researcher **Sarah Blair**

"Processes that appear to be linear might not be linear at all when you look at them more closely," Doucet said. "Getting to that structure as a function of time is the hard part. The technique we developed for this experiment allowed us to do just that."

Hanyu Wang, an ORNL instrument scientist who also works closely with users at ORNL's Spallation Neutron Source, said, "These time-dependent experiments will draw scientists who study separation chemistries."

ORNL Neutron Reflectometry group leader Jim Browning added, "Their approach can answer a lot of questions for separation chemistries, batteries and an entire gamut of different areas of interest, like energy production, energy storage and conservation of energy."

3D-printed turbine blades a first

by Heather Duncan
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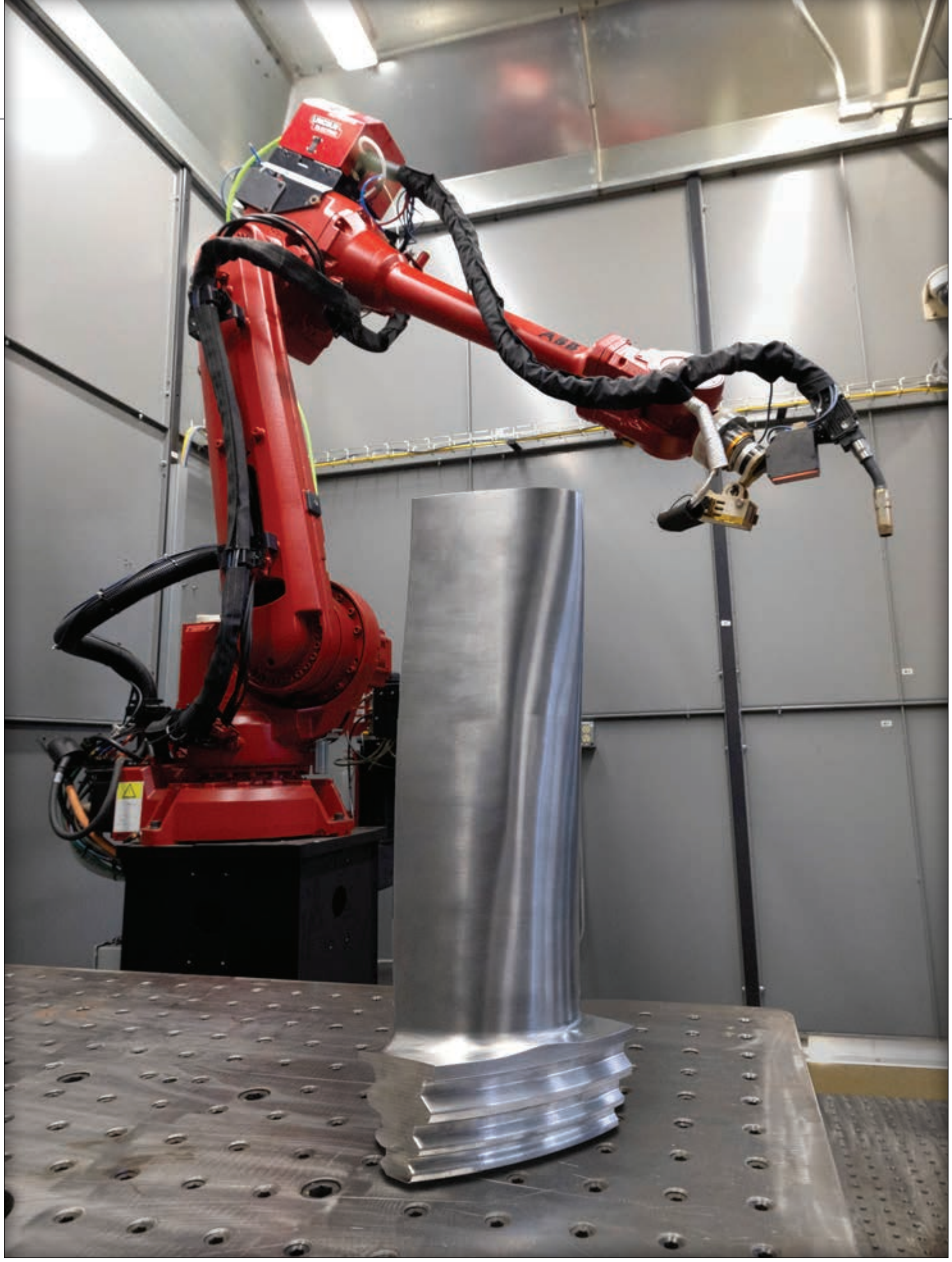
ORNL researchers have become the first to 3D-print large rotating steam turbine blades for generating energy in power plants.

Led by partner Siemens Technology, the U.S. research and development hub of Siemens AG, the project demonstrates that wire arc additive manufacturing is viable for the scalable production of critical components exceeding 25 pounds. These parts have traditionally been made using casting and forging facilities that have mostly moved abroad.

"There's now a realization that we cannot get low-volume castings and forgings that exceed 100 or 200 pounds from the domestic supply chain," said Michael Kirka, the project's lead researcher and leader of ORNL's Deposition Science and Technology group. "It's put us in an untenable position, especially as we see how international conflicts have affected the international movement of critical supplies."

Wire arc additive manufacturing uses an electric arc to melt metal wire in a process controlled by a robotic arm. Thin layers of metal are gradually built up into the desired shape. Once printed, the part is machined to meet final design requirements. The wire-arc technology used to manufacture the turbine blade was developed in collaboration with Lincoln Electric under a cooperative research and development agreement.



Wire arc additive manufacturing allowed this robot arm at ORNL to transform metal wire into a complete steam turbine blade like those used in power plants. Image credit: Carlos Jones, ORNL

Because wire arc manufacturing is based on welding technology, it is easily used for repairing existing parts. When the Siemens wire arc research began in 2019, it focused on component repair. However, the scope expanded during the COVID-19 pandemic, when the wait for new cast steam turbine blades stretched to two years. Then the project broadened to include printing entire replacement parts for turbine engines for gas, coal and nuclear power plants, Kirka said.

ORNL researchers experimented with materials and developed better ways to evaluate the mechanical performance of printed parts. The large steam turbine blade, made from a steel alloy, was the culmination of these efforts.

"The original intent was to just print 25 percent of the top section of the blade," said Anand Kulkarni, senior principal key expert for Siemens Technology. "But when we saw the potential of the wire arc setup at ORNL, we thought we could do the whole blade in one build. The capability to scan the part while it was being built gave us the right information that could be fed to our machining staff and enabled us to reduce production time."

ORNL was able to print the blade in 12 hours, then machine it and complete the part in two weeks, Kulkarni said.

> *The original intent was to just print 25 percent of the top section of the blade. But when we saw the potential of the wire arc setup at ORNL, we thought we could do the whole blade in one build. The capability to scan the part while it was being built gave us the right information that could be fed to our machining staff and enabled us to reduce production time.*
>
> — Siemens Technology **Anand Kulkarni**

Although wire arc is a prominent 3D-printing technology, it had not previously been used to make a rotating component of this scale, Kirka said. Turbine blades typically have no parallel or perpendicular surfaces. Their contoured curves narrow toward the tip.

"Being able to print and finish something with no locating features is a challenge," he said. In addition, heavier parts of this size cool more slowly, adding sensitivity to the speed of deposition and order of the layers.

Siemens continued testing the part with the Electric Power Research Institute.

"We're still to see how results compare with traditional methods," Kulkarni said.

Properties don't have to be identical for repairs needed to keep engines running, he said, "but if the quality of the part is good, that opens doors to more on-demand manufacturing. And this case study opens the envelope to large components."

The steam turbine blade was funded by the DOE Office of Fossil Energy and Carbon Management and printed in DOE's Manufacturing Demonstration Facility. The MDF, supported by DOE's Advanced Materials and Manufacturing Technologies Office, is a nationwide consortium of collaborators working with ORNL to innovate, inspire and catalyze the transformation of U.S. manufacturing.

ORNL researchers Chris Masuo, left, and Luke Meyer monitor the heat signatures of a steam turbine blade that was additively manufactured in a wire arc 3D printer at DOE's Manufacturing Demonstration Facility at ORNL. Image credit: Carlos Jones, ORNL

Medium-voltage research

promotes clean, reliable power

by Heather Duncan
duncansh@ornl.gov

ORNL scientists are looking for a happy medium to enable the grid of the future, filling a gap between high and low voltages for power electronics technology that underpins the modern U.S. electric grid.

Today's power electronics, which take split seconds to perform tasks such as converting the direction of current or adjusting voltages, tend to operate at the extremes. Charging personal vehicles or storing energy from a commercial solar panel requires low voltage, while high voltage is used for utility-scale projects like wind and solar farms or interconnecting power distribution and transmission systems.

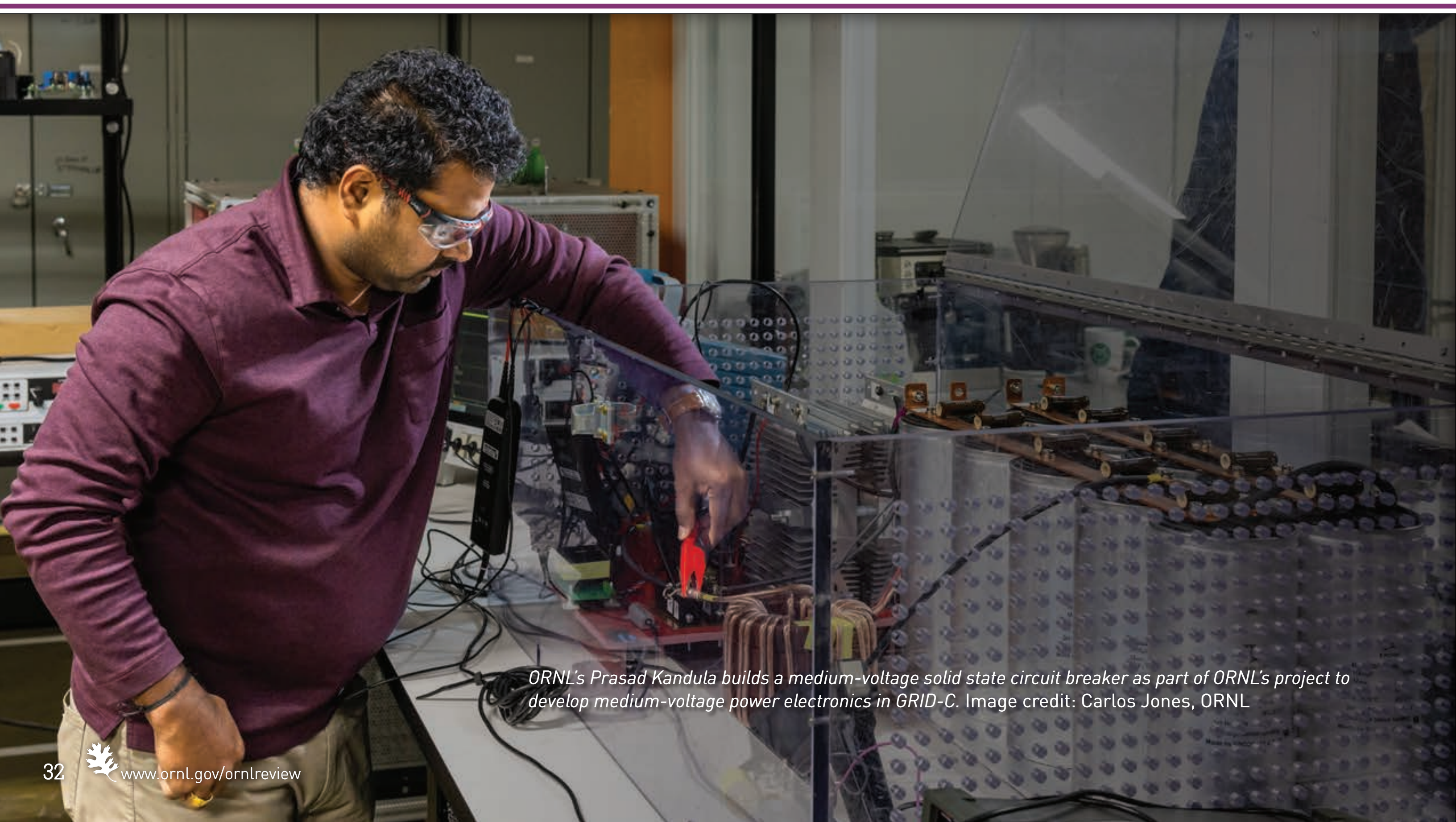
But there is a power electronics gap between 1,500 and 50,000 volts — the "medium-voltage" range — that is critical to larger-scale renewable energy projects, larger equipment such as wind turbines, and larger electric vehicles like trains and vertical-takeoff aircraft.

Bridging that gap will help the U.S. achieve clean energy goals and expand capacity in an overburdened power grid — without erecting thousands of miles of new transmission lines.

"There are many applications that can fit here, but the technology for that middle space hasn't been proven to be reliable or cost-effective," said Prasad Kandula, leader of ORNL's Grid Systems Hardware group.

To help meet the need, ORNL will be guiding DOE's new Medium Voltage Resource Integration Technology program, or MERIT, which teams four national labs and five universities to develop devices that operate efficiently in that middle range.

Kandula notes that medium-voltage power electronics could increase efficiency by reducing the size, weight and



ORNL's Prasad Kandula builds a medium-voltage solid state circuit breaker as part of ORNL's project to develop medium-voltage power electronics in GRID-C. Image credit: Carlos Jones, ORNL

ORNL researcher Prasad Kandula is leading ORNL's effort to develop medium-voltage building blocks, such as converter modules and specialized magnetics, in the Medium-Voltage Laboratory at GRID-C. Image credit: Carlos Jones, ORNL

volume of a system. Plus, they could serve a pressing need by expanding electric grid capacity to meet today's demands and provide tomorrow's economic development opportunities.

Most of the North American electric grid uses alternating current, or AC. But renewable energy generation and electric cars require direct current, or DC. Power electronics are used to switch between these flows and to link separate systems.

Expanding these capabilities to medium voltages could enhance electric reliability. For example, medium-voltage power electronics could be used to feed electricity from a region with extra supply to a neighboring system struggling to meet demand. This could prevent rolling blackouts, price spikes and activation of polluting backup power plants.

ORNL researchers have been developing a menu of medium-voltage building blocks, such as converter modules, specialized magnetics and protection mechanisms that isolate electrical problems.

"With MERIT, we'll develop building blocks of varying types to increase reliability, then stack multiple blocks to reach higher voltages," Kandula said.

This will enable the exploration of new power applications, from recharging long-haul electric trucks to producing green hydrogen for the steel industry. The effort relies on capabilities in ORNL's Grid Research Integration and Deployment Center, or GRID-C.

"We are developing a matrix of technology across components that can go into many applications," said Madhu Chinthavali, head of ORNL's Energy Systems Integration and Controls Section. "GRID-C is uniquely equipped with the component-building proficiency, test beds and expertise to fully develop and test these power electronics components."

For MERIT, ORNL will expand existing relationships with utilities to identify medium-voltage needs. This dovetails with the DOE Office of Electricity's initiative called Power Electronics Accelerator Consortium for Electrification, or PACE, created in 2022 to increase collaboration among research institutions, power companies and manufacturers.

Individual labs can join forces with industrial partners to pursue specific advances in medium-voltage power electronics.

"The end goal for us is to pick a use case, work with a partner, build a full system, install it, show it operational in the field, and show the financial implications," Kandula said.

Other MERIT research partners include the National Renewable Energy Laboratory, Sandia National Laboratories, Pacific Northwest National Laboratory, the University of Arkansas, Virginia Polytechnic Institute and State University, and Florida State University.

Tennessee's nuclear renaissance

East Tennessee's nuclear industry is growing rapidly. Businesses are introducing new reactor and fuel designs. Institutions such as ORNL, the Tennessee Valley Authority and the University of Tennessee are providing knowledge and support. And local colleges are ensuring this growing industry has a skilled workforce. Here are just a few of the region's major players.

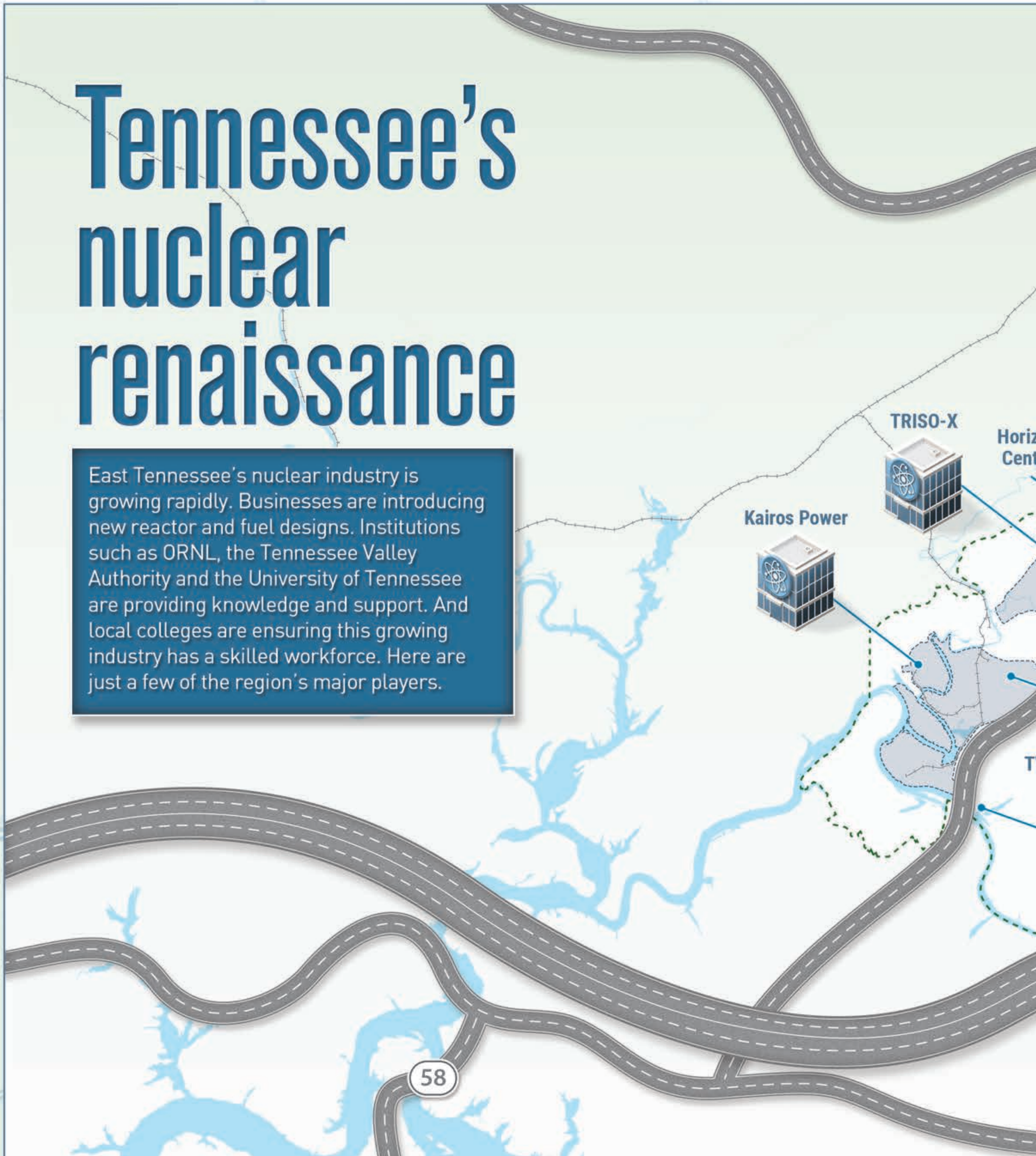
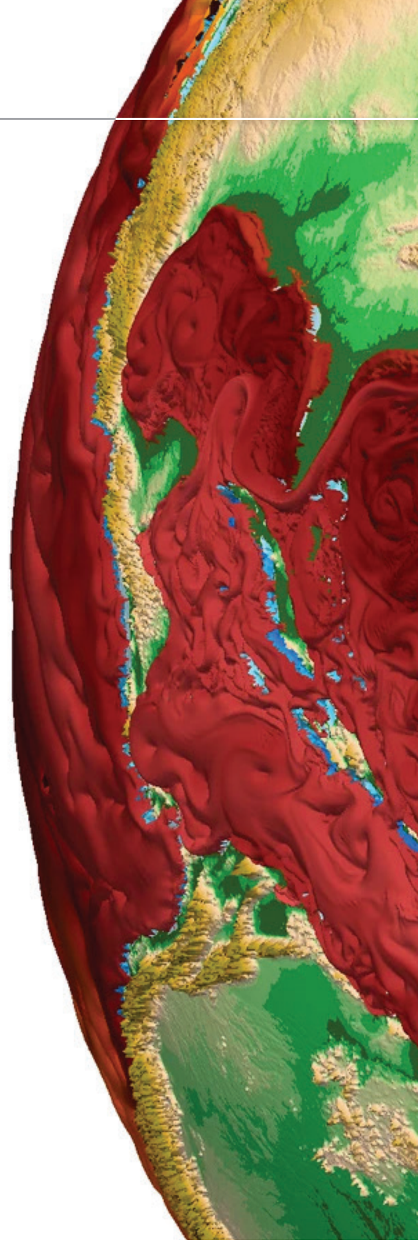


Image credit: Brett Hopwood, ORNL



Custom software speeds up,

stabilizes high-profile ocean model

By Elizabeth Rosenthal
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On the beach, ocean waves provide soothing white noise. But in scientific laboratories, they play a key role in weather forecasting and climate research. Along with the atmosphere, the ocean as a whole is typically one of the largest and most computationally demanding components of Earth system models like DOE's Energy Exascale Earth System Model, or E3SM.

Most modern ocean models focus on two categories of currents: fast, or barotropic, systems and slow, or baroclinic systems. To help address the challenge of simulating these two modes simultaneously, a team from ORNL and Los Alamos and Sandia national laboratories has developed a new solver algorithm that reduces the total run time of the Model for Prediction Across Scales-Ocean, or MPAS-Ocean, E3SM's ocean circulation model, by 45 percent.

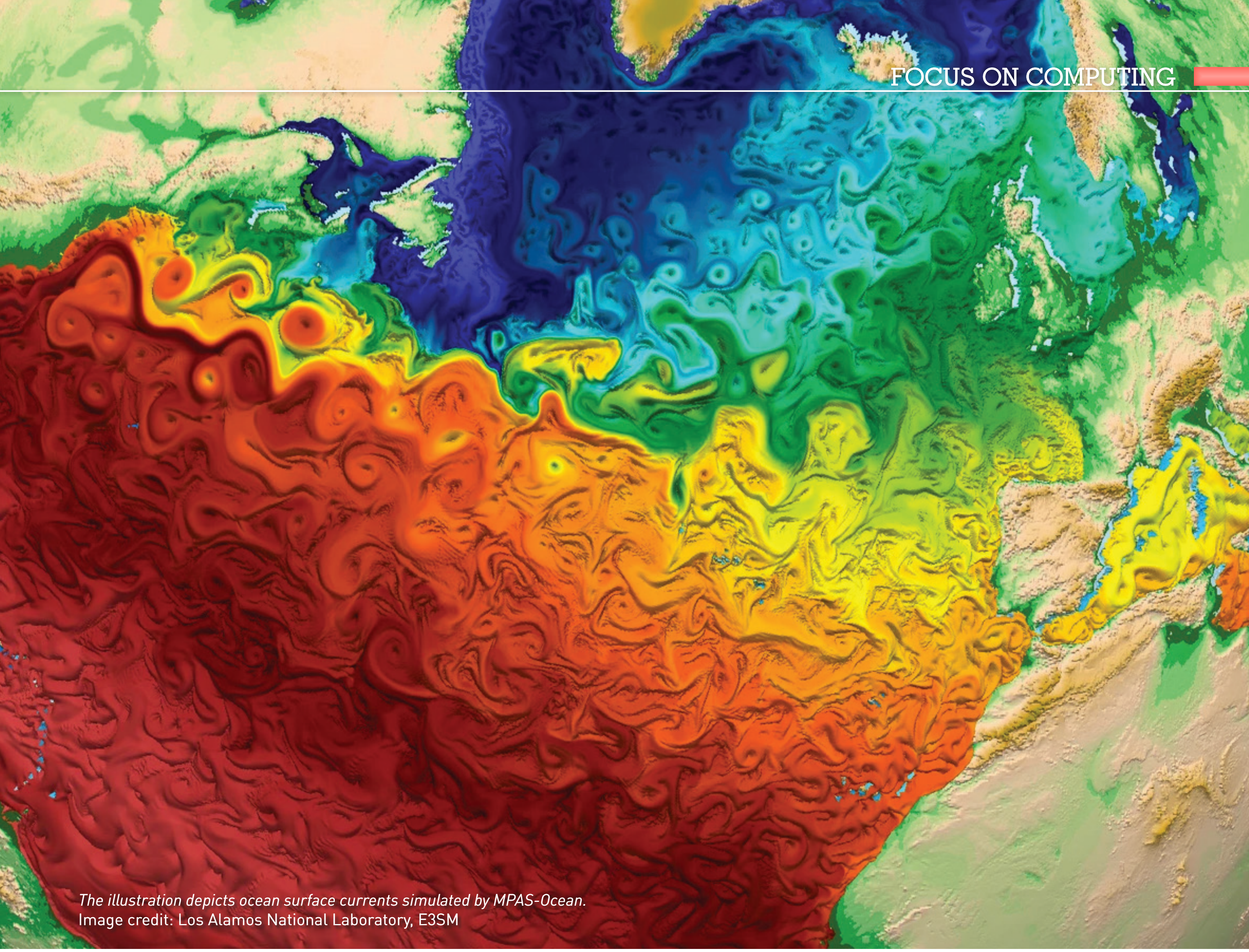
The researchers tested their software on supercomputers at ORNL as well as Lawrence Berkeley and Pacific Northwest national laboratories, and their results were published in the *International Journal of High Performance Computing Applications*.

Trilinos, a database of open-source software ideal for solving scientific problems on supercomputers, is written in the C++ programming language, but Earth system models like E3SM are typically written in Fortran. To overcome this programming language barrier, the team took advantage of ForTrilinos, a software library that incorporates Fortran interfaces into existing C++ packages, to design and customize their barotropic wave-focused algorithm.

"A useful feature of this interface is that we can use every component of the C++ package in the Fortran language so we don't need to translate anything, which is very convenient," said lead author Hyun Kang, a computational Earth system scientist at ORNL.

This work builds on research results published in a previous paper in which researchers from ORNL and Los Alamos produced a code by hand to improve MPAS-Ocean. Now, the ForTrilinos-enabled solver has overcome the remaining drawbacks of the solver from the previous study, especially when users run MPAS-Ocean using a small number of compute cores for a given problem size.

MPAS-Ocean's default solver requires about 20 to 40 times more barotropic calculations than baroclinic calculations to accurately characterize both types of waves, which takes a massive amount of computing power. The new solver allows



The illustration depicts ocean surface currents simulated by MPAS-Ocean.
Image credit: Los Alamos National Laboratory, E3SM

researchers to run the same number of calculations for both types of waves without sacrificing accuracy, saving significant time and computing power.

"If we had to individually code every algorithm, it would require so much more effort and expertise," Kang said. "But with this software, we can run simulations right away at faster speeds by incorporating optimized algorithms into our program."

> *Extensive use of computational resources requires an enormous amount of electricity and energy, but by speeding up this model we can reduce that energy use, improve simulations and more easily predict the effects of climate change decades or even thousands of years into the future.*
>
> — ORNL computational Earth system scientist **Hyun Kang**

Although the current solver still has scalability limitations on high-performance computing systems, it performs exceptionally well up to a certain number of processors. This disadvantage exists because of the need for processors to constantly communicate with one another, which can slow down MPAS-Ocean's performance. To overcome this obstacle, the researchers have plans to port the solver to the GPUs that power those systems, as well as to speed up communications between processors and continue improving the ocean model itself.

These advancements aim to make climate predictions faster, more reliable and more accurate, which are essential to ensuring climate security and enabling timely decision-making and high-resolution projections.

"This barotropic mode solver enables faster computation and more stable integration of models, especially MPAS-Ocean," Kang said. "Extensive use of computational resources requires an enormous amount of electricity and energy, but by speeding up this model we can reduce that energy use, improve simulations and more easily predict the effects of climate change decades or even thousands of years into the future."

Illuminating

the mechanics of solid-state batteries

by Reece Brown
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As current courses through a battery, its materials erode over time. Mechanical influences such as stress and strain affect this trajectory, although their impacts on battery efficacy and longevity are not fully understood.

A team led by ORNL researchers has developed a framework for designing solid-state batteries with a focus on mechanics. Their paper, published in Science, reviewed how these factors change batteries during their cycling.

"Our goal is to highlight the importance of mechanics in battery performance," said Sergiy Kalnaus, a scientist in ORNL's Multiphysics Modeling and Flows group. "A lot of studies have focused on chemical or electric properties but have neglected to show the underlying mechanics."

The team spans several ORNL research areas, including computation, chemistry and materials science. Its review painted a more cohesive picture of the conditions that affect these batteries by using perspectives from across the scientific spectrum.

"We're trying to bridge the divide between disciplines," Kalnaus said.

In batteries, charged particles flow through materials known as electrolytes. Most are liquids, like in the lithium-ion batteries found in electric cars — but solid electrolytes also are being developed. These conductors are typically made from glass or ceramic and could offer advantages such as enhanced safety and strength.

"True solid-state batteries don't have flammable liquids inside," said Kalnaus. "This means that they would be less hazardous than the batteries commonly used today."

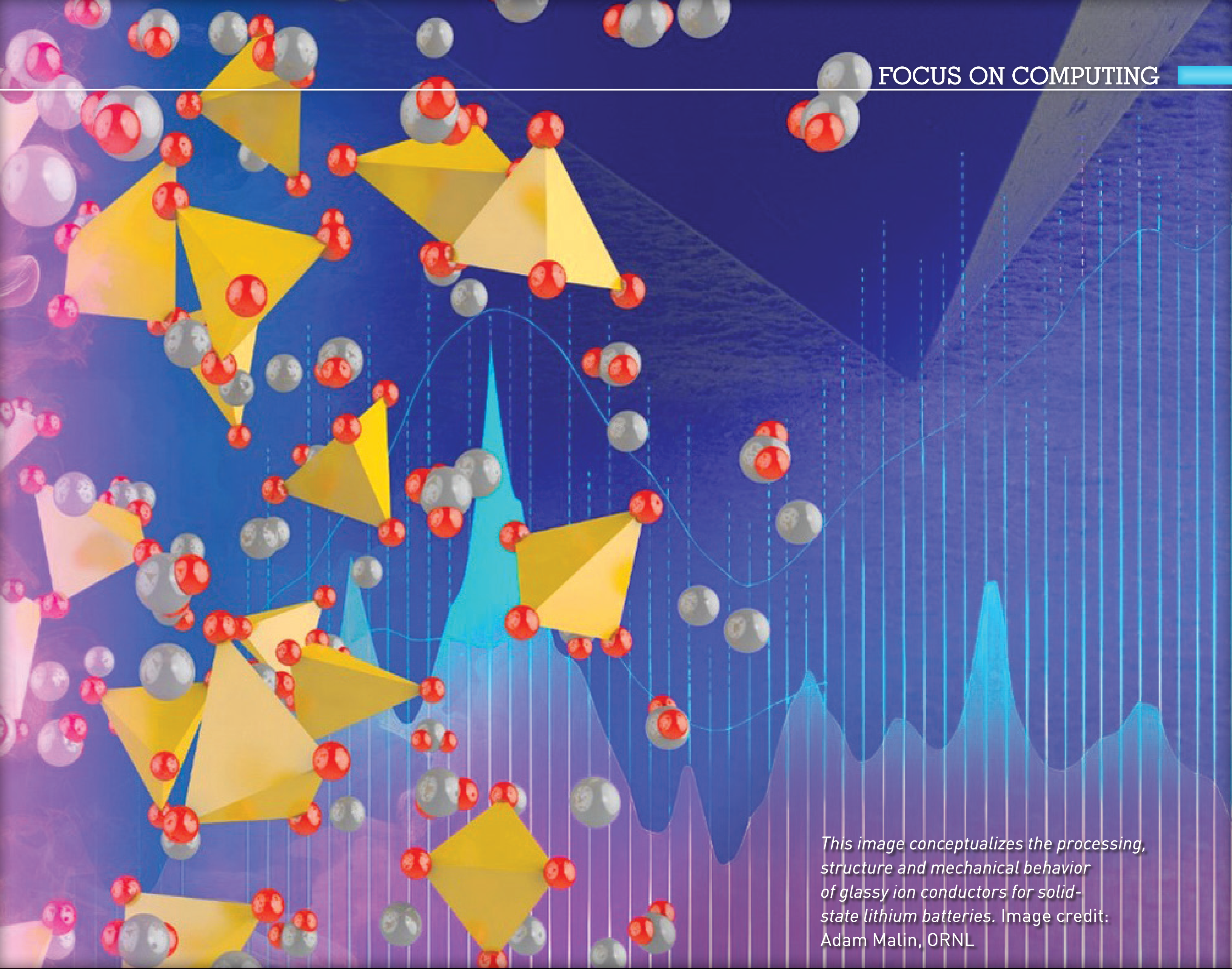
Solid electrolytes remain in the early stages of development due to the challenges associated with these novel materials. Their components swell and shrink during charge and mass transport, which alters the system and damages the electrolytes.

"Electrodes constantly deform during the battery operation," Kalnaus said. "In today's systems, the best solution is applying a large amount of pressure to keep everything together."

Making electrolytes from more ductile materials would allow them to better withstand stress. This behavior can be achieved with some techniques that introduce small crystal defects into ceramic electrolytes.

Electrons leave a system through anodes. In solid-state batteries, this component can be made from pure lithium, the most energy dense metal. Although lithium offers advantages for a battery's power, it also creates pressure that can damage electrolytes.

"During charging, nonuniform plating and an absence of stress-relief mechanisms can create stress concentrations.



This image conceptualizes the processing, structure and mechanical behavior of glassy ion conductors for solid-state lithium batteries. Image credit: Adam Malin, ORNL

These can support large amounts of pressure, enabling the flow of lithium metal," said Erik Herbert, the leader of ORNL's Mechanical Properties and Mechanics group. "In order to optimize the performance and longevity of these batteries, we need to engineer the next generation of anodes and solid electrolytes that can maintain mechanically stable interfaces without fracturing the solid electrolyte separator."

> *The research community needed a road map. Our paper outlined the mechanics of materials for solid-state electrolytes, encouraging scientists to consider these when designing new batteries.*
>
> — ORNL researcher **Sergiy Kalnaus**

The team's work is part of ORNL's long history of researching materials for solid-state batteries. In the early 1990s, a glassy electrolyte known as lithium phosphorous oxynitride, or LiPON, was developed at the lab. LiPON has become widely used as an electrolyte in thin-film batteries that have a metallic lithium anode. This component can withstand many charge-discharge cycles without failure, largely due to the ductility of LiPON. When met with mechanical stressors, it flows instead of cracking.

"In recent years we have learned that LiPON has robust mechanical properties to complement its chemical and electrochemical durability," said Nancy Dudney, a retired ORNL scientist who led the team that developed the material.

The team's effort highlights an understudied aspect of such batteries — the factors that shape their lifespan and efficacy.

"The research community needed a road map," Kalnaus said. "Our paper outlined the mechanics of materials for solid-state electrolytes, encouraging scientists to consider these when designing new batteries."

Study projects massive savings from geothermal heat pumps

by Jennifer Burke
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An ORNL-led modeling simulation estimates that carbon emissions could be reduced by more than 7,000 million metric tons if geothermal heat pumps, or GHPs, were mass deployed across the United States over the next few decades.

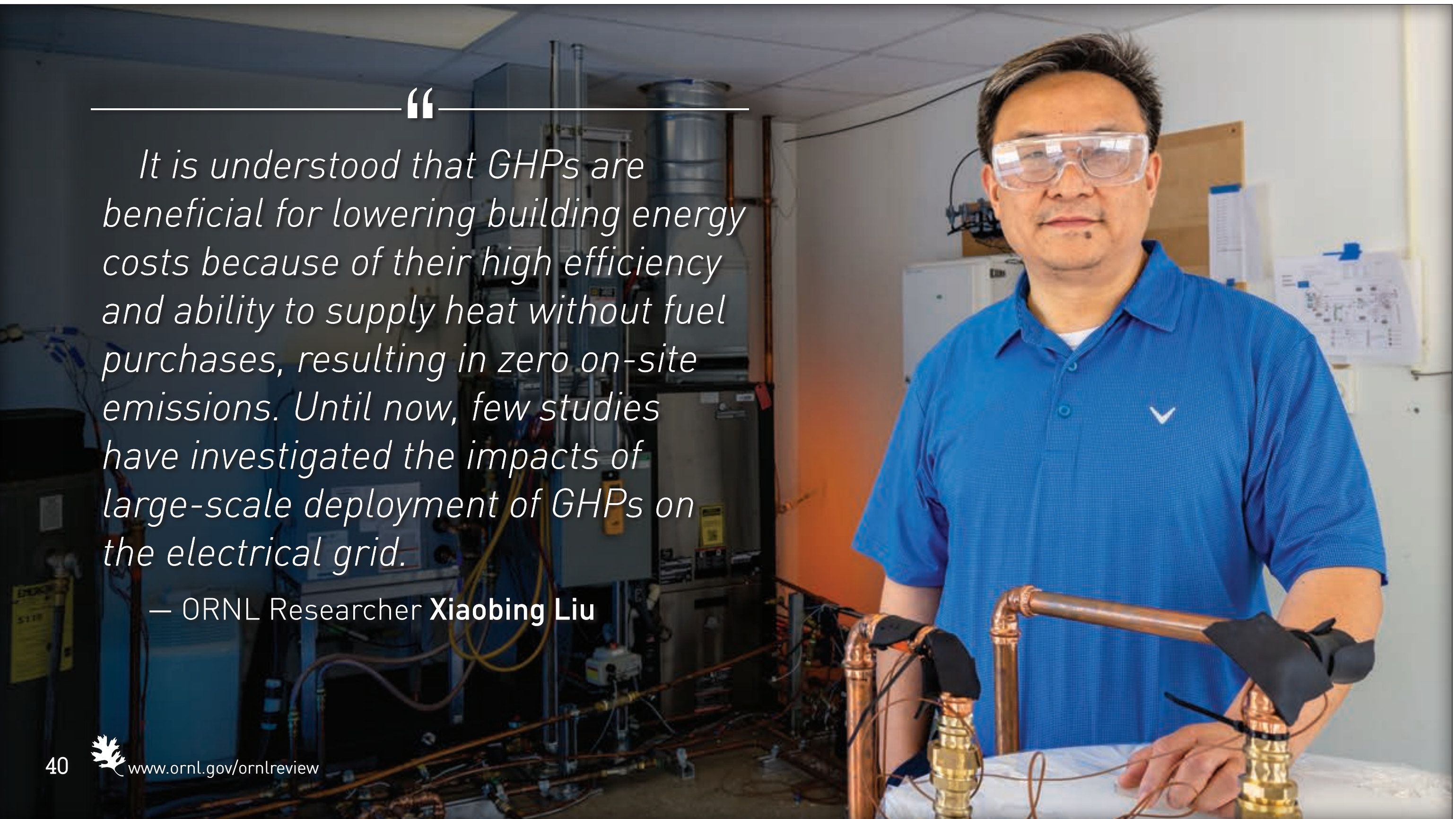
The study highlighted the impact of a nationwide rollout of GHPs in commercial and residential buildings from 2022 through 2050. It determined that the generation and capacity needs of the electric power system could also be reduced by up to 13 percent.

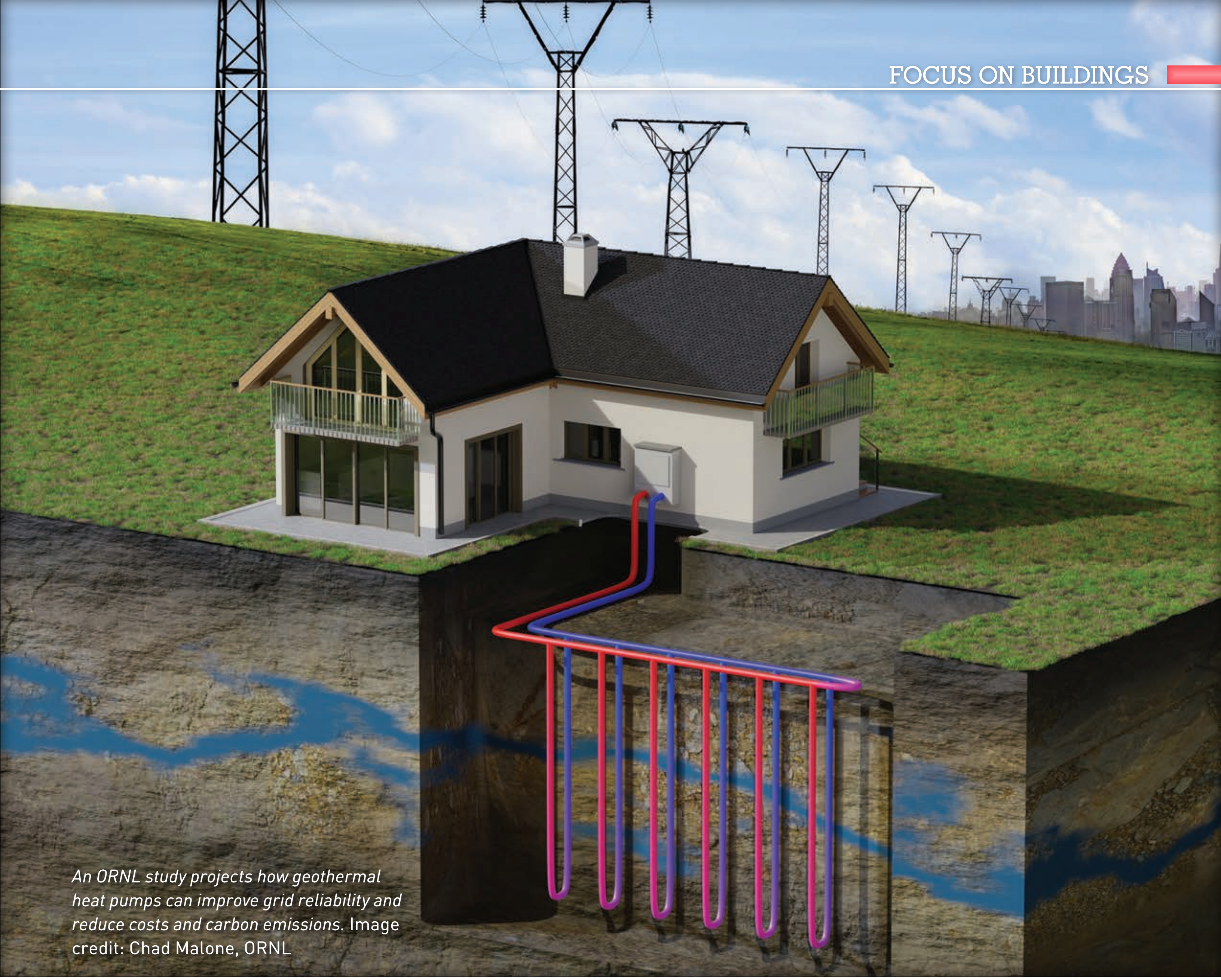
"GHPs have traditionally been seen as a building energy efficiency technology," said ORNL's Xiaobing Liu, principal investigator and buildings scientist. "This analysis found that GHPs can have a tremendous impact on electric power systems by reducing the requirements in capacity, generation and transmission, as well as carbon emissions."

GHPs, also known as ground source heat pumps, provide an environmentally friendly, energy-efficient alternative to conventional heating, ventilation and air-conditioning systems. They operate by transferring heat to and from the ground through underground pipes. The pipe system extracts heat from the ground to warm buildings in the winter while using the ground as a heat sink to cool buildings in the summer.

Researchers simulated the impacts if GHPs were deployed in 68 percent of existing and new building floor space across the contiguous U.S. Three scenarios were analyzed: continuing to operate the grid as it is today; reducing 95 percent of grid emissions by 2035 and achieving 100 percent clean electricity by 2050; and expanding grid decarbonization to include the electrification of

Xiaobing Liu, who directs the Thermal Energy Storage group at ORNL, led a study that analyzed the potential impact of geothermal heat pumps. Image credit: Carlos Jones, ORNL





An ORNL study projects how geothermal heat pumps can improve grid reliability and reduce costs and carbon emissions. Image credit: Chad Malone, ORNL

wide portions of the economy, including building heating.

Liu said the results translate into savings of approximately 600 terawatt-hours of electricity while eliminating more than 5,000 billion megajoules of fossil fuels — equivalent to 5 percent of the primary energy, including natural gas, heating oil and propane, that was consumed in the U.S. in 2022. Deploying more than 5 million GHPs per year could save over $300 billion in electricity payments as well.

"It is understood that GHPs are beneficial for lowering building energy costs because of their high efficiency and ability to supply heat without fuel purchases, resulting in zero on-site emissions," Liu said. "Until now, few studies have investigated the impacts of large-scale deployment of GHPs on the electrical grid."

In hot climate zones in the U.S., GHPs provide higher electricity savings, with modeling showing that peak electricity demand could be reduced by as much as 28 percent. GHPs were most effective at reducing carbon emissions and energy consumption in colder climates because natural gas furnaces are displaced and electric heaters are no longer used.

Liu said GHPs could also improve grid stability during extreme weather, particularly in Texas, where a severe ice storm in 2021 strained electrical infrastructure and led to widespread power outages. The study allows utilities to evaluate investment in GHPs given that a mass deployment requires ground drilling. To better understand the economic impacts, researchers further developed a consumer-friendly, web-based tool that estimates GHP cost and benefits and calculates potential energy savings for any type of residential or commercial building in U.S. climate zones.

"When there is a massive deployment of GHP systems, we now have a starting point for what it would look like in terms of capacity, generation, emissions, cost and resilience for the electric power systems," Liu said. "That picture looks very promising."

The analysis was funded by DOE's Geothermal Technologies Office and produced in collaboration with the National Renewable Energy Laboratory.

Additive boosts building heating, cooling tech

by Jennifer Burke
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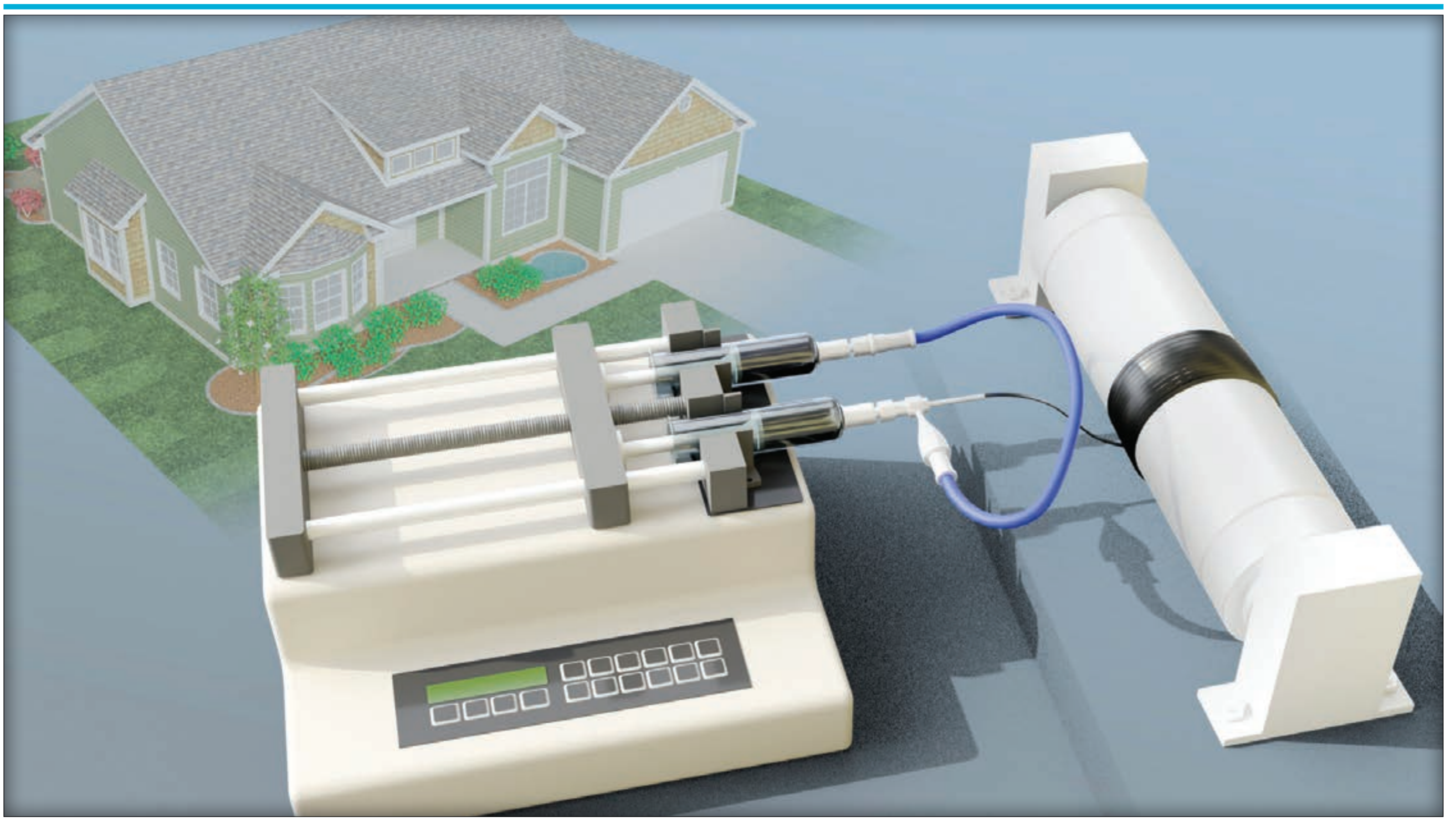
ORNL researchers have demonstrated a novel way to encapsulate materials that can be used to heat and cool buildings and proved how a polymer and electrolyte-based additive can stabilize them — findings that could accelerate their widespread use.

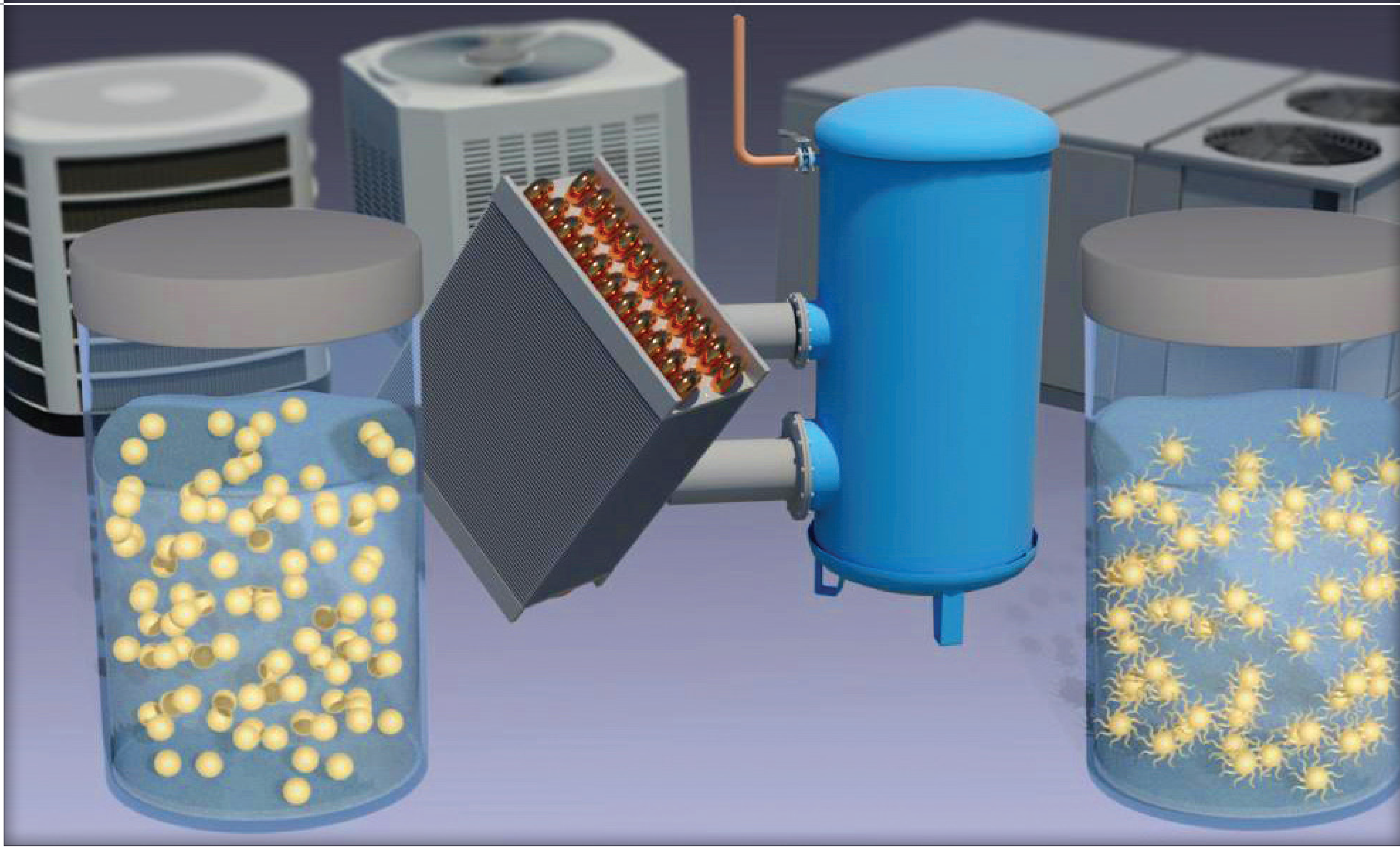
Environmentally friendly salt hydrates are a type of phase-change material, or PCM, that can function as a thermal battery, providing heating and cooling by storing and releasing energy when changing from solid to liquid. While these materials release minimal carbon and can retain heat, they can also leak. The challenge to using them as insulation for walls and roofs is how they are enclosed to prevent leaking. The new coaxial technique pulled polymer and salt together in one direction to form core-shell fibers that contain a salt core and polymer shell.

"Coaxial pulling lowers the cost of encapsulation and offers better thermal conductivity and energy density, all while being easy to reproduce and scale up," said ORNL's Jaswinder Sharma, who led development of the encapsulation process. "The fibers are flexible and can be seamlessly incorporated into current building materials and products."

In addition to insulation, PCMs can be integrated into heat pumps, a carbon-reducing alternative to furnaces and air



An encapsulation system developed by ORNL researchers prevents salt hydrates, which are environmentally friendly thermal energy storage materials, from leaking and advances their use in heating and cooling applications. Image credit: Andy Sproles, ORNL



ORNL researchers found that a polyelectrolyte additive can improve the stability and performance of a salt hydrate phase-change material, enhancing its usefulness in heat pumps. Image credit: ORNL

conditioners. Heat pumps extract heat from the surrounding air, ground or nearby sources of water or waste heat. The system includes a compressor to move refrigerants and a heat exchanger that amplifies and transfers heat to where it's needed. PCMs can provide the heat in heat pumps, but they're also prone to phase separation and instability — two conditions that also limit energy storage.

To improve their stability, ORNL researchers studied eight polymer mixtures and tested their impact when added to PCMs. Synthetic and naturally occurring polymers were included. Results showed that the polyelectrolyte additive dextran sulfate sodium can achieve the best performance.

"The pure salt hydrate PCM cannot sustain up to 10 melt-freeze cycles, but with the additive, stability is retained after 150 cycles," said ORNL's Damilola Akamo, a primary researcher on the study. "This determination will help inform the design of thermal storage materials in low-carbon-emitting heat pumps for residential and commercial buildings."

ORNL is conducting PCM research as part of a DOE consortium, Stor4Build, that's focused on thermal energy storage to accelerate the growth, optimization and deployment of technologies in buildings. Cost-effective energy storage is necessary for the large-scale deployment of renewable electricity, electrification and decarbonization.

Currently, as much as 50 percent of electricity consumed by buildings in the United States goes toward heating and cooling. Thermal energy storage shows promise as a cost-effective alternative and refers to energy that can be stored in a material as a heat source or a cold sink, rather than as electrical energy. This solution can increase the flexibility of adjusting electricity loads to match demand, promote the use of renewable energy sources and allow heat pumps to function more effectively and in more extreme climates.

"By shifting heating, ventilation and air-conditioning loads off-peak, thermal energy storage addresses grid challenges associated with electrification and decarbonization. Becoming impactful nationwide requires new materials and new methods of integrating storage," said Kyle Gluesenkamp, ORNL senior R&D scientist and Stor4Build co-director. "Stor4Build brings together the stakeholders necessary to accelerate development and market adoption of scalable thermal energy storage technologies."

Research areas identified as foundational to consortium activities include materials optimization and manufacturing; modeling and analysis; system optimization and integration; and market, policy and equity. A community-scale demonstration of technologies developed from Stor4Build will serve as a foundation for large-scale deployments of thermal energy storage as well as electrochemical battery energy storage and systems capable of satisfying both the heating and cooling needs in buildings.

Research shows novel uses for hafnia

by Scott Gibson
gibsonws@ornl.gov

ORNL scientists have explained unusual phenomena associated with hafnium oxide, or hafnia, material that could be used in novel semiconductor applications.

"We have proved that the ferroelectric behavior in these systems is coupled to the surface and is tunable by changing the surrounding atmosphere," said Kyle Kelley of the lab's Center for Nanophase Materials Sciences. "Previously, the workings of these systems were speculation, a hypothesis based on a large number of observations both by our group and by multiple groups worldwide."

Materials such as hafnia exhibit ferroelectricity, which means that they are capable of extended data storage even when power is disconnected and that they might be used in the development of new, so-called nonvolatile memory technologies. Innovative nonvolatile memory applications will pave the way for the creation of bigger and faster computer systems by alleviating the heat generated from the continual transfer of data to short-term memory.

The scientists explored whether the atmosphere plays a role in hafnia's ability to change its internal electric charge arrangement when an external electric field is applied. Their findings were published in the journal *Nature Materials*.

Kelley performed the experiments and envisioned the project in collaboration with Sergei Kalinin of the University of Tennessee, Knoxville.

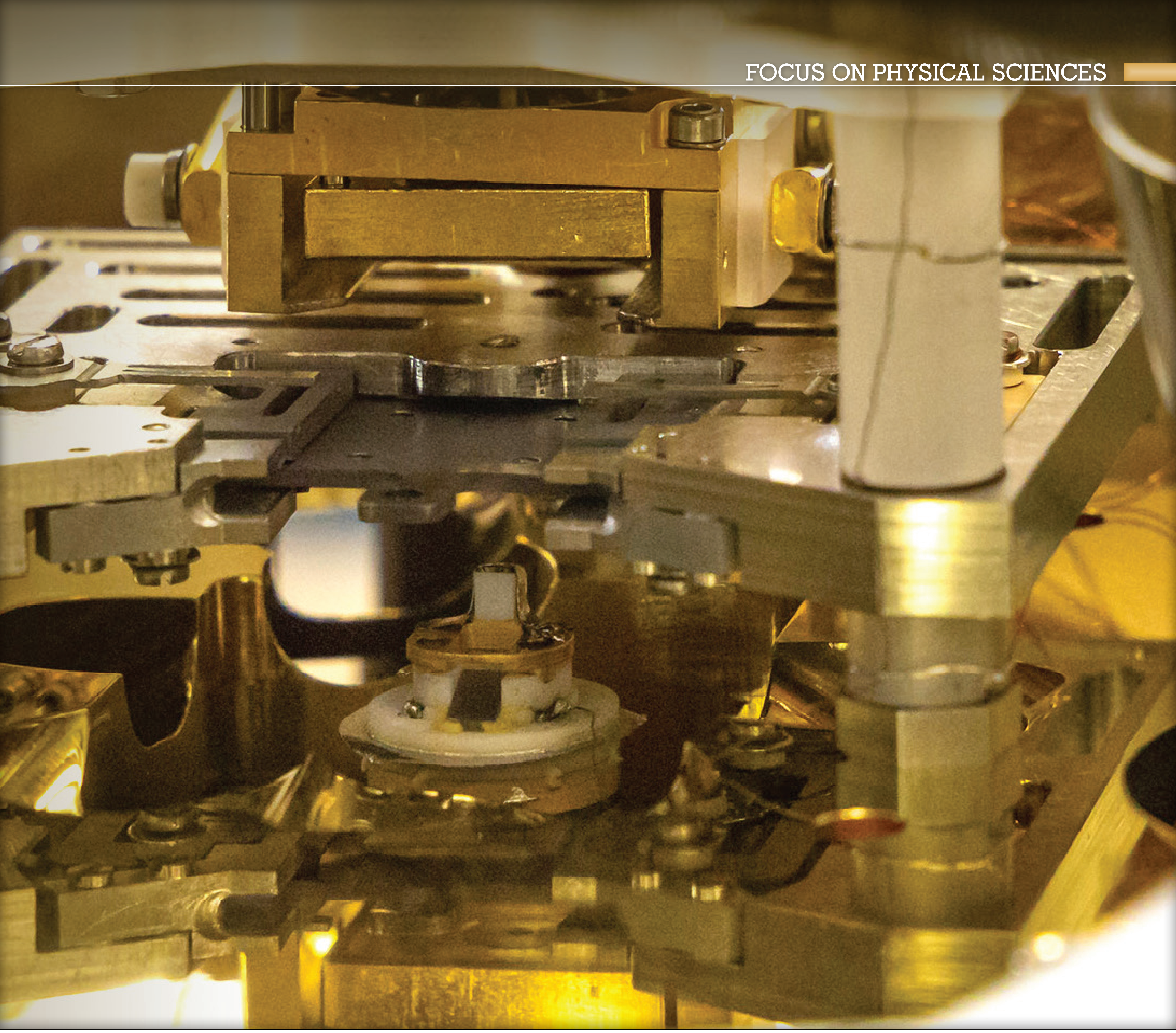
Materials commonly used for memory applications have a surface, or dead, layer that interferes with the material's ability to store information. As materials are scaled down to only several nanometers thick, the effect of the dead layer becomes extreme enough to completely stop the functional properties. By changing the atmosphere, the scientists were able to tune the surface layer's behavior, which, in hafnia, transitioned the material from the antiferroelectric to the ferroelectric state.

"Ultimately, these findings provide a pathway for predictive modeling and device engineering of hafnia, which is urgently needed, given the importance of this material in the semiconductor industry," Kelley said.

Predictive modeling enables scientists to use previous research to estimate the properties and behavior of an unknown system. The study focused on hafnia alloyed, or blended, with zirconia, a ceramic material containing zirconium.

"
Ultimately, these findings provide a pathway for predictive modeling and device engineering of hafnia, which is urgently needed, given the importance of this material in the semiconductor industry.
— ORNL researcher **Kyle Kelley**

Using the ultrahigh-vacuum atomic force microscope at DOE's Center for Nanophase Materials Sciences at ORNL, researchers found unique, environmentally induced ferroelectric phase transitions in hafnium zirconium oxide, a material important in developing advanced semiconductors.
Image credit: Arthur Baddorf, ORNL



But future research could apply the findings to anticipate how hafnia may behave when alloyed with other elements.

This study relied on atomic force microscopy both inside a glovebox and in ambient conditions, as well as ultrahigh-vacuum atomic force microscopy, methods available at the CNMS.

"Leveraging the unique CNMS capabilities enabled us to do this type of work," Kelley said. "We basically changed the environment all the way from ambient atmosphere to ultrahigh vacuum. In other words, we removed all gases in the atmosphere to negligible levels and measured these responses, which is extremely hard to do."

Team members from the Materials Characterization Facility at Carnegie Mellon University played a key role in the research by providing electron microscopy characterization, and collaborators from the University of Virginia led the materials development and optimization.

ORNL's Yongtao Liu, a researcher with CNMS, performed ambient piezoresponse force microscopy measurements.

The model theory that underpinned this research project was the result of a long research partnership between Kalinin and Anna Morozovska at the Institute of Physics, National Academy of Sciences of Ukraine.

"Future studies can extend this knowledge to other systems to help us understand how the interface affects the device properties, which, hopefully, will be in a good way," Kelley said. "Typically, the interface kills your ferroelectric properties when scaled to these thicknesses. In this case, it showed us a transition from one material state to another."

Super supercapacitor

sets energy-storage record

by Dawn Levy
levyd@ornl.gov

Guided by machine learning, ORNL chemists have designed a record-setting carbonaceous supercapacitor material that stores four times more energy than the best commercial material. A supercapacitor made with the new material could improve regenerative brakes, power electronics and auxiliary power supplies.

Without the goal that machine learning set, we would have kept optimizing materials through trial and error without knowing their limit.
— ORNL researcher **Sheng Dai**

"By combining a data-driven method and our research experience, we created a carbon material with enhanced physicochemical and electrochemical properties that pushed the boundary of energy storage for carbon supercapacitors to the next level," said chemist Tao Wang of ORNL and the University of Tennessee, Knoxville. He led the study with chemist Sheng Dai of ORNL and UTK.

"This is the highest recorded storage capacitance for porous carbon," said Dai, who conceived and designed the experiments with Wang. "This is a real milestone."

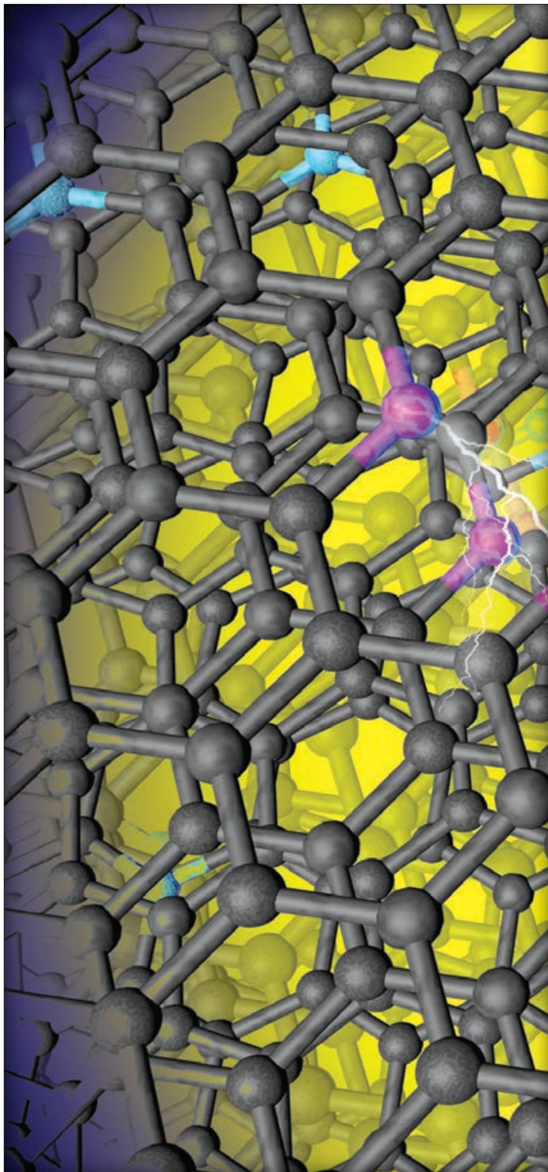
The researchers conducted the study at the Fluid Interface Reactions, Structures and Transport Center, or FIRST, an ORNL-led DOE Energy Frontier Research Center that operated from 2009 to 2022. Their partners at three national labs and seven universities explored fluid-solid interface reactions having consequences for capacitive electrical energy storage. Capacitance is the ability to collect and store electrical charge.

When it comes to energy storage devices, batteries are the most familiar. They convert chemical energy to electrical energy and excel at storing energy. By contrast, capacitors store energy as an electric field, akin to static electricity. They cannot store as much energy as batteries in a given volume, but they can recharge repeatedly and do not lose the ability to hold a charge. Supercapacitors, such as those powering some electric buses, can store more charge than capacitors and charge and discharge more quickly than batteries.

The materials of choice for making electrodes for supercapacitors are porous carbons. Pores provide a large surface area for storing electrostatic charge.

The ORNL-led study used machine learning to guide the discovery of the superlative material. Runtong Pan, Musen Zhou and Jianzhong Wu from the University of California, Riverside, a FIRST partner university, built an artificial neural network model and trained it to set a clear goal: develop a "dream material" for energy delivery.

The model predicted that the highest capacitance for a carbon electrode would be 570 farads per gram if the carbon were co-doped with oxygen and nitrogen.



The highly porous carbon doped with oxygen and nitrogen that Wang and Dai designed and synthesized had a capacitance of 611 farads per gram — four times higher than a typical commercial material. Pseudocapacitance is storage of charge based on continuous, fast and reversible oxidation-reduction reactions at the surface of electrode materials. Pseudocapacitance at the oxygen/nitrogen sites contributed to 25 percent of the overall capacitance. The material's surface area was among the highest recorded for carbonaceous materials — more than 4,000 square meters per gram.

This success came quickly. The data-driven approach allowed Wang and Dai to achieve in three months what would have previously taken at least a year.

"We achieved the performance of carbon materials at the limit," Wang said. "Without the goal that machine learning set, we would have kept optimizing materials through trial and error without knowing their limit."

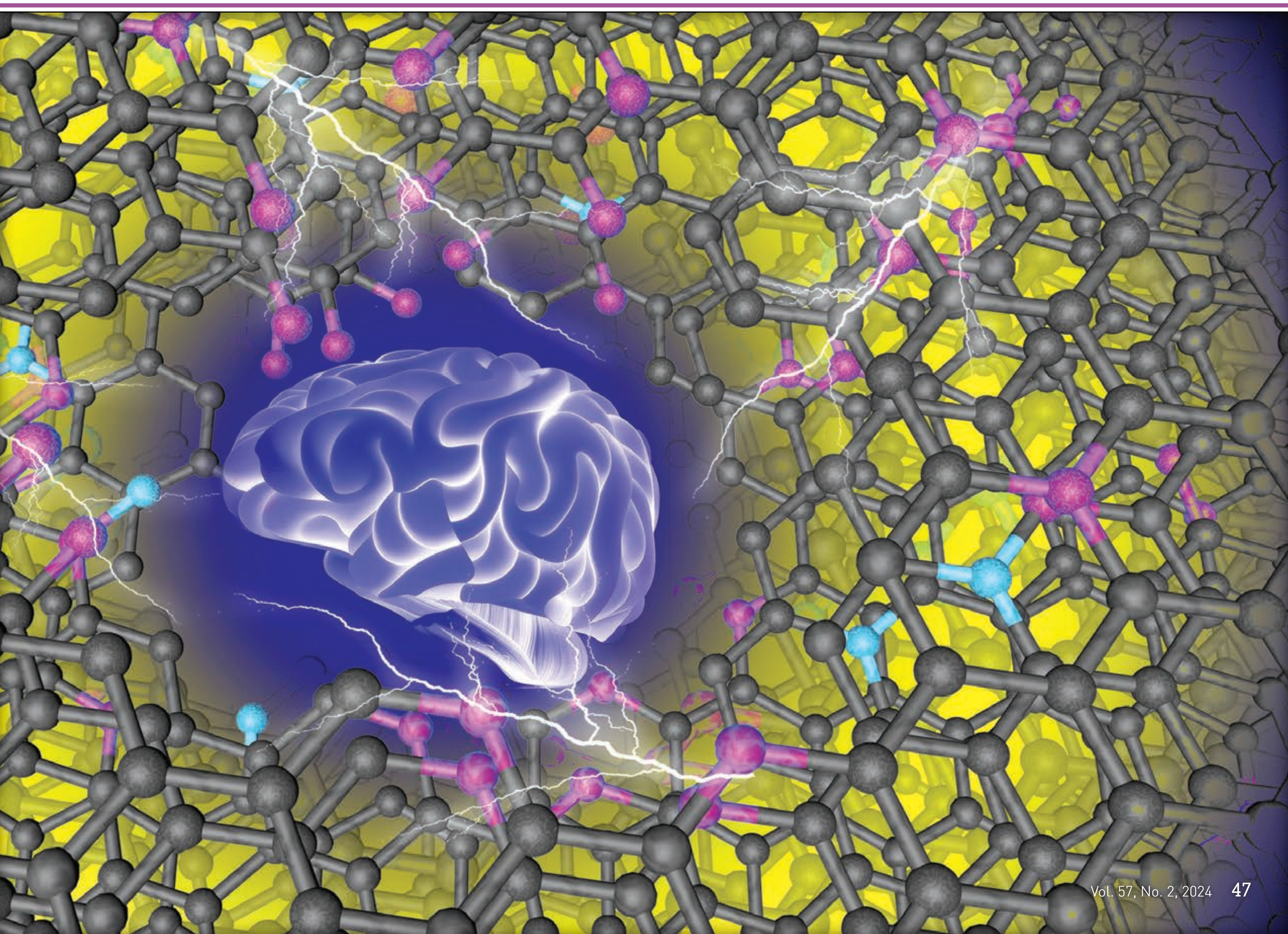
The key to success was achieving two kinds of pores — mesopores between 2 and 50 nanometers, or billionths of a meter, and micropores tinier than 2 nanometers. Miaofang Chi and Zhennan Huang at ORNL's Center for Nanophase Materials Sciences performed scanning transmission electron microscopy to characterize pores. Murillo Martins and Eugene Mamontov of ORNL's Spallation Neutron Source performed neutron scattering that revealed the electrolyte moved at different speeds: quickly in mesopores and slowly in micropores.

"You are building a highway for ion transport," Dai said. "Supercapacitors are all about high-rate performance — fast charging, fast discharging. In this structure that Tao and I designed, you have a larger pore, which you can view as a superhighway. This is connected to smaller roads, or tinier pores."

Wang said, "A balanced amount of small and large pores can realize the best performance, as predicted by the artificial neural network model."

For more information: bit.ly/3Tv0pv4

Conceptual art depicts machine learning finding an ideal material for capacitive energy storage. Part of the image, the brain, was generated by Fotor, Aug. 10, 2023. Image credit: Tao Wang, ORNL



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.

Małgorzata Makoś

Postdoc, Chemical Sciences Division
Ph.D., Computational Chemistry, Southern Methodist University
Hometown: Zawoja, Poland

What are you working on at ORNL?

My research at ORNL focuses on developing advanced computational methods and machine learning techniques that efficiently and comprehensively explore chemical reactions aiming to enhance our understanding of catalytic processes for diverse applications in materials science and beyond.

What would you like to do in your career?

In my career, I aim to advance the field of artificial intelligence in chemistry and materials science. I want to contribute to this field within research institutions or national laboratories such as ORNL, focusing on developing cutting-edge computational methods and applying them to solve complex chemical problems.

Why did you choose a career in science?

From my earliest memories, I have been fascinated by science, always wondering about the intricate nature of atoms and how they form the world around us. This curiosity has driven my passion for quantum mechanics, motivating me to pursue a career dedicated to tackling complex computational challenges.

Ernesto Camilo Zuleta Suarez

Postdoc, Chemical Sciences Division
Ph.D., Energy Science and Engineering, University of Tennessee (Bredesen Center)
Hometown: Valledupar, Colombia

What are you working on at ORNL?

I'm a postdoc in the Energy Storage and Conversion group, focusing on redox flow batteries for grid storage. My research aligns with the lab's mission of pioneering energy storage science to address crucial challenges vital to U.S. economic development and security.

What would you like to do in your career?

I aspire to be an energy science researcher, innovating efficient methods for generation and storage. Beyond research, I envision contributing to education, fostering a commitment to teaching in the future. My passion lies in advancing sustainable energy solutions and sharing knowledge to inspire future generations.

Why did you choose a career in science?

Since my childhood in Colombia, an enduring passion for science and nature has been the driving force behind my motivation. I take delight in unraveling the mysteries of the natural world and exploring ways to harness its benefits for our collective advancement.

ChristiAnna Brantley

Postdoc, Radioisotope Science and Technology Division
Ph.D., Inorganic Chemistry, University of Florida
Hometown: Rocky Mount, North Carolina

What are you working on at ORNL?

My research at ORNL focuses on the development of novel radiopharmaceutical therapies where, through synthetic organic chemistry, we modify existing FDA-approved medications to incorporate radioisotopes while retaining their therapeutic efficacy. Our research merges protein inhibition with targeted alpha therapy to provide new cancer treatments to those who have no other options.

What would you like to do in your career?

In my career I would like to make a lasting impact with my efforts. I enjoy following a project from inception to completion, seeing the resulting butterfly effect of this work. I want to develop new technologies that help people, especially in their greatest times of need.

Why did you choose a career in science?

I have always been fascinated by bringing small things into focus. I am an avid macro photographer, and I find beauty in magnifying and understanding the small things, as changes in small things lead to greater impacts. I chose science, chemistry specifically, because how much smaller can you get than atoms?

Aidan Klemm

Graduate student, Manufacturing Science Division
Ph.D. student, Chemical Engineering, Case Western Reserve University
Hometown: Chicago, Illinois

What are you working on at ORNL?

My research at ORNL is investigating the behavior of magnetic nanoparticles suspended in ionic liquids (salts that are liquid at room temperature) during microwave heating, in order to better understand the fundamental processes involved in the electromagnetic regeneration of direct air capture sorbents.

What would you like to do in your career?

I have always enjoyed teaching, so eventually I plan to become a professor of chemical engineering. However, in the two months I have been at ORNL, I have been amazed and inspired by the incredible resources and people at the lab and hope to continue working in the DOE national lab system for the foreseeable future.

Why did you choose a career in science?

Math and science courses, particularly chemistry and calculus, came more naturally to me when I was in grade school, but I struggled with writing and creative endeavors. When I finally started to explore scientific writing, those more creative subjects started to click. This — along with my passion for answering the question "why?" — drove me to a career in science.

Mercy Sammy

Graduate student, Buildings and Transportation Science Division
Ph.D. student, Computational Science, Tennessee State University
Hometown: Addis Ababa, Ethiopia

What are you working on at ORNL?

My research at ORNL focuses on enhancing refraction-based air leak detectors and moisture detector devices to meet building energy codes, enhance energy efficiency, and diminish buildings' carbon footprints. I will leverage image analysis software to validate experimental work and enhance detection capability, thereby contributing to innovative energy-efficient technologies.

What would you like to do in your career?

In my career, I aspire to develop sustainable solutions that are critical in combating climate change, focusing particularly on optimizing building energy efficiency, reducing greenhouse gas emissions, and enhancing indoor air quality through engineering building energy simulation and modeling. My graduate student internship aids in cultivating expertise for impactful contributions to cutting-edge research in this field.

Why did you choose a career in science?

I chose science as my career because it infuses our lives, prompting the exploration of untouched mysteries. It aligns with my passion for problem-solving and innovation, enabling me to address urgent global issues like net-zero energy building and sustainability while pursuing what truly excites me as a researcher.

Lucas Bowman Sutton

Graduate student, Neutron Scattering Division
Ph.D. student, Biology, Rensselaer Polytechnic Institute
Hometown: Binghamton New York

What are you working on at ORNL?

Currently I am working in the Large Scale Structure Section under the guidance of Dr. Hugh O'Neill. I am studying the structure of protein complexes in the circadian clock using the Bio-SANS beamline at HFIR to differentiate proteins within these complexes.

What would you like to do in your career?

My career aspirations are to go into either industry or governmental research. I have always enjoyed biomedical research, so I would like to continue that after graduate school. However, my current field will allow me to have diverse opportunities after I graduate, which is exciting.

Why did you choose a career in science?

As a kid I always loved puzzles, which is why I originally got into research. I realized experiments are puzzles that you have to build from the ground up and solve using a variety of skills and knowledge. To be honest, I did not know a lot of careers existed in science while growing up, so my real interest in biomedical research really sparked while I was an undergrad.

ORNL's nonproliferation history

by Chris Driver and Liz Neunsinger
neunsingerel@ornl.gov

The global commitment to prevent the spread of nuclear weapons is preserved in a single document, the Treaty on the Non-Proliferation of Nuclear Weapons, signed in 1970. Commonly known as the NPT, 191 countries signed the treaty, agreeing to protect nuclear materials and associated technology while receiving support in areas such as food and water management, sustainable development and clean energy.

The needs of war drove nuclear science forward to develop an atomic bomb during World War II, but there are also many peace-time uses of nuclear technology, including cancer treatments, food preservation, the sterilization of goods and nuclear power, which

ORNL's Ana Raffo Caiado (center) demonstrates a handheld radiological detection meter to Jean-Pierre Cayol (left), Departmental Programme Coordinate from the IAEA, during a tour of ORNL's Safeguards Lab. Image credit: Genevieve Martin, ORNL

ORNL's Angie Lousteau (center) briefs Jean-Pierre Cayol (right), Departmental Programme Coordinate from the IAEA, during a tour of ORNL's Safeguards Lab. Image credit: Genevieve Martin, ORNL

has become a key tool to combat climate change. Shortly after the war ended, the U.S. Atomic Energy Commission was established and charged with managing peacetime nuclear science and technology.

"The AEC acknowledged the need for national laboratories to maintain national research capabilities and was responsible for establishing Oak Ridge National Laboratory as a premier research center," said Angie Lousteau, a nuclear safeguards and security expert at the lab.

ORNL's commitment to nuclear nonproliferation predates the NPT.

"From the beginning, the U.S. realized the financial importance of accounting for all our nuclear material," Lousteau said. "We could account for material, but after the bombs were dropped, it was clear we also had to *protect* the nuclear materials and technologies that could be used for weapons development."

Lousteau believes nonproliferation expertise was born at ORNL. "Here at the lab, we implemented new and enhanced accounting and control practices, new measurement technologies, and verification methods from the onset. Over the years, we have shared our stories, our lessons learned, and our best practices."

From teaching member states' regulatory agencies to set up their own material accounting or licensing structure to developing technology for International Atomic Energy Agency inspectors to use in the field, the U.S. is a leader in preventing the proliferation of nuclear weapons.

Ana Raffo Caiado, an international safeguards and nonproliferation expert at ORNL, has witnessed how the treaty has kept its signatories safe over the last 34 years. She advocates for the NPT because it allows the peaceful use of nuclear science to benefit communities around the world while preventing nuclear material and nuclear facilities from being misused.

"The NPT shows how a country can belong to a community that not only protects them from nuclear weapons and explosions, but also helps them achieve their social and economic development," she said. "The treaty enables the goodness of cooperation among the world."

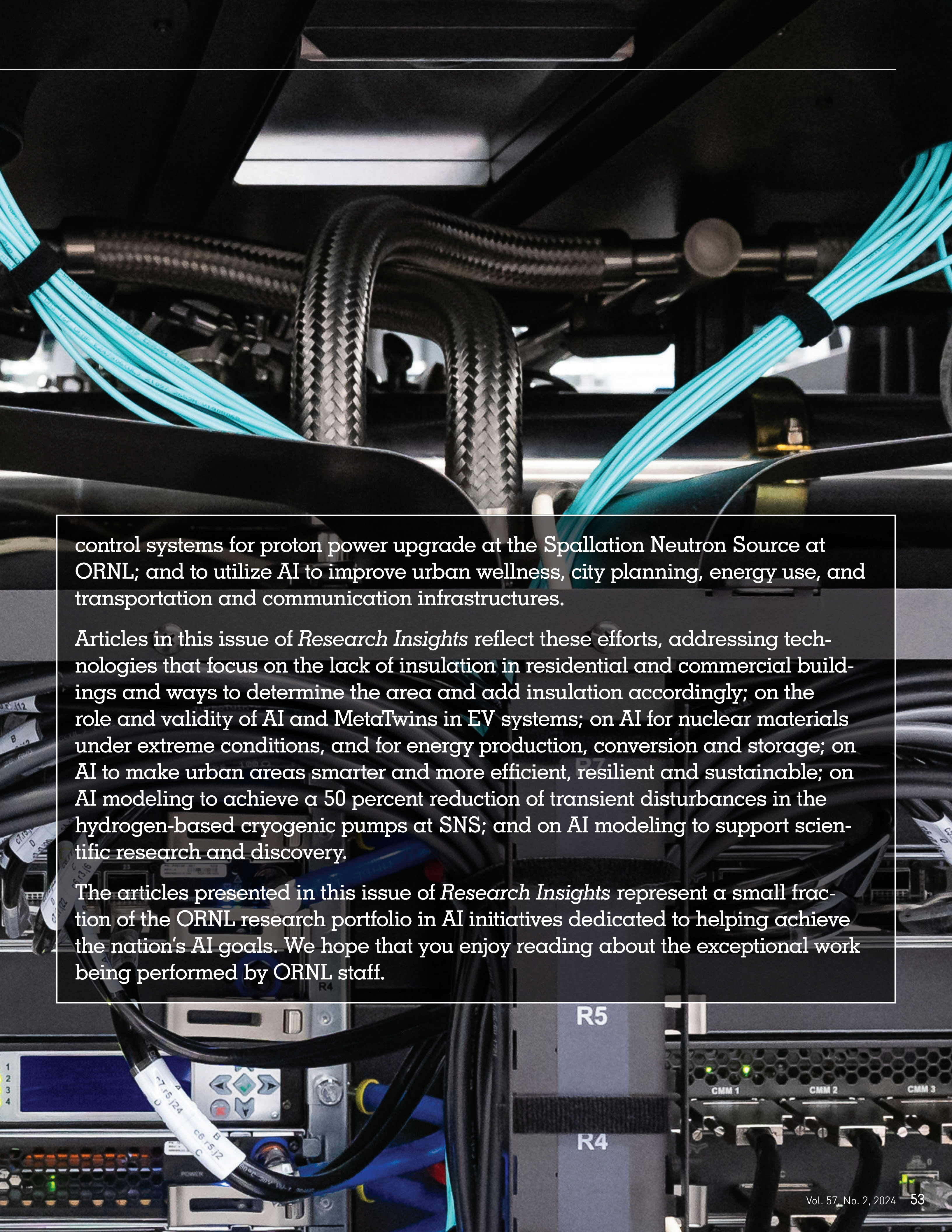
Eight decades after its inception, ORNL remains at the vanguard of essential IAEA-supporting research and technology. The complementary approach to nonproliferation research — which includes the creation of innovative nuclear technology while safeguarding from threats — underpins ORNL's enduring commitment to the goals of the NPT.

Welcome to Research Insights

AI of the Future: Impact of Artificial Intelligence Modeling

ORNL Review is pleased to present the seventh issue of *Research Insights*, a collection of research articles from our scientific and technical staff. *Research Insights* was created to showcase the world-leading science being performed at ORNL, with each issue addressing an important theme.

This issue highlights recent advances by ORNL staff in artificial intelligence modeling. ORNL has in recent years developed a substantial fundamental and applied research program as part of our AI Initiative. Within this initiative, ORNL is working to improve the efficiency of old residential and commercial buildings through AI-assisted algorithms that enable placement of insulation into buildings and roofs autonomously; to couple AI with network digital twins known as MetaTwins for improving electric vehicle charging infrastructures; to leverage AI for the design of new molecules and structures for experimental validations; to develop AI tools for language processing, texting and answering questions through high-performance computing facilities; to create AI-based cryogenic



control systems for proton power upgrade at the Spallation Neutron Source at ORNL; and to utilize AI to improve urban wellness, city planning, energy use, and transportation and communication infrastructures.

Articles in this issue of *Research Insights* reflect these efforts, addressing technologies that focus on the lack of insulation in residential and commercial buildings and ways to determine the area and add insulation accordingly; on the role and validity of AI and MetaTwins in EV systems; on AI for nuclear materials under extreme conditions, and for energy production, conversion and storage; on AI to make urban areas smarter and more efficient, resilient and sustainable; on AI modeling to achieve a 50 percent reduction of transient disturbances in the hydrogen-based cryogenic pumps at SNS; and on AI modeling to support scientific research and discovery.

The articles presented in this issue of *Research Insights* represent a small fraction of the ORNL research portfolio in AI initiatives dedicated to helping achieve the nation's AI goals. We hope that you enjoy reading about the exceptional work being performed by ORNL staff.

Using AI to Revolutionize the Construction Industry

N. W. Hayes, B. P. Maldonado, D. E. Hun, M. M. Salonvaara

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INTRODUCTION

Modern-day building construction is not quite as productive as in 1947 [1]. Although industries such as agriculture and manufacturing have increased productivity by adopting advanced technologies, the construction industry has experienced minimal innovation. This is partly because industry members are risk-averse and are sometimes unwilling to try new technologies that could save time and money. Low productivity is further exacerbated by a shortage of ~500,000 skilled workers [2], contributing to a housing shortage now estimated at 3.8 million units [3]. To address these issues, emerging research efforts are industrializing building construction through mechanization, automation, and digitization.

State-of-the-art techniques such as modularization, prefabrication, preassembly, and mass production can increase productivity significantly. These techniques relocate the labor from the construction site to an off-site manufacturing facility. If assemblies are prefabricated, then laborers will spend less time on the jobsite, resulting in a safer work environment and potentially higher-quality construction. Off-site construction naturally enables repeatable tasks that are automatable using artificial intelligence (AI). In recent years, AI has helped industrialize the construction industry to improve productivity, safety, quality, and affordability [4,5,6]. For example, research has enabled the use of machine vision to monitor progress of prefabricated component construction in the manufacturing facility, and digital models and sensing systems are being used to assess construction quality through machine learning. Oak Ridge National Laboratory (ORNL) is using AI to improve the speed and quality of various efforts such as building envelope retrofits, spray foam insulation installation, and specification compliance of floors and roofs.

AUTOMATED DIMENSIONING OF BUILDINGS

More than half of residential and commercial buildings in the United States were constructed before energy codes were established. These older buildings consume most of the energy that residential buildings use to heat and cool the living space. These buildings usually have little or no insulation because of the practices that were in place at the time of construction. Retrofits to add insulation to walls and roofs would drastically reduce their energy consumption.

Adding insulation to existing walls is difficult, often requiring destructive methods to open the walls and place insulation inside. Furthermore, because older buildings with brick walls have no cavities to contain insulation, overclad retrofits can be used in which prefabricated insulated panels are placed on the exterior of existing walls. This is often the only option to add insulation to these older buildings. One of the most difficult aspects of an overclad retrofit is determining the dimensions of the existing building in a cost-effective and accurate manner so that the overclad panels can be customized. Older buildings rarely have documentation detailing the design dimensions of the building; more importantly, it is highly unlikely that the as-built dimensions match the design intent. Therefore, it is necessary to measure the actual dimensions of all key features of the existing envelope to be retrofitted.

Current practices consist of hand-measuring key features and specifying that contractors verify all measurements in the field to ensure seamless installation. If designed dimensions are inaccurate, panels will likely be prefabricated incorrectly, and installation problems are certain to occur, leading to downtime and additional expenses to correct the issue.

Modern surveying instruments can quickly and accurately capture point cloud data using light detection and ranging (lidar), providing a complete measurement of all key features of a building. However, point cloud data are difficult to analyze manually because of their high point density. Extracting dimensions of key features such as walls, doors, and window edges routinely requires several hours of manual labor to produce the simple dimensions necessary to design the panelized retrofit.

ORNL developed AI-assisted algorithms that automate the dimensioning of key building features from point cloud data. The Automatic Point Cloud Building Envelope Segmentation (Auto-CuBES) takes a building's raw point cloud data as input and generates a wireframe model of the key features of the building façade, including windows, walls, and doors [7]. The highly dense point cloud in Figure 1 (left) consists of ~32 million points; Auto-CuBES generated the corresponding wire frame (right) in 12 min, whereas the task took over 4 h when manually measured. Auto-CuBES also extracts planarity to determine the degree to which existing walls are out of plumb, out of level, or otherwise

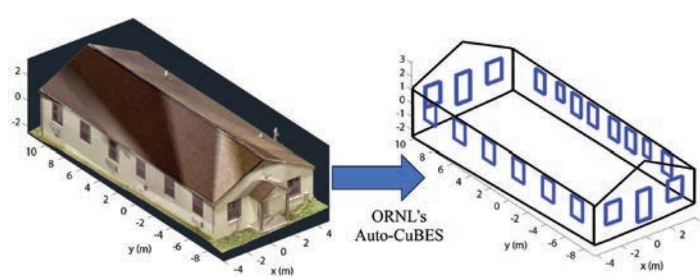

Figure 1. Automated transformation of (left) raw point cloud to (right) a wireframe model. (Credit: ORNL)

crooked. The retrofit designer can use this information to accurately plan and size retrofit panels that can easily be installed to ensure a high-performance new envelope.

AUTOMATED INSTALLATION OF SPRAY FOAM

Spray foam insulation offers benefits over rigid foam board, batt, blown-in, and other insulation types; spray foam insulation not only insulates but also seals potential air leaks. However, personal protective equipment is required during application of the commonly used isocyanate-based spray foam because uncured isocyanate is toxic. Moreover, foam installation by humans is often imprecise and wasteful.

ORNL developed an autonomous spray foam installer (ASFI) that uses *machine vision*, a form of AI, to automate the spray foam process (Figure 2). A lidar sensor installed on the robot provides a continuous point cloud data stream to define its location with respect to the wall cavity to be sprayed. AI algorithms analyze the data to position the robot and plan spray paths to install the required amount of insulation. Spray path planning is achieved by using unsupervised machine learning methods to identify geometrical trends in the wall and then separating wall framing from cavities. Within the cavity spaces, spray paths are generated using optimization methods. ASFI will reduce labor costs by ~50%, improve installation safety, increase the yield of installed insulation by ~10%, and reduce the overall cost by ~20%.

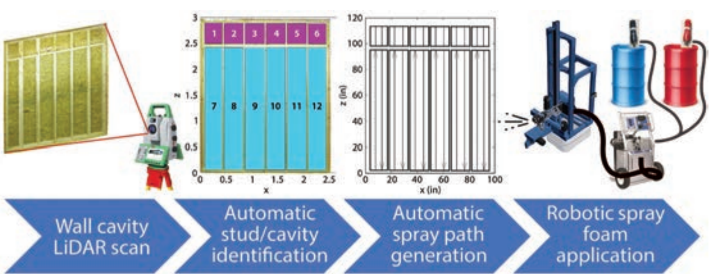

Figure 2. Spray foam robot and automated planning of spray path. (Credit: ORNL)

AUTOMATED ASSESSMENT OF FLOORS AND ROOFS

All buildings have floors and roofs. However, floors are usually flat and level, whereas roofs are usually sloped to drain water. Ensuring the flatness and levelness (F&L) of floors is critical to maintaining building function. For example, a warehouse requires a certain degree of floor F&L to ensure that stacked storage shelves sit plumb and level and that people can adequately and safely traverse the space. Low-slope roofs are designed with a small slope to drain water. Traditional methods to measure floor F&L or roof drainage require many hours of manual labor to collect and analyze the data and generate a report.

Modern surveying instruments such as laser scanners allow near real-time measurement of object positions in an environment; however, processing the raw point cloud data produced by these instruments takes hours of manual labor. AI enables faster automated analysis of point cloud data.

ORNL developed algorithms for the Flat and Level Analysis Tool (FLAT) and Roof Drainage Analysis Tool (RDAT) to analyze point cloud data of a construction site, identify errors, and provide real-time feedback. Figure 3 shows the process of analyzing the raw lidar scan data of a construction site with a concrete slab. This process produces useable information on the slab's F&L in real time. First, a point cloud of the entire construction site is captured, including the concrete slab. A machine learning algorithm segments the construction site's raw point cloud data and identifies near-flat planes (e.g., floor and low-slope roof). Then the algorithm extracts the near-flat plane's flatness, levelness, or slope. An automated analysis compares these measurements to a digital twin to determine areas that are not flat or level in floors or areas where the slope does not match the intended design and potential locations for ponding water in low-slope roofs. Generating an F&L report for a 50,000 ft^2 slab takes 1 to 3 days when measured manually, whereas FLAT can execute this task in less than 45 min.

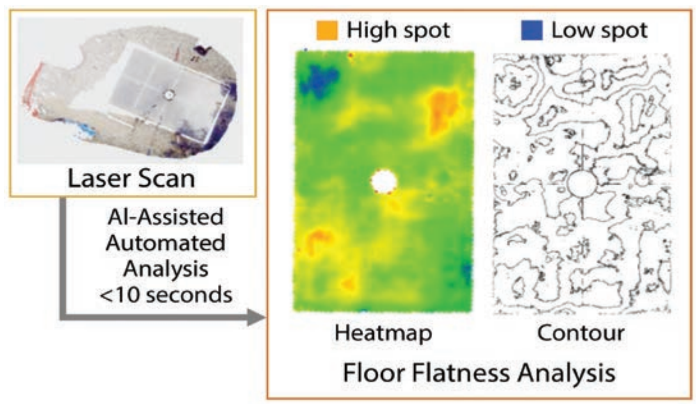

Figure 3. Automated analysis of floor flatness. (Credit: ORNL)

Because FLAT and RDAT run in minutes, they can be used in real time to detect and correct errors. For concrete floors, real-time evaluation enables proactive correction of F&L issues by filling low spots or trimming high spots while the concrete is still workable, reducing the need for costly corrections such as grinding of hardened concrete. For low-slope roofs, real-time evaluation enables proactive correction of installed slopes to prevent water ponding that can lead to roof leaks.

CONCLUSIONS

To address shortages of skilled labor and affordable housing, the construction industry must incorporate innovative technologies that produce higher quality, efficiency, and productivity with increased safety. When combined with digital tools and advanced sensing systems, AI enables automation of many otherwise inefficient construction tasks that currently require significant human labor.

IMPACT

Auto-CuBES, ASFI, FLAT, and RDAT improve productivity, safety, quality, and affordability in building construction. Specifically, Auto-CuBES's automated dimensioning of buildings enables ~50% faster and more affordable planning of building wall retrofits. ASFI reduces the cost of installed spray foam insulation in residential and commercial buildings by ~20%. FLAT and RDAT reduce the human labor required to monitor the as-built conditions by ~75% and enable higher-quality construction output.

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The AI MetaTwin: A Leap Toward Intelligent Electric Vehicle Infrastructure

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INTRODUCTION

In recent months, dramatic exponential growth in artificial intelligence (AI) capabilities has been observed in the electric vehicle (EV) ecosystem, especially in the charging infrastructure and the vehicles themselves.

A robust and efficient EV ecosystem requires a highly integrated network of vehicles, chargers and the electrical grid; the challenge lies in achieving seamless integration. The solution? An overarching AI-driven platform that enables bidirectional communication among all three entities. This platform serves as a linchpin to ensure the system's efficient operation and to facilitate data-driven decisions.

A central factor supporting this complex interaction and decision-making algorithm is the exchange of data between these entities—an exchange facilitated by digital twins (DTs). The DTs are high-fidelity simulations of physical systems, operating synchronously with their physical counterparts in real time [1].

However, individual DTs have limited capability and cannot oversee and monitor the entire system, which is essential for the well-knit EV ecosystem [2]. To address these limitations, the DT should be developed into what will be referred to as a *MetaTwin*. Unlike a DT, which models a single physical entity, a MetaTwin represents a network of interconnected DTs, effectively simulating a larger, more complex system. This approach allows for management and coordination of data from multiple DTs, thus enabling greater insight, robust data analysis and effective decision making.

BACKGROUND

To gain a better understanding of the MetaTwin concept, the EV drivetrain can be used as an example. Each drivetrain component, including the battery pack, power electronics converters, motor and gear, has its own MetaTwin (shown in Figure 1). These MetaTwins are composed of several DTs, and they operate synchronously, generating a wealth of data and enabling high-level functionalities, including system diagnostics, as well as deep analytics such as design root-cause analysis (shown in Figure 2). In the realm of deep analytics, advanced machine learning techniques and statistical analysis are executes specific tasks while maintaining effective communication with its counterparts.

This intercommunication among the digital twins, coupled with the regular exchange of information, gives the MetaTwin an enhanced level of functionality. By training a machine learning model using both a healthy motor and a motor with defects and then embedding the mode in diagnosis DT (dDT), the MetaTwin can perform advanced tasks such as diagnostics and prognosis and can recommend preemptive measures. For example, if the motor's DT reports unusual heat or current patterns using ML algorithms, then the MetaTwin can flag this as a potential sign of impending motor failure. Furthermore, the MetaTwin could then recommend preemptive measures such as scheduling a service appointment to repair or replace a malfunctioning motor. The MetaTwin can also identify the pattern and frequency of failures and can suggest design optimizations such as changing motor slot dimensions or winding schemes in the next product generation.

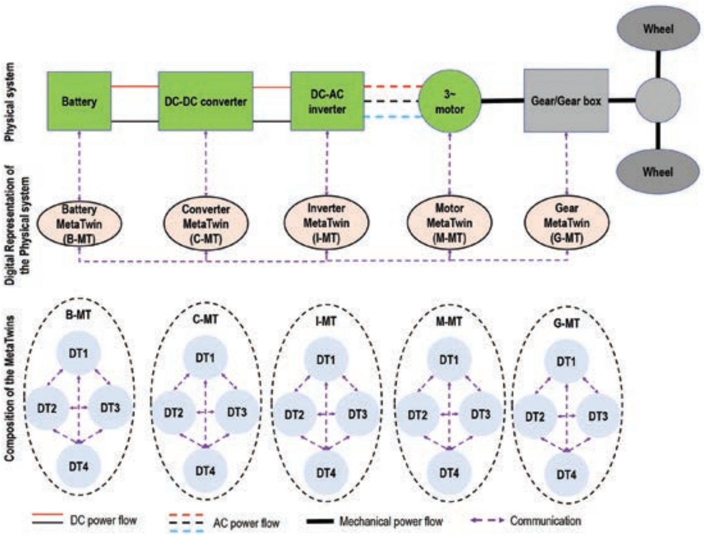

Figure 1. Generic diagram showing the major components of an EV drivetrain. Each major component has its own MetaTwin, and each MetaTwin comprises multiple DTs modeled and configured to represent the MetaTwin of a subsystem (e.g., motor, battery pack, power electronics converters and mechanical transmission). Thus, the drivetrain has several MetaTwins that communicate with each other using wired or wireless communication channels. (Credit: ORNL)

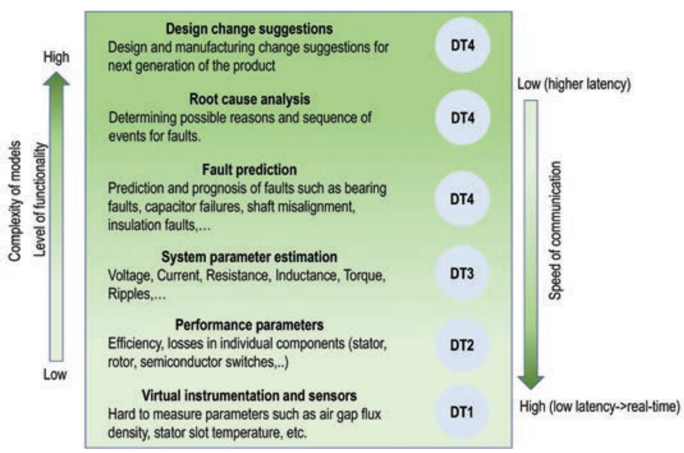

Figure 2. MetaTwin comprising multiple DTs, each with a set of functionalities to execute. Levels of complexity increase from bottom to top as the dependency of inputs from base DTs and the requirement of data volume increase and the model becomes more complex. Note that the top DT (DT4) performs operations that do not need an immediate response, so communication speed is not a necessity for these DTs. (Credit: ORNL)

applied to extract valuable insights from this vast complex data. The process involves data filtering, mining complex data sets, discovering underlying patterns and predicting potential trends, thereby transforming raw data into actionable intelligence. The integral role of deep analytics allows for failures to be detected early, fostering a proactive maintenance approach and thus curtailing overall downtime to reduce economic losses [3]. Furthermore, failure analysis can lead to design improvements in the product's next generation [4].

RESULTS

The MetaTwin serves as an overarching structure in which numerous DTs coexist and function as its subsets. Each DT

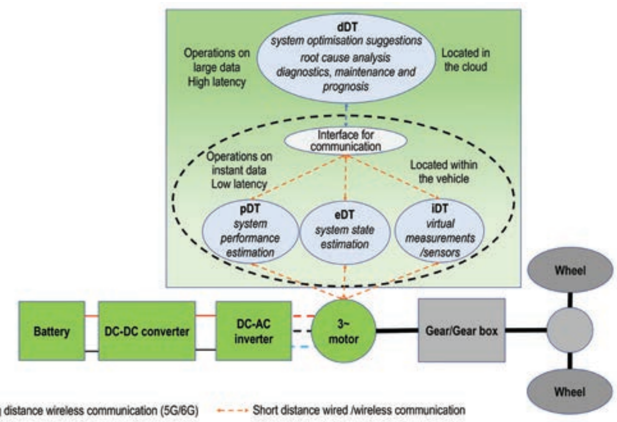

Figure 3. Descriptive MetaTwin of the motor. All types of DTs—performance DT (pDT), estimation dT (eDT), instrumentation DT (iDT) and diagnosis DT (dDT)—are interconnected via communication channels. The pDT, eDT and iDT support operations requiring a faster response, so they are connected with faster communication channels. Meanwhile, dDT, which performs operations not requiring immediate attention, requires inputs from other DTs and an extensive amount of data and is connected via long-distance wireless communication channels. Data storage for executing dDT functionalities is in a cloud infrastructure with data servers. (Credit: ORNL)

The architecture of a MetaTwin is inherently difficult to comprehend, especially for complex items such as an entire EV drivetrain. To facilitate comprehension, the focus was narrowed to a single fundamental component of the EV drivetrain: the motor. Figure 3 is a detailed illustration of the motor's MetaTwin architecture, offering a glimpse into this novel system.

CONCLUSIONS

When MetaTwins are coupled with AI, they have the capacity to diagnose and prognose the EV system, and they can also recommend changes to the system. However, the progression and use of this technology within the automotive industry necessitate rigorous research to answer several key questions. How can AI and machine learning techniques be applied effectively at different stages? What is the compromise between the computational complexity, fidelity and transparency of these models? What is the optimal approach for intelligent perception and interconnection of multisource heterogeneous physical entities and acquiring multidimensional real-time data of these entities?

Furthermore, the effective representation of large-scale data remains a challenge. How can we ensure interoperability between different DTs and operating platforms?

IMPACT

The MetaTwin can redefine the EV ecosystem and has five critical functionalities:

- Preventive diagnostics
- Automated fault detection
- Remaining useful life estimation
- Root cause analysis of failures
- Design flaw detection

These functionalities signify more than technical enhancements in EVs; they foreshadow a foundational shift in our understanding and implementation of not only EVs, but also the larger EV ecosystem that includes charging infrastructures.

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AI-Based Control for Optimized Operation of the Cryogenic Moderator System at the Spallation Neutron Source in Preparation for Proton Power Upgrades

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INTRODUCTION

The Spallation Neutron Source (SNS) at Oak Ridge National Laboratory (ORNL) generates neutrons with an accelerator-based system that delivers microsecond proton pulses to a steel target containing liquid mercury through a process called *spallation* [1]. These neutrons are directed toward more than 20 cutting-edge instruments, offering a diverse range of research capabilities across physics, chemistry, biology, and materials science. High-energy neutrons can pass through materials, potentially damaging both the instruments and the samples. Therefore, for some of the instruments at SNS, neutrons are moderated by liquid hydrogen (H_2) at cryogenic temperatures. The H_2 moderators remove heat from the neutron beam, causing them to slow down and allowing the neutrons to scatter off the nuclei of atoms in the sample. This process provides valuable information about the sample's structure and properties. The Cryogenic Moderator System (CMS) is responsible for maintaining the cryogenic thermal and hydraulic conditions in the H_2 moderators [2]. The CMS transfers the heat extracted from the neutron beam by the 20 K H_2 moderators to a 17 K He Brayton refrigeration cycle, also known as *cold box*. Finally, the heat is dissipated by an expansion turbine in the He refrigerator connected to a compressor-brake system.

Sporadic losses in beam power, referred to as *beam trips*, cause large disturbances in cooling requirements for the CMS. Beam trips are instantaneous changes in power from nominal conditions (1.4 MW) to 0 MW. Such a disturbance causes temperature and pressure spikes in the H_2 conditions. When the CMS recovers from a beam trip, the increase in heat load can cause a large H_2 pressure change because supercritical H_2 at 20 K behaves as an incompressible fluid. Loss of moderation can then occur if a beam trip causes overpressurization, forcing rupture discs to vent the H_2 to protect the physical integrity of the system. Nonetheless, over-pressurization of the system could be prevented by appropriate calibration of the CMS transient response.

As the disturbance caused by the beam trip propagates through the system, the He refrigerator also experiences transients in its thermodynamic conditions. In particular, the turbine embedded in the Brayton cycle shows large perturbations in its shaft rotational speed. The turbine speed transients from beam trips have caused eventual shutdown of the CMS for corrective actions. Downtime for a CMS system trip, including repair and recovery, is approximately 5 days. Given that SNS operates 200 days/year, CMS downtime corresponds to 2.5% of lost beam availability per CMS trip. Moreover, with an SNS availability goal of 90%, one CMS trip has a notably adverse impact on that goal. Similar to the H_2 pressure issue, the turbine speed transients can be reduced by appropriate control of the pressure across the turbine.

The CMS transient issues after beam trips have been observed at 1.4 MW beam power. However, the beam power of the SNS accelerator is currently being upgraded to reach 2.8 MW by 2028 through the Proton Power Upgrade (PPU) effort [3]. Although this effort includes the construction of a second target station [4], the CMS in the current target station must be capable of moderating 2.0 MW of beam power. Therefore, as SNS beam power is increased according to the PPU schedule, larger beam trips will result in larger transients and longer periods with a loss of moderation capabilities after transients. More importantly, larger temperature and pressure spikes during transients can cause CMS to be shut down for corrective actions. To mitigate current and future beam trip disturbances, optimization of the control logic is needed to ensure improved moderation performance under transients.

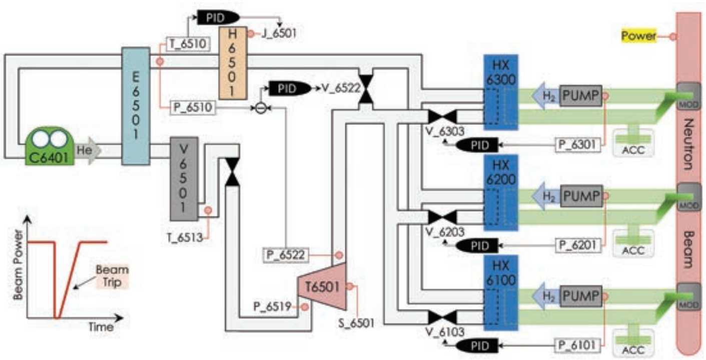

Figure 1. Simplified control-oriented model of CMS. The letters P, T, V, S, and J represent pressure, temperature, valve opening, speed, and electric power, respectively. (Credit: ORNL)

CRYOGENIC MODERATOR SYSTEM OVERVIEW

Figure 1 shows a simplified model of CMS. The heat transfer process starts at the 1.4 MW neutron beam. Three H_2 moderators are located around the mercury target vessel to absorb the nuclear heating produced by high-energy neutrons. The heat from each moderator is removed by the H_2 circulation system, which consists of a pump, an accumulator, and an He-H_2 heat exchanger. Given that cryogenic H_2 is incompressible, the accumulators use He-backed bellows to adjust the expansion without the need to add or subtract H_2 to or from the system. Thus, the accumulator serves as a passive volume controller to minimize H_2 pressure swings [5]. Nonetheless, the accumulators cannot provide the required pressure control to compensate for beam trips. For this reason, the H_2 pressure is actively controlled by a proportional-integral-derivative (PID) controller that adjusts the corresponding He flow.

The heat removed from the neutron beam by the H_2 moderators at 20 K is transferred to the He refrigeration system at 17 K. Starting at the He-H_2 heat exchanger and following the flow of He in Figure 1, the main components of the He refrigeration system are (1) He bypass valve V_{6522} to redirect flow depending of cooling demands and different beam power levels, (2) electrical heater H6501 to compensate for the lack of heat transferred to the He refrigerator during beam trips, (3) regenerative heat exchanger E6501, (4) ambient condition gaseous screw compressor C6401, (5) absorber V6501 for removal of air and moisture, and (6) turbine T6501 that rejects the heat extracted from the H_2 moderators to a compressor-brake system.

Because beam trips cause a disturbance in the thermodynamic conditions of the He, the heater power and bypass valve opening are controlled by independent PID controllers to minimize fluctuations of He pressure and temperature, thus mitigating the loss of moderation during beam trips. Given the requirement to maintain a constant H_2 density in each moderator loop and the desire to dampen He temperature and pressure fluctuations, a closed-loop model of the CMS is needed for optimization.

DATA-DRIVEN MODEL OF THE CMS

A control-oriented model blending zero-dimensional physics and machine learning techniques was introduced.

Helium refrigeration loop. The system was modeled using fundamental physics principles such as the first law of thermodynamics, the ideal gas law, turbulent compressible flow through an orifice, and the principle of mass conservation. A system identification approach was used to obtain the model's parameters. The resulting model corresponded to a continuous-time, nonlinear, dynamic system of the form $\dot{x} = f(x,u)$, where u are the control variables or inputs (left column of Figure 2) and x are the relevant thermodynamic states of He (middle column of Figure 2). The states can be used to calculate other variables in the He refrigeration system such as the turbine speed S_{6501} and the pressure difference across the bypass valve ΔP_{6523} used for the PID controller [6].

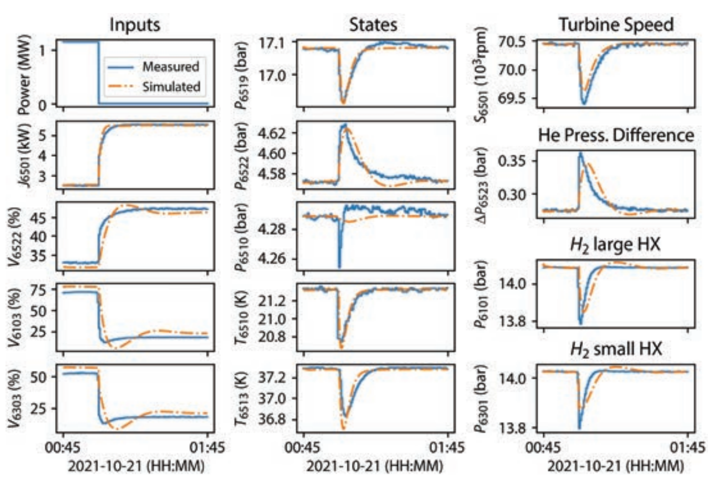

Figure 2. Comparison of closed-loop CMS simulated model vs. measurements. (Credit: ORNL)

Liquid hydrogen circulation system. Unlike the modeling of the He refrigeration loop, it was not possible to model the H_2 system with simple physics-based equations because of the complexity of the accumulators and the moderators. Thus, a multilayer perceptron (MLP) was trained using historical input data already available in the He submodel, resulting in the following relation: $P_{6i01} = MLP(\text{Power}, P_{6522}, V_{6i03})$ for $i \in \{1,2,3\}$. Given that the He–H_2 heat exchangers HX6200 and HX6300 and their H_2 circulation systems are roughly the same size, it was assumed that $V_{6203} = V_{6303} \Rightarrow P_{6201} = P_{6301}$. Putting all the control-related outputs together, the model can be augmented with $y = g(x,u)$, where $y = [T_{6510}\ \Delta P_{6523}\ P_{6101}\ P_{6301}]^T$. The two bottom-right plots of Figure 2 show how closely the MLP model matches the measured H_2 pressure.

PID controllers. For every output in the model, a setpoint y^{SP} was calibrated to maintain desired thermodynamic conditions in the He and H_2 subsystems. Therefore, the feedback control can be calculated as $u = PID_\theta(y - y^{SP})$, where θ are the gains of the PID controller. Figure 2 shows the closed-loop simulation (dash-dotted line) of the CMS during a beam trip from 1.15 MW, followed by an inactive period long enough to allow transients to settle. Note that the only input needed for the model is the beam power; all the other signals can then be calculated.

RESULTS

The turbine speed was chosen as the performance variable in order to minimize beam trip disturbances by recalibrating the controller. Thus, consider the following optimization problem for choosing the PID gains:

$$\theta^* = \underset{\theta \in \Theta}{\operatorname{argmin}} \| S_{6501} - \mathrm{E}[S_{6501}] \|_2 \ \text{subject to} \quad \begin{aligned} \dot{x} &= f(x, u) \\ y &= g(x, u) \\ u &= PID_\theta(y - y^{SP}) \end{aligned}$$

The methodology attempts to choose the PID gains so that S_{6501} stays as close as possible to its nominal value $\mathbb{E}[S_{6501}]$. The optimal parameters were found using the nonlinear least squares methods, and the proposed gains were tested experimentally. Figure 3 shows the experimental data collected during an accelerator physics study performed in February 2023. The black solid line shows the response of the turbine speed after a beam trip from 1.4 MW using the baseline PID gains. On the other hand, the red dash-dotted line shows the S_{6501} response under a similar beam trip with the recalibrated controlled gains. In the second case, the turbine speed did not decrease as much as in the first case, resulting in a reduction of 50% in S_{6501} fluctuations compared to the baseline case. This result suggests that artificial intelligence (AI)–based methods, combined with physics-informed models, can be used to optimize CMS operations and reduce downtime.

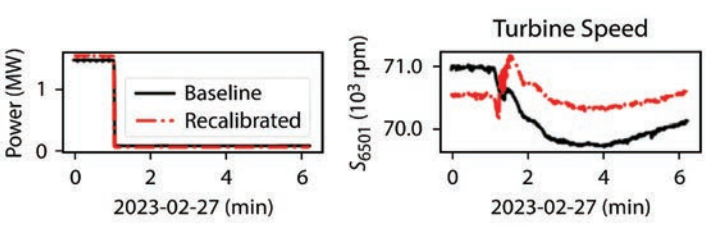

Figure 3. Experimental results showing advantages of control optimization. (Credit: ORNL)

CONCLUSIONS

CMS has historically sustained large pressure and temperature transients during beam trips. A hybrid physics-based and AI-based approach with a neural network component was used to simulate the dynamic behavior of the CMS using a closed-loop model. The model was used to formulate an experimental test plan to reconfigure PID gain settings in the control system. The experiment results show a 50% reduction of the transient disturbances in the turbine speed using the proposed methodology.

IMPACT

Significant improvement was observed in the cryogenic system cold-end temperature and the pressure behavior, with an optimistic outlook for handling 1.7 MW beam power operation. This is the first time that a large-scale cryogenic facility in the U.S. Department of Energy has successfully used a model-based approach for tuning.

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AI for Scientific Discovery of Materials with Desired Functional Properties

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INTRODUCTION

The design and discovery of materials with desired functional properties is are pivotal to the scientific mission of the U.S. Department of Energy (DOE), which includes several important applications for the national economy and security. Examples of DOE-relevant applications are nuclear materials capable of withstanding extreme environments, molecules and materials for energy-efficient solar power conversion, and compounds capable of removing undesirable greenhouse gases or industrial waste products through secure storage or conversion into value-added compounds.

Understanding materials at the atomic scale is crucial for designing the macroscopic functional behavior of a material; the arrangement, bonding, and interactions of atoms determine the material's properties and behavior. The study of multicomponent materials at the atomistic scale requires exploring a vast chemical space with a large dimensionality determined by the variety of chemical compositions (e.g., concentration of each chemical species), atomic configurations (e.g., arrangement of atoms of different chemical species), and geometrical orientations of interatomic angles in the 3D space. The high dimensionality of the chemical space to be explored poses significant challenges to the state-of-the-art experimental (in vivo) and computational (in vitro) approaches. Although experiments are labor-intensive and time consuming, physics-based models are computationally expensive and require massive dedicated computational resources that exceed even the more advanced leadership-class supercomputing capabilities.

Recently, artificial intelligence (AI) has shown remarkable promise in overcoming experimental and computational barriers to enable effective (fast and still sufficiently accurate) screening of large chemical spaces. This will facilitate identification of materials with desired functional properties. A team of Oak Ridge National Laboratory (ORNL) researchers supported by the AI for Scientific Discovery and Design project in the ORNL AI Initiative has made significant progress using AI to address fundamental materials science problems. The team has developed AI techniques in specific areas, including (1) causal reasoning, which identifies relevant multiscale features that determine the functional behavior of the material; (2) scalable surrogate models to perform estimates of material properties using relevant physical descriptors provided by the causal models; (3) generative AI models for the design of organic molecules with desired properties; and (4) generative AI models for inorganic materials design.

BACKGROUND

Causal AI for atomistic materials modeling. Current machine learning (ML) approaches for materials design and discovery fail to determine important physics-based causal relationships such as what causes influence the target and how and which features can be efficiently tuned to reach a target property of interest. Causal models, combined with standard ML approaches, have the potential to uncover fundamental physical principles that traditional ML methods alone cannot. Aside from a few successful studies, applications of such models to the domain of materials science are still in their infancy. In general, ML models informed with structured causal connections work well when the relationship between the target and feature spaces is well-defined, as in theoretical sciences. Studying multifunctional materials from the perspective of causal relations using atomic information constitutes a promising arena in which ML models informed with structured causal connections can be explored.

If successful, causal models will identify the relevant input features that reduce the risk of overfitting and will increase the robustness (accuracy and trustworthiness) of the surrogate model predictions.

Scalable graph neural network surrogate models. Deep learning models effectively capture nonlinearities arising from interatomic interactions. These models can be trained on a subset of data from first-principles calculations to predict properties for new inputs. Graph neural networks (GNNs) accurately predict material properties by mapping atomic configurations onto graphs on which each atom becomes a node connected by edges representing bonding interactions. This representation captures the local environment and coordination, crucial information for material formation energy. GNNs require a large dataset of known material properties for training to maintain generalizability and robustness across the parameter space; this approach requires high-performance computing (HPC) resources for efficient data processing.

Using GNN models on HPC significantly reduces prediction time compared with full first-principles calculations while also maintaining accuracy. This accelerated approach holds promise for expediting material discovery and design.

Generative AI for the design of organic molecules. State-of-the-art statistical approaches for exploring high-dimensional chemical spaces for materials discovery can be computationally expensive and time consuming. Generative ML models such as genetic algorithms, generative adversarial networks (GANs), and language models expedite the search for new materials by suggesting novel atomic structures or compositions with desired properties, allowing researchers to focus on promising candidates.

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In high-throughput screening for functional molecules, synthesizability is a crucial criterion. Retrosynthesis-based methods offer insights into synthesis costs and yields, but their need for a vast reagent library and significant computing resources makes them computationally expensive. To address this challenge, RetroGNN, a GNN model, was integrated into the workflow. RetroGNN is based on Chemprop, which enhances the robustness of the selection criteria for synthesizable drug candidates during high-throughput screening.

Generative AI for design of inorganic compounds. GAN continues to be explored and developed for materials design applications such as generation of viable 3D structures of solid materials under periodic boundary conditions (PBCs). Specifically, this effort focused on generating novel zeolite structures with maximal cavity space for storage of CO_2 or CH_4 greenhouse gases. The resulting PBC-GAN software was developed using PyTorch and can be easily integrated into surrogate models for targeted inverse design problems.

RESULTS

Causal AI for atomistic materials modeling. The causal AI team elucidated the atomic-scale mechanism for A-site cation ordering in double perovskite oxides [1]. This study involved first-principles computations on 145 double perovskite oxides using a combination of standard input features and those derived from first-principles calculations with structural modes to generate feature spaces. These findings introduce a new design principle for stable A-site cation ordering in perovskites that can be applied to a broader range of materials.

The outcomes of causal AI models will enhance the performance of surrogate models for atomistic materials modeling by identifying critical atomic descriptors, thereby increasing surrogate accuracy and reducing the risk of overfitting.

Scalable graph neural network surrogate models. The surrogate model team developed HydraGNN [2], a flexible GNN architecture for HPC, to ensure compatibility with updated software packages. Large publicly available datasets, *GDB-9-Ex* and *ORNL_AISD-Ex*, were created containing nearly 100,000 and over 10,000,000 organic molecules, respectively [3]. A scalable workflow supports first-principles calculations with different quantum chemical methods and is portable across HPC systems. These datasets, along with the workflow software, are freely accessible for training surrogate models.

HydraGNN was trained for two applications: predicting the HOMO-LUMO gap (HLG) [4] in organic molecules and forecasting the formation energy [5] in solid solution alloys. Linear scaling of HydraGNN training was achieved using up to 1,024 NVIDIA V100 graphics processing units on the Oak Ridge Leadership Computing Facility (OLCF) Summit and 1,024 NVIDIA A100 graphics processing units on Perlmutter at the National Energy Research Scientific Computing Center.

The trained HydraGNN model enables efficient exploration of high-dimensional chemical spaces to identify compounds with desired properties.

Generative AI for the design of organic molecules. A strategy to generate molecules surpassing the limitations of the original dataset was developed by automating mutation rules through iterative dataset expansion. A masked language model (MLM) approach enhances the efficiency of generating molecules with improved properties [6].

The methodology focuses on minimizing the HLG in organic molecules, which is crucial for applications such as semiconductors, photodetectors, catalyzers, batteries, and light-emitting materials. HydraGNN predicts the HLG of new molecules generated by the MLM and guides identification of promising chemical regions for exploration.

The approach harnesses hybrid language models to streamline molecular sequence design, aiding experimental discovery efforts.

Generative AI for design of inorganic compounds. PBC-GAN was used to generate chemically stable zeolite structures. The PBC-GAN was trained using a public dataset with 31,713 zeolites. PBC-GAN has outperformed comparable models for zeolite design in terms of the chemical validity of the generated structures, as measured by simple chemical rules, including Si:O ratio and bond connectivity information. For example, the success rate of PBC-GAN was 5.86%, whereas the state-of-the-art model for zeolite design achieved only 2.68%.

The scalable PBC-GAN model enables identification of atomic structures of inorganic compounds with promising functional properties for carbon capturing and sequestration.

CONCLUSIONS

The research conducted by the AI for Scientific Discovery and Design thrust of the ORNL AI initiative is developing scalable, robust AI methodologies to enable a systematic, principled, and effective exploration of large parameter spaces for the design of organic and inorganic compounds with desired functional properties. This has been achieved through ongoing collaborations with different organizations and user facilities at ORNL to ensure that the algorithmic and computational capabilities developed within the AI Initiative are relevant for the scientific mission of DOE.

IMPACT

The goal in chemical and materials sciences is the rational design of compounds and materials with specific properties. Currently, the discovery process relies on a trial-and-error approach, which is costly and inefficient given the vast range of chemical structures and elements. To tackle this challenge, a workflow that combines computational methodologies with advanced ML was developed for the inverse design of materials with user-defined properties. These applications include renewable energy (e.g., solar cells, organic photovoltaics, and light-emitting diodes), energy storage (e.g., batteries and supercapacitors), carbon capture, materials innovation (e.g., drugs and materials with desired properties), and nuclear energy (e.g., high-performance fuels and materials with improved shielding properties). The goal is to create a virtual lab in which simulations can rapidly predict chemical compositions and structures for experimental validation.

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Building Open Foundation Models for Sciences

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INTRODUCTION

The past few years have witnessed the rise of large language models (LLMs) as a powerful tool in the field of artificial intelligence (AI), demonstrating remarkable success in various natural language processing tasks like text generation, machine translation, and question answering. A common pattern has since emerged: LLMs are used as foundation models upon which downstream applications can be built through fine-tuning.

However, a deficit in investigating LLMs specifically designed and tailored for scientific tasks is in part caused by the prohibitive cost of training such models and the lack of a sufficiently large pool of scientific downstream tasks for evaluation. For the scientific community at large, U.S. Department of Energy leadership computing platforms are some of the most viable and accessible resources. This study focused on building LLMs for science by running them on leadership high-performance computing (HPC) platforms and using a large corpus of scientific articles. The end-to-end building process involves data collection and processing, model pretraining, and downstream tasks evaluation. In this paper, *model pretraining* refers to the method and process for teaching these LLMs the general rules and dependencies within a language, which can be compute-intensive and data-intensive, even for modest model sizes.

Pretraining LLMs for science on HPC systems presents a unique set of challenges, including the absence of best practices for large-batch training, scaling questions in terms of training and model performance, and unknowns regarding the optimal LLM model size for scientifically relevant tasks. This paper presents best practices for end-to-end building of LLMs for science on HPC systems, including optimizing batch size and scaling strategies. A set of foundation models called FORGE was released with up to 22 billion (22B) parameters using 257 tokens from more than 200M scientific articles, along with domain-specific datasets specifically centered around scientific corpora. Science-related downstream benchmarks are proposed to evaluate the effectiveness of LLMs for science. The scaling of optimal model size to data size and the efficacy of generic vs. domain-specific LLMs are also presented. This contributions of this effort include a framework for effectively using the computational power of HPC systems to develop LLMs for science-related tasks.

BACKGROUND

Since the introduction of the transformer [1] architecture, the LLM has become the centerpiece not only in natural language processing but also in computer vision. Its variants—Bidirectional Encoder Representations from Transformers (BERT) [2] and generative pretrained transformers (GPTs) [3]—have become the dominant architectures for LLMs. One key factor that drives the success of transformer-based LLMs is that the model performance scales with the number of model parameters (P) and input tokens (D), following the aptly named *scaling law* [4]; the total number of floating-point operations (FLOPs) needed to train the LLM is calculated approximately using

$$T_{\text{FLOPs}} \sim 6 \times P \times D. \qquad (1)$$

Typically, input token D is comparable in size to model parameter P. The Chinchilla study [5] found a ratio of 20 for D/P to be optimal, although a more recent work [6] demonstrates that better results can be obtained with an even larger ratio. However, the model behaviors for scientific texts are mostly unexplored.

Pretraining-related works [1–8] are largely limited to NVIDIA graphics processing unit (GPU)-based systems. However, the emergence of supercomputers equipped with other vendors' GPUs, such as Oak Ridge National Laboratory's (ORNL's) Frontier, an Advanced Micro Devices GPU-based supercomputer, requires further exploration of computation strategies.

RESULTS

Feasibility study. Based on Eq. (1) and Chinchilla scaling (20 tokens per parameter), the computation needed for pretraining LLMs is quadratically proportional to the number of model parameters (P), as shown in Figure 1. For example, training a 175B parameter GPT3 model requires 3.7×10^{24} FLOPs, and it quickly grows to 1.2×10^{26} FLOPs for a 1 trillion (1T) parameter GPT-style model. Even with an exascale platform like Frontier, it takes the entire machine over 3 months to train a GPT-1T model, assuming theoretical peak performance and linear scaling. In practice, the achievable performance is approximately 40% of the peak, and the scaling efficiency strongly depends on the model size: the larger the model, the greater the challenge to achieve a good scaling because communication becomes a bottleneck.

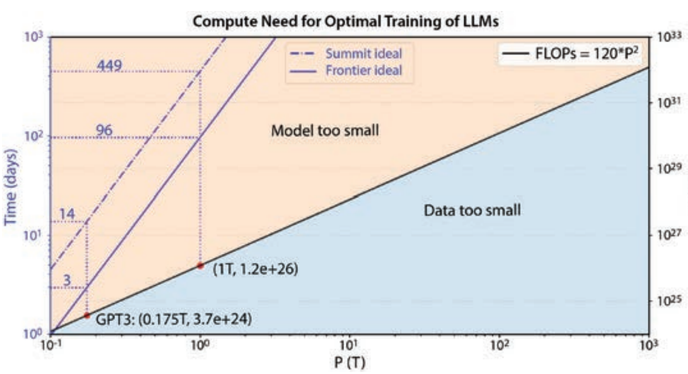

Figure 1. Computation needs (FLOPs) and ideal training time (days), assuming peak performance and perfect scaling for optimal training of LLMs on ORNL's Summit and Frontier, respectively. For a given model size (with P parameters), the blue region below the solid line indicates that data size is insufficient (i.e., the number of tokens is less than 20P). Conversely, for a given compute budget, the orange region above the solid line indicates that the output accuracy would likely benefit from increasing the model size. (Credit: ORNL)

To estimate the actual cost in terms of computation time and energy, the training performance was measured from approximately 100 iterations of the execution, excluding the initial warm-up. The total run time and energy cost were then projected based on the number of steps needed to process the entire input data. Table 1 lists the estimations for three model sizes: 13B, 175B, and 1T parameters. For larger models (175B and 1T), considering the limitation of data, a range is provided, with the lower and upper bounds being 1× and 20× of the model parameters.

Model	Time (node hours)	Energy (MWh)	Efficiency (TFLOPS/watt)
GPT-13B	12,000	24	0.239
GPT-175B	[0.1M–2.6M]	[217–4338]	0.235
GPT-1T	[8M–160M]	[4,727–94,539]	0.343

Table 1. Computation time, energy, and efficiency for pretraining GPT models on Frontier.

FORGE architecture and scientific corpora. This work bases the construction of FORGE on the GPT-NeoX architecture [7], which largely follows GPT-3 [8] with some small deviations. These deviations include using rotary positional embeddings instead of absolute positional embeddings using parallel computation of the attention and feed-forward layers rather than executing sequentially and using full dense layers. The details of the architecture are listed in Table 2. FORGE was mainly trained in three sizes: 1.44B (FORGE-S), 13B (FORGE-M), and 22.4B (FORGE-L) parameters, which should fit into a modern GPU for inference downstream tasks. FORGE-S has a comparable number of parameters to GPT2-XL, with 24 layers and a hidden dimension of 2,064. FORGE-M increases to 40 layers and a hidden dimension of 5,120, resulting in approximately one order of magnitude more parameters. FORGE-L further doubles the model parameters by increasing to 48 layers.

Model	No. of parameters	No. of layers	No. of heads	Hidden size
FORGE-S	1.44B	24	24	2,064
FORGE-M	13B	40	40	5,120
FORGE-L	22.4B	48	48	6,144

Table 2. FORGE model architectures.

This effort draws upon a diverse set of scientific texts collected from multiple sources. Specifically, data were gathered from (1) Connecting Repositories (CORE) [9], which provides access to abstracts and full texts of 52M papers, (2) Open Academic Graph, which consists of Microsoft Academic Graph (MAG) [10] and Aminer [11] and contains 151M abstracts, (3) 2.2M abstracts from ArXiv, and (4) 6.4M abstracts from SCOPUS [12]. Because a large portion of the collected texts are in English, non-English entries were filtered out to narrow the focus and scope of the model. Additionally, a preliminary deduplication of data was conducted from CORE, MAG, and Aminer based on cross-reference indexes. Table 3 lists the details of the preprocessed data used for training.

Training performance. LLMs are commonly trained on cloud-based computing platforms, which differ in architecture and scale from leadership computing platforms like Frontier. One major advantage of Frontier is its larger scale, which allows for training LLMs with particularly large batch sizes.

As shown in Figure 2, for FORGE-S, the scaling efficiency is about 95% up to 512 GPUs. Larger models see a performance drop across nodes, but the efficiency afterward is approximately 90% up to 1,024 GPUs. The ideal line (dotted) is based on the FORGE-S single-node performance (63 teraflops). The per-device performance of training the 175B model only drops slightly, from 33.4 to 31.4 teraflops for 384 and 1,024 GPUs, respectively. Therefore, the main bottleneck stems from the high communication bandwidth requirement.

Source	No. of docs	No. of tokens	Size (GB)
CORE	52.3M	225B	764
Aminer	47.1M	10B	55
MAG	103.8M	20B	108
SCOPUS	6.3M	1.5B	6.5
ArXiv	2.2M	0.8B	3.4
Total	~212M	~257B	937

Table 3. Scientific data corpora.

In terms of the time to solution, once a working batch size (that converges) is determined, the per-device batch size can be reduced to scale up to more devices if the computation performance per device still maintains. For a fixed batch size of 16.8M, the time to solution can be reduced from 20 h to 6 h by adding 4× more devices (512 to 2,048 GPUs).

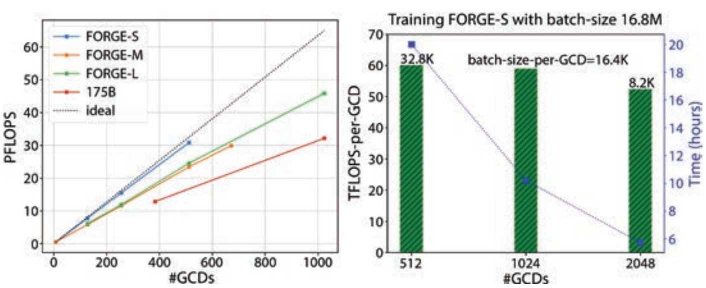

Figure 2. Scalability of training FORGE models and 175B parameters up to 2048 GCDs on Frontier. (Credit: ORNL)

Downstream evaluation: generic language benchmarks. In Figure 3, the training losses of FORGE models are plotted with respect to the number of input data (tokens) that the models have learned. As expected, for all model sizes, the loss value (a measurement of the deviation between the model prediction and ground truth) continues to decrease because the model has been trained on more data. Compared with FORGE-S, larger models such as FORGE-M and FORGE-L have more learning capabilities, as indicated by the lower loss values.

To further validate model performance, FORGE models were evaluated against established benchmarks [13] for language models, including SciQ, PIQA, ARC-easy, and ARC-challenge. Those models include lists of question and answer pairs and are evaluated based on the accuracy of the model-generated answers. As shown in Figure 3, the accuracy of FORGE models continues to improve with more training data, with FORGE-L performing the best for these tasks.

Downstream evaluation: scientific tasks. Scientific databases contain publications from diverse scientific domains. Depending on the application, it can be beneficial to tokenize and pretrain models on related fields. Considering the practical implications, a task was established to fine-tune models for domain classification. To generate the labelled data set, approximately 1,000 entries were randomly sampled for each of six domains (biology/medicine, chemistry, engineering, materials, physics, and social science/art) from the CORE data set. The LLMs are fine-tuned for the task, and the evaluation metric is the classification accuracy.

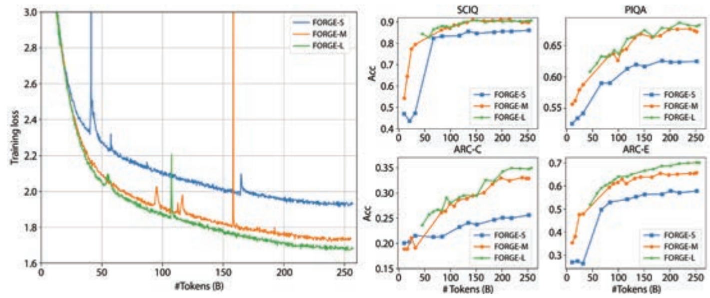

Figure 3. Training performance: evolution of loss and accuracy during training for FORGE models of varying sizes. (Credit: ORNL)

To demonstrate the labeled data and task, the FORGE models were fine-tuned on the data, and the 2D t-distributed stochastic neighbor embedding (t-SNE) clustering generated by the fine-tuned model was plotted. As shown in Figure 4, six distinctive local clusters are formed by scientific domains, indicating the effectiveness of using LLMs to filter out domain texts from the large corpus.

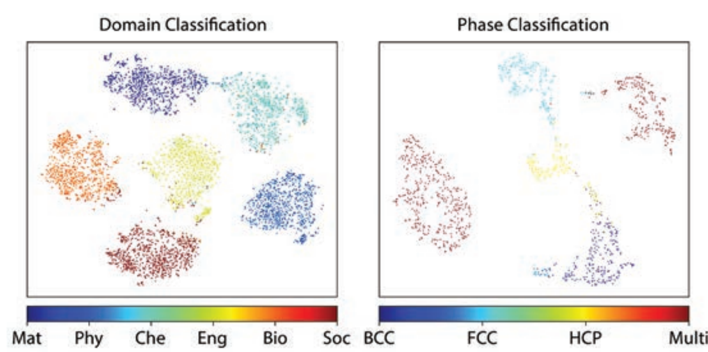

Figure 4. Visualization of domain and phase classifications using t-SNE clustering from fine-tuned model. (Credit: ORNL)

Domain classification is designed for models trained on generic texts. A more fine-grained task is to test the model's capability within a particular domain, especially for research questions. To this end, an evaluation of material phase classification is proposed. The data set was first introduced [14] to show how elemental properties (e.g., molar volume, melting point) can be used as an indicator for the phase of alloys such as body-centered cubic, face-centered cubic, hexagonal closest packed or a combination of these phases. Understanding phases is a fundamental problem in understanding the structure of materials and can impact the design of new high-entropy alloys. This data set consists of a list of alloy formulas, and in principle, embedding the formulas encodes the information within the literature, and the elements provide context for each other. An LLM that is fine-tuned on this data set can serve as a descriptor for phase classification. As shown in Figure 4, the fine-tuned FORGE model can effectively distinguish different material structures.

Model and data size considerations. The optimal data-to-model size ratio is debatable [5,6]. To address this debate for scientific texts, the evolution of loss and accuracy was shown during training for FORGE models in Figure 3. Although the improvement in accuracy begins slow down near 100B tokens for FORGE-S4 (1.44B parameters), the improvement trend continues. This indicates that the model is still learning, even after 257B tokens (data-to-model ~178), which is in agreement with the observations of training LLM Meta AI (LLaMA) [6]. A capable, smaller model is more applicable (less demanding for hardware) for downstream applications, and the larger model likely requires more than 20× the number of tokens per parameter.

FORGE models and usages. FORGE models are released [15] according to Hugging Face's API and documentation standard. This common interface will make FORGE easier to use for downstream tasks. Furthermore, the model checkpoints will be released in a format compatible with the GPT-NeoX code base, allowing the community to train the models on Frontier or other platforms.

FORGE models are trained on five data sources (Table 3), which contain publications without peer review; the data quality may impact the model performance. FORGE models are intended for research purposes only and have not been evaluated for bias, toxicity, and misinformation.

CONCLUSIONS

This paper presents a comprehensive approach to developing LLMs specifically designed for scientific knowledge. The research team conducted an end-to-end analysis of pretraining LLMs on the Frontier supercomputer and proposed an LLM-based method for filtering out domain-specific texts, along with heuristics for large-batch training. This effort thoroughly evaluated various performance aspects of training LLMs on HPC platforms and presents results that were run on Frontier.

A set of open foundation models for science— FORGE—was released, and three scientific downstream tasks were proposed. The FORGE models are available in three different sizes designed for general scientific and domain-specific texts. When compared with other similar-sized models, the FORGE models performed comparably or better for scientific tasks.

IMPACT

The approach and findings have significant implications for developing language models that can improve understanding and interpretation of scientific language and thus support scientific research and discovery. Although these approaches primarily involve using model embeddings as a knowledge representation (e.g., phase classification and energy regression) or model-generated sequences (e.g., chemical or genomic sequences) to navigate a large search space, in the future, the research team will experiment with scientific applications that will include combining LLMs with data of different modalities such as instrument parameters and images. These diverse applications will highlight the versatility of LLMs and their potential to enhance scientific research and analysis.

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Urban AI Emerges

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INTRODUCTION

Urban artificial intelligence (AI) is an emerging field that blends technology and cities to tackle complex urban challenges. In our ever-smarter and more efficient cities, urban AI taps into data from devices like wearables, sensors, and internet of things devices to make informed decisions. It examines factors such as weather, energy consumption, connectivity, and human interactions to devise strategies for safer, more adaptable, environmentally friendly cities. Experts in this domain use sophisticated computer programs and data analysis to engineer systems that optimize city functions and services. These systems harmonize various systems like energy and transportation to ensure seamless operations. They also deploy these programs to anticipate urban growth patterns and enhance disaster preparedness.

A team of Oak Ridge National Laboratory (ORNL) researchers is pioneering innovative AI applications to enhance urban environments. They are exploring how AI can aid in city planning, boost urban wellness, and refine energy, transportation, and communication infrastructures. The overarching goal is to harness technology's potential to create safer, more livable, inclusive urban spaces.

CREATING NEW NEIGHBORHOODS USING AI

As cities plan, they must consider how neighborhoods evolve with population expansion and new construction. This transformation has implications for the environment, too. Melissa Allen-Dumas employs computer programs to visualize potential future neighborhoods [1]. These programs are trained using *generative adversarial networks*, a type of AI that comprises two components: one crafts images, and the other evaluates their authenticity. These components learn from each other, gradually improving image quality. This methodology was applied to create alternate visions of prospective Los Angeles neighborhoods, factoring in existing building placements and functions. (see Figure 1.)

Figure 1. Land cover image (left), target image (center), and generated image (right) for a high-density urban residential area in Los Angeles. [1]

Why is this significant? Envisioning diverse trajectories for neighborhood growth aids in understanding how new construction might impact microclimate and weather patterns. This type of analysis is invaluable in climate research and represents cutting-edge exploration.

AI FOR INTELLIGENT TRAFFIC CONTROL

Optimizing traffic signal timing across a network is a vital research domain. Yan Liu spearheads a project leveraging deep learning techniques to improve traffic prediction and signal control on urban networks. This initiative contributes to broader efforts aimed at using AI for intelligent transportation systems. Liu's team employs graph-based machine learning (ML) to capture traffic flow and signal patterns on an urban network. Coupled with reinforcement learning–based control agents, graph-based ML allows signaled intersections to harness learned traffic patterns in a neighborhood to optimize local signal timings. This AI approach effectively addresses the data scarcity challenge and improves computational scalability in traffic control on large networks.

Why is this significant? Once fully developed, these innovations will be deployed in *digital twin cities*, or in digital replicas of cities, including Chattanooga and Nashville. The anticipated outcomes include improved traffic flow, expedited travel for all, energy savings, and reduced emissions.

HAZARDS IN URBAN INFORMATION TECHNOLOGY

As highlighted in the Introduction, contemporary cities are heavily reliant on information technology, demanding seamless operation. Urban information technology systems generate copious data, and pivotal events are crucial for decision-making and urban service enhancements. However, detecting hazards in these systems poses challenges; issues range from temporal variations of events, sparse abnormal event data for learning, and intricate event relationships for handling the large volume of data. Recent advances employ intelligent computer programs with deep learning to uncover anomalies, particularly within data sequences. However, these techniques have limitations in urban contexts. They might misclassify normal occurrences as anomalies or overlook vital information, thus requiring substantial computational resources. The associated computational cost of these limitations in urban applications is unfathomable.

Femi Omitaomu and Ph.D. student Haoran Niu introduced a novel method for identifying anomalies within data sequences [2]. Their approach leverages sequential masked token prediction (SMTP), which treats data as linguistic sentences. It learns sequential event patterns and discerns deviations from

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the norm by comparison. The application of SMTP to medical data yielded superior anomaly detection without introducing new challenges or straining computational resources. (see Figure 2.) This indicates that SMTP can be a powerful tool for enhancing urban systems efficiently.

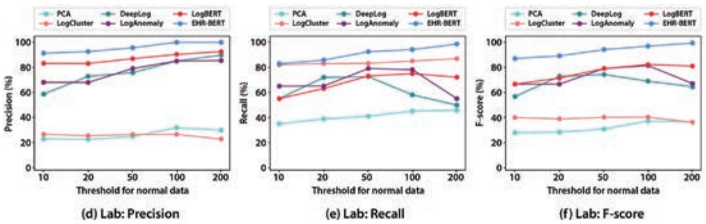

Figure 2. Comparison evaluation results on electronic health record bidirectional encoder representations from transformers with five baselines.) [2]

Why is this significant? This new method has the potential to greatly reduce errors related to anomalous events and could become a valuable tool for improving urban safety and the overall quality of urban services.

AI FOR HIGH-RESOLUTION CLIMATE MODELING

Enabling cities to withstand extreme climate challenges is the focus of Deeksha Rastogi, who is actively exploring AI methods to enhance climate modeling. For climate applications at the urban scale, high-resolution datasets serve as a crucial resource for understanding the characteristics of extreme weather events and their impacts on infrastructure, such as the electric grid and associated climate change impacts. Extreme events, including heat waves, storms and hurricanes, have the potential to cause devastating impacts on human settlements, a threat that is expected to intensify under a changing climate. The integration of AI-based methods with conventional climate downscaling techniques to generate high-resolution climate data offers significant advancement. This approach allows domain knowledge to be incorporated into AI models and enables faster computations. Using these techniques can effectively bridge existing gaps between the scales at which climate models are run and the scales at which the impacts on human systems are experienced.

Why is this significant? These extreme events can wreak havoc on infrastructure and settlements, underscoring the importance of gaining insight into these occurrences.

AI-INFORMED DIGITAL TWIN CITIES

Developing methodologies to examine future scenarios is imperative for the inevitable increase of urbanization. This approach helps planners anticipate the consequences of present choices. In this pursuit, Haowen Xu crafts digital replicas, known as *digital twins*, of cities. These virtual twins employ real-time data and AI algorithms to replicate urban landscapes. The pioneering Chattanooga Twin Project (CTwin) replicates Chattanooga's primary roads, aiming to study urban mobility challenges [3]. CTwin is an end-to-end web-based platform (see Figure 3) that incorporates various aspects of the decision-making process for optimizing urban transportation systems in Chattanooga, Tennessee, to reduce traffic congestion, incidents and vehicle fuel consumption. The platform enables advanced capabilities for (a) real-time situational awareness of traffic and infrastructure conditions on highways and urban roads, (b) cyber-physical control for optimizing traffic signal timings and (c) interactive visual analytics on big urban mobility data and various metrics for traffic prediction and transportation performance evaluation. CTwin is the first known digital city twin and was featured in a recent CNN article [4].

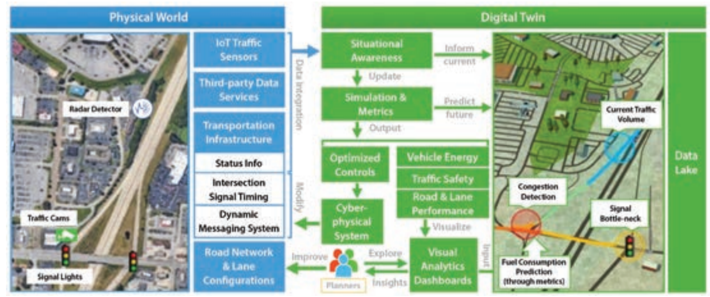

Figure 3. The workflow for CTwin. [3]

Why is this significant? By harnessing real-time data and AI, digital twins open doors to simulating a wide range of scenarios, spanning from infrastructure and construction to traffic dynamics and energy usage.

SOLAR AI TECHNOLOGIES

As the global population continues to urbanize and electrification increases, city planners will play a critical role in addressing climate change and achieving sustainable development goals. Integrating renewable energy sources such as solar and wind into urban infrastructure will be a significant factor. Solar energy has been primed as one of the most promising renewable energy sources. Femi Omitaomu is developing solar AI technologies that combine big data and ML to analyze rooftop solar potential and to estimate savings virtually. This has traditionally been a laborious task and a significant bottleneck that limits solar energy providers from scaling their reach to potential customers. The process to produce a utility value is highly inferential because it is dependent on geographical and contextual information. Therefore, this task is well suited to be performed by ML. The task to estimate the solar potential of rooftops is divided into several competing subtasks, and an ML model is built for each subtask. In the field of ML, this is known as an *ensemble model*, which is a model that is composed of smaller, simpler models. These smaller models tend to perform better on simpler tasks, and when they are brought together, they outperform a single model trained to perform the task as a single problem. Solar AI divides the task of solar potential estimation into subtasks such as rooftop segmentation, obstacle detection, and weather forecasting.

Why is this significant? Solar soft costs account for 65% of the total solar installation cost. The solar AI technologies will effectively reduce the soft costs of solar energy and provide immense value to solar energy suppliers by reducing their customer acquisition costs.

ENGINEERING URBAN BIG DATA

Amid the accumulation of diverse data for urban AI methods, effective data organization is pivotal. Sarah Tennille and Brandon Miller employ a series of tools and processes that systematically collect, process, and store data, facilitating optimal utilization.

Why is this significant? Data are the foundation upon which AI systems are built and developed. Without data, AI models lack the necessary information to learn, adapt, generalize, and perform the tasks for which they are designed. The quality, quantity, and diversity of data directly impact the performance and capabilities of AI systems

CONCLUSIONS

As the global population continues to urbanize, ORNL is championing the development of novel AI methods that will make our urban areas become smarter and more efficient, resilient, and sustainable. As a complement to these initial research endeavors, ORNL orchestrated the First International Workshop on Advances in Urban AI (Urban-AI 2023). The event united scholars and practitioners to discuss progress and future trajectories in urban AI. Urban-AI 2023 (https://urbanai.ornl.gov/urbanai2023/) coincided with the 31st ACM SIGSPATIAL International Conference in Hamburg, Germany, in November 2023. A second workshop, Urban-AI 2024, is scheduled for October 2024, in Atlanta, Georgia (https://urbanai.ornl.gov/urbanai2024/).

IMPACT

In the era of urbanization and technological advancement, ORNL scientists are developing methods and tools that use data-driven approaches to help decision makers enhance operational efficiency, public safety, and cost-effectiveness of our urban systems.

COLLABORATE WITH ME

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