ARGONNE NOW
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HOW THINGS BREAK

AND WHY SCIENTISTS WANT TO KNOW

ALSO IN THIS ISSUE:

WEATHER OR NOT WE'RE READY | THE COMPLEX CHEMISTRY OF COMBUSTION

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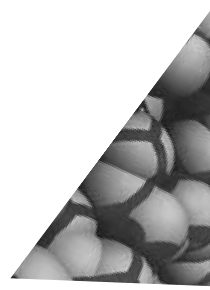


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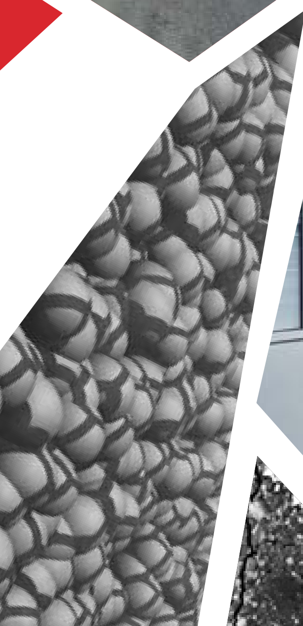

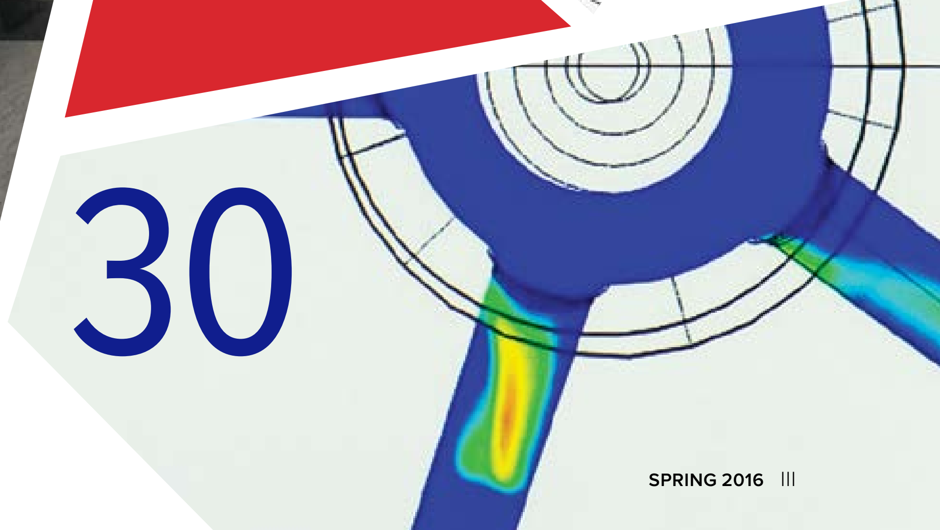
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Argonne NATIONAL LABORATORY

NOTE FROM THE DIRECTOR

Dear reader,

Seventy years ago, Argonne's founding scientists put the "break" in breakthrough when they set out to create energy by splitting atoms.

Today, the scientists and engineers of Argonne continue to break new ground in search of understanding how and why things break. By understanding how something breaks, we can make it work better.

In this issue you'll meet a cross-section of talented researchers working here at Argonne, including: scientists who run batteries in special chambers until they break down; physicists who smash atoms to find out what makes up the smallest parts of matter; modelers who build elaborate simulations of car engines and nuclear reactors; and analysts who work to prevent our country's infrastructure from breaking down amid violent storms.

The work happening at Argonne is designed to answer big questions—so big, in fact, that our researchers are constantly collaborating to answer them. Take, for example, the scientists and engineers examining the microstructures of a material used in nuclear reactors in order to build more robust power plants. At ATLAS, our linear accelerator, they use xenon ions to mimic the effects of radiation on the metal they're studying. The next stop is the Advanced Photon Source, a powerful X-ray source, to see how the metal behaves under intense heat and pressure. Finally, this data is combined with complex simulations of reactors at the Argonne Leadership Computing Facility to strengthen our understanding of reactor materials behavior and safety.

In fact, all of the grand challenges that Argonne is built to address—safe, sustainable energy, clean environment, and a thriving economy—are so complex that they require multidisciplinary teams with many different backgrounds coming together. And those teams need large facilities, techniques, and instruments—precisely what we bring to bear as a national laboratory.

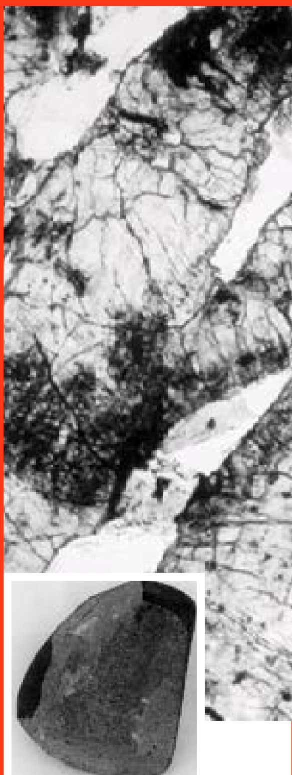
As we look forward to another 70 years of ambitious research and exciting discoveries, we appreciate your interest and your support. Find out more about us on our website, www.anl.gov, or follow us on social media for the latest updates on the very important work we're doing.

Thank you, and I hope you enjoy this issue of *Argonne Now*.

Peter B. Littlewood
Director
Argonne National Laboratory

THIS YEAR IN SCIENCE HISTORY

151 YEARS AGO



1865

A BIT OF MARS ON EARTH

Witnesses retrieve an 11-pound meteorite after its fall to earth in India. The Shergotty Meteorite is thought to be about 165 million years old and was ejected from the surface of Mars 11 million years ago. It wasn't til 1962 that we saw another Martian rock land on Earth.

75 YEARS AGO

1941

Russian explorer Tatyana Ustinova discovers the "Valley of Geysers" in eastern Russia—one of just five major geyser fields in the world. Her valley turned out to contain 20 geysers and more than 200 thermal pools.

50 YEARS AGO

1966

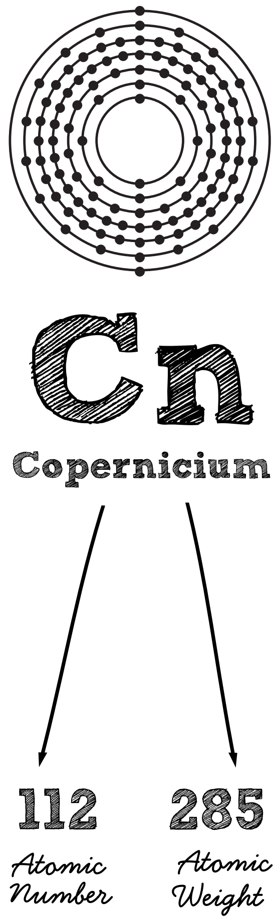
ROYALTY AT ARGONNE

King Simeon II (left) and Queen Margarita, exiled monarchs of Bulgaria, tour Argonne. Simeon would later become one of only two monarchs to become head of government through democratic elections.

20 YEARS AGO

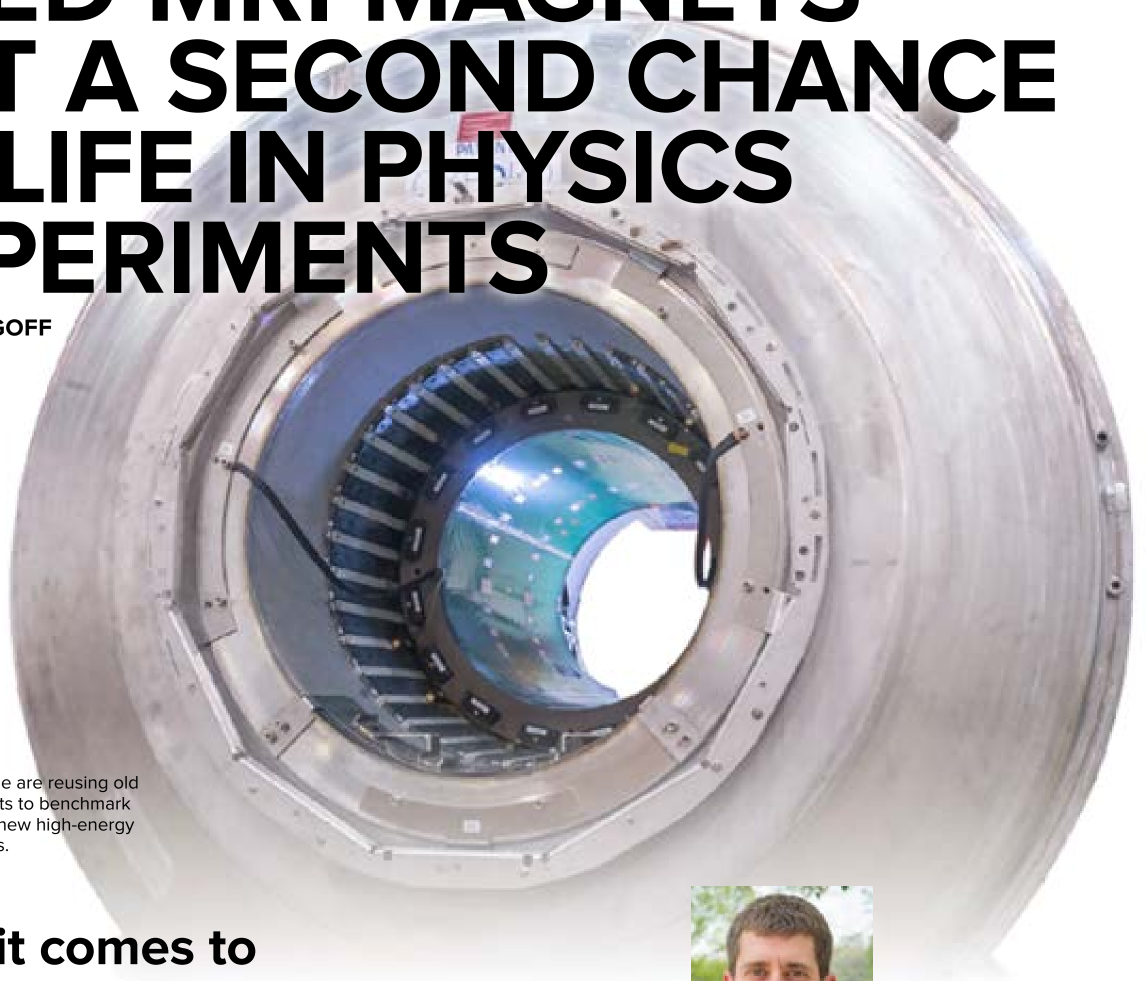
1996

Inside a German accelerator, scientists produce a single atom of element 112, later named copernicium, for the first time. This radioactive metal is so highly unstable that only a few atoms have ever been produced.



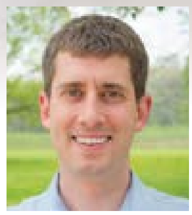
USED MRI MAGNETS GET A SECOND CHANCE AT LIFE IN PHYSICS EXPERIMENTS

BY JARED SAGOFF



Scientists at Argonne are reusing old hospital MRI magnets to benchmark instrumentation for new high-energy physics experiments.

When it comes to magnets, a doctor's trash is a physicist's treasure.



Peter Winter works to adapt the magnets for their new homes in a muon experiment.

Researchers at Argonne recently acquired two decommissioned magnets from MRI scanners from hospitals in Minnesota and California that will find a new home as proving grounds for instruments used in high-energy and nuclear physics experiments.

The two new magnets have a strength of 4 Tesla, not as strong as the newest generation of MRI magnets but ideal for benchmarking experiments that test instruments for the g minus 2 ("g-2") muon experiment currently being assembled at Fermilab.

The Muon g-2 experiment will use Fermilab's powerful accelerators to explore the interactions of muons, which are short-lived particles, with a strong magnetic field in "empty" space.

To measure and calibrate the custom-built probes, scientists needed a magnet that could provide not only a strong field but one that was uniform and stable. Solenoid MRI magnets like the ones Argonne has acquired are perfect for that purpose.

The repurposed magnets have another notable advantage: originally used as a human patient MRI magnet, they have a wide bore so that large detector components can easily fit inside.

"By using these new magnets, we can fit the entire half-meter-long probe system in the magnet, which will give us a very precise measurement of the intensity of the magnetic fields," said Argonne high-energy physicist Peter Winter. "These MRI magnets produce a very stable, homogenous magnetic field that is ideal and crucial for getting technology ready for the larger g-2 experiment."

NEWS

SIMULATING SAFER TRANSPORT OF EXPLOSIVES

BY JIM COLLINS

In 2005, a semi truck hauling 35,000 pounds of explosives through the Spanish Fork Canyon in Utah crashed and caught fire, causing a dramatic explosion that left a 30-by-70-foot crater in the highway.

Fortunately, there were no fatalities. With about three minutes between the crash and the explosion, the driver and other motorists had time to flee. Some injuries did occur, however, as the explosion sent debris flying in all directions and produced a shock wave that blew out nearby car windows.

Such accidents are extremely rare but can obviously have devastating results. So understanding better exactly how such explosions occur can be an important step to learning how better to prevent them.

The cause of the massive blast on the Utah highway, brought on by a process called deflagration-to-detonation transition (DDT), posed something of a mystery. The semi was transporting 8,400 cylinders of explosives intended for blasting operations in the mining industry. Despite the cargo's volatile nature, it was not supposed to detonate violently as it did.

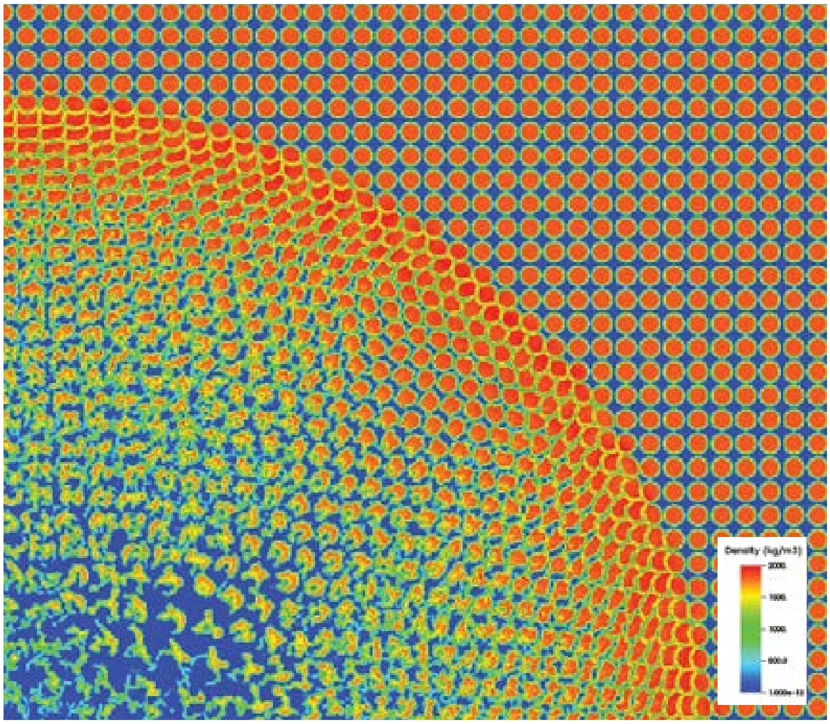
In the case of an accidental fire, the explosive cylinders were supposed to burn rapidly in a type of combustion called deflagration. Limited by heat transfer, deflagration events spread at a velocity lower than the speed of sound. Detonation, on the other hand, occurs when the combustion spreads at a supersonic rate and triggers a high-pressure shock wave.

Researchers from the University of Utah are using supercomputing resources at the Argonne Leadership Computing Facility (ALCF), a U.S. Department of Energy Office of Science User Facility, to recreate

Crews work on a section of highway in the Spanish Fork Canyon in Utah destroyed by an explosion when a truck hauling explosives crashed. Photo courtesy Utah Department of Transportation.

the 2005 explosion virtually. Led by Professor Martin Berzins, the research team is performing large-scale 3-D simulations on Mira, the ALCF's 10-petaflops IBM Blue Gene/Q supercomputer, to study the physical mechanisms that led to DDT.

"Ultimately," said Berzins, "we hope our research will result in strategies that can prevent accidents like the one we are studying."



Researchers are using Argonne's supercomputer Mira to model how explosives detonate and how to pack them more safely.

REAL-WORLD INSPIRATION

"The main focus of our simulations is to determine why the fire escalated to detonation," said Jacqueline Beckvermit, a Ph.D. student and research assistant at the University of Utah.

While the real-world accident only took a few minutes to transition from deflagration to detonation, achieving virtual detonation required considerable time and effort.

"We set out to simulate one-eighth of the actual truck with the explosives in their original packing configuration, but it was not an easy feat," Beckvermit said. "After two years of work and more than 100 million computing hours, we finally reached detonation this fall."

The simulations were a challenge due to the complex nature of DDT, which involves several strongly correlated processes, such as chemical kinetics, pressure waves, and turbulence, all occurring in multiple spatial and temporal scales.

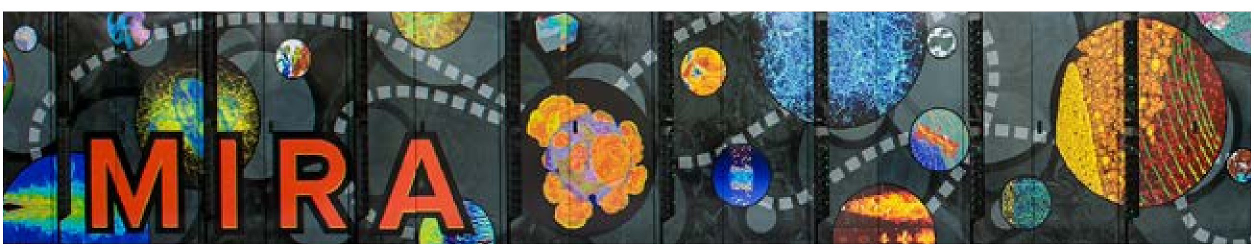
EXPLOSIVE RESULTS

Thus far the team's simulations have led them to two possible mechanisms for DDT in large arrays of explosives. One hypothesis points to inertial confinement, a process in which damaged cylinders of explosives form a barrier that traps product gases, creating a pocket of high pressure that could initiate DDT. The other proposed mechanism involves a shock-to-detonation transition caused by the impact of explosive cylinders colliding in a high-pressure environment. But more analysis is required before these theories can be confirmed or rejected.

In addition to investigating why DDT occurred, the researchers are using Mira to examine how different packing densities and configurations could be used to prevent such explosions. They are also working to scale up their simulations to run on the entire supercomputer as a means to achieve even higher fidelity results in the future.

"The ultimate goal of our project is to propose ideas on how to package explosives for transport to make sure accidents like this don't happen anymore," Beckvermit said.

The project received computing time at the ALCF through the DOE Office of Science's Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program.



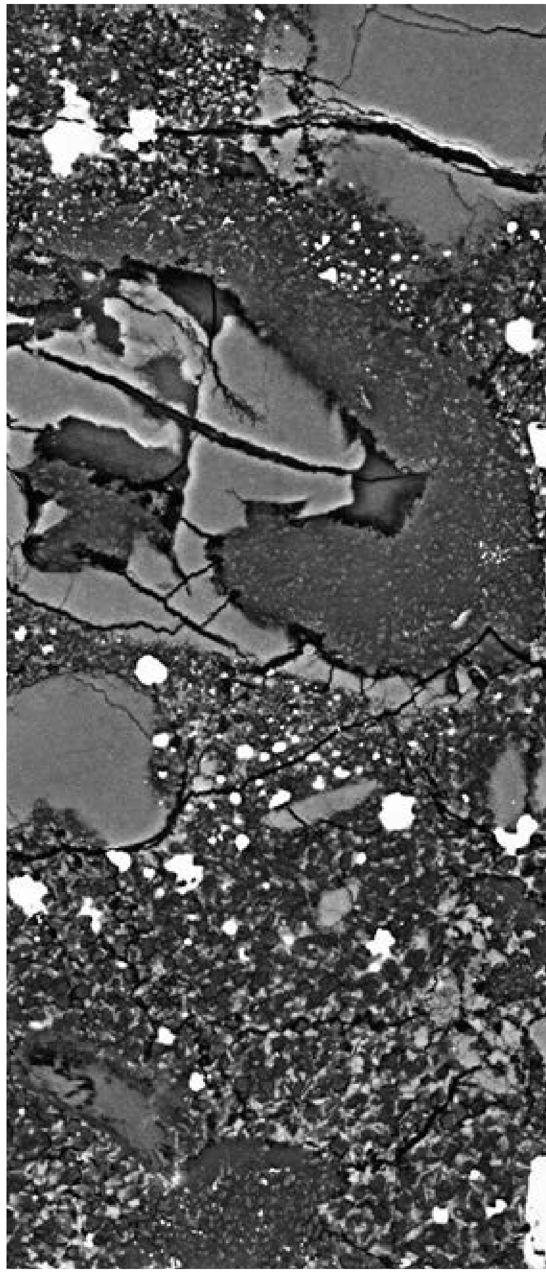
Argonne's supercomputer Mira is capable of 10 quadrillion calculations per second.

NEWS

EARTH'S MOST ABUNDANT MINERAL FINALLY HAS A NAME

BY TONA KUNZ

An ancient meteorite and high-energy X-rays have helped scientists conclude half a century of effort to find, identify, and characterize a mineral that makes up 38% of the Earth.



And in doing so, a team of scientists clarified the definition of the Earth's most abundant mineral—a high-density form of magnesium iron silicate, now called Bridgmanite. The naming does more than fix a vexing gap in scientific lingo; it also will aid our understanding of the deep Earth.

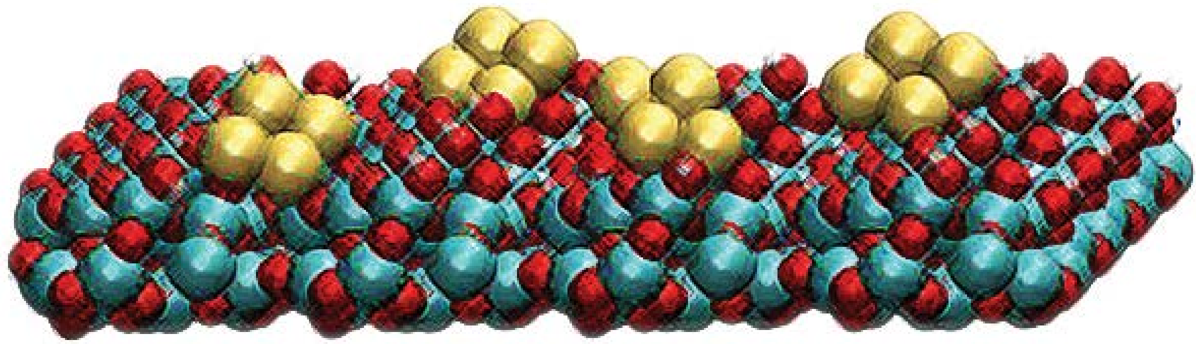
To determine the makeup of the inner layers of the Earth, scientists need to test materials under extreme pressure and temperatures. For decades, scientists have believed a dense perovskite structure makes up 38% of the Earth's volume, and that the chemical and physical properties of Bridgmanite have a large influence on how elements and heat flow through the Earth's mantle. But since the mineral failed to survive the trip to the surface, no one has been able to test and prove its existence.

Shock-compression that occurs in collisions of asteroid bodies in the solar system create the same hostile conditions of the deep Earth—roughly 3,800 degrees Fahrenheit and pressures of about 240,000 times greater than sea-level air pressure. Part of the debris from these collisions falls on Earth as meteorites, with the Bridgmanite "frozen" within a shock-melt vein. But previous tests on meteorites using electron microscopy caused radiation damage to the samples and incomplete results.

So the team decided to try a new tactic: non-destructive X-rays at GeoSoilEnviroCARS, a University of Chicago-operated beamline at the Advanced Photon Source, a U.S. Department of Energy Office of Science User Facility located at Argonne. The X-rays' high energy allows them to penetrate the meteorite, and their intense brilliance leaves little of the radiation behind to cause damage. The team examined a section of the meteorite Tenham, which crashed in Australia in 1879. The GSECARS beamline was optimal for the study because it is one of the nation's leading locations for conducting high-pressure research.

This research was funded by the DOE, NASA, and NSF.

Scientists used samples from this 1879 Australian meteorite containing Bridgmanite, a mysterious mineral that also exists deep within the Earth, to finally clarify its structure using the Advanced Photon Source.



CLUSTERS CAPTURE CO_2

BY PAYAL MARATHE

A new copper catalyst could help capture carbon dioxide to make fuel.

Capture and convert—this is the motto of carbon dioxide reduction, a process that stops the greenhouse gas before it escapes from chimneys and power plants into the atmosphere and instead turns it into a useful product.

One possible end product is methanol, a liquid fuel and the focus of a recent study conducted at Argonne. The chemical reactions that make methanol from carbon dioxide rely on a catalyst to speed up the conversion, and Argonne scientists identified a new material that could fill this role. With its unique structure, this catalyst can capture and convert carbon dioxide in a way that ultimately saves energy. They call it a copper tetramer.

It consists of small clusters of four copper atoms each, supported on a thin film of aluminum oxide. These catalysts work by binding to carbon dioxide molecules. The structure of the copper tetramer is such that most of its binding sites are open, which means it can attach more strongly to carbon dioxide and can better accelerate the conversion. (In the catalyst currently used by industry, a number of binding sites are occupied merely in holding the compound together, which limits how many atoms can catch and hold carbon dioxide.)

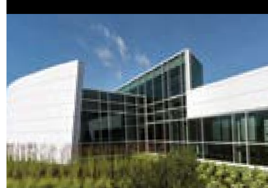
"With our catalyst, there is no inside," said Stefan Vajda, a chemist at Argonne and the Institute for Molecular Engineering and co-author on the paper. "All four copper atoms are participating because with only a few of them in the cluster, they are all exposed and able to bind." The benefit of enhanced binding is that the new catalyst requires lower pressure and less energy to produce the same amount of methanol. Copper tetramers could allow us to capture and convert carbon dioxide on a larger scale—reducing an environmental threat and creating a useful product like methanol that can be transported and burned for fuel.

The team used the Center for Nanoscale Materials as well as the Advanced Photon Source, both U.S. Department of Energy Office of Science User Facilities, which allowed them to observe ultralow loadings of their small clusters, down to a few nanograms, which was a critical piece of this investigation.

This study, which used beamline 12-ID-C of the APS, was funded by the DOE's Office of Basic Energy Science.

LEED GOLD FOR NEW BUILDINGS

Two newly finished buildings at Argonne were awarded LEED Gold. In the **Energy Sciences Building**, the countertops are recycled glass, the fume hoods and air handling are energy-efficient, and the large windows and skylights save electricity by lighting offices and lobbies naturally.



The Advanced Protein Characterization Facility has a reflective roof to keep the building cool, sensors to minimize energy use when offices are empty, and trees and drought-tolerant native vegetation to reduce water use.

NEWS

CARBON SURPRISES UNDER THE SEA

BY SARAH SCHLIEDER

Some of the world's tiniest organisms may have a large impact on climate change.

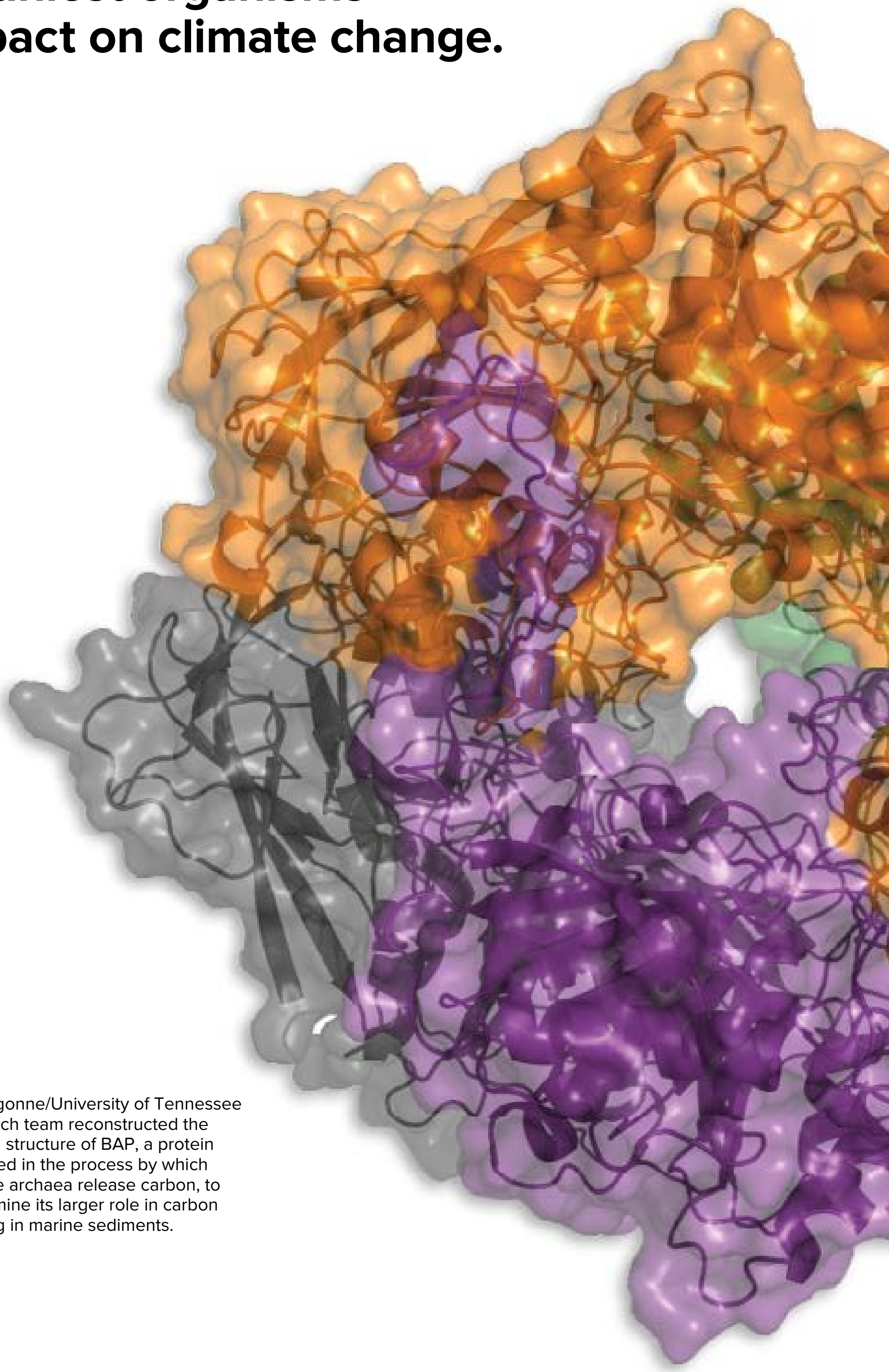
Researchers from Argonne and the University of Tennessee found that microorganisms called archaea living in marine sediments use completely novel enzymes to break down organic matter into carbon dioxide.

These single-celled archaea eat organic carbon in marine sediments. Enzymes in the archaea break down large carbon molecules into smaller units. This process releases carbon dioxide and methane into the water and eventually, into the atmosphere.

However, as the temperature of oceans and bodies of freshwater increases, this carbon cycling process accelerates. The temperature at the bottom of the ocean, for example, is approximately 35 to 39°F. According to Andrzej Joachimiak, Argonne distinguished fellow and director of the Structural Biology Center, if the ocean temperature rises, the rate of carbon release might increase.

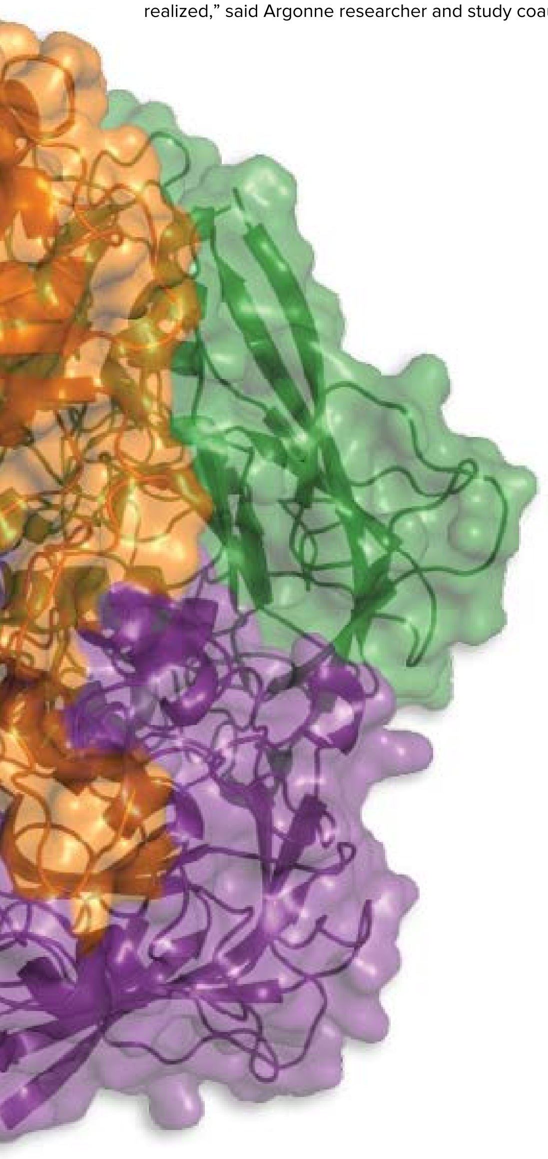
"ABOUT 40 PERCENT OF EARTH'S ORGANIC CARBON IS STORED IN MARINE SEDIMENTS,"

Joachimiak said. "An increase in temperature and acceleration of the carbon cycling process in these sediments is a major concern."



An Argonne/University of Tennessee research team reconstructed the crystal structure of BAP, a protein involved in the process by which marine archaea release carbon, to determine its larger role in carbon cycling in marine sediments.

"It seems that archaea have a larger role in organic carbon, or protein, degradation than we previously realized," said Argonne researcher and study coauthor Karolina Michalska.



Joachimiak said scientists are uncertain about how fast archaea process carbon and whether the release is accelerating. Once researchers have these statistics, they may find ways to better predict the environment's response to a changing climate.

This understanding starts at the molecular level. Using resources at the Advanced Photon Source, a DOE Office of Science User Facility, and the Advanced Protein Characterization Facility, the research team produced and crystallized bathyaminopeptidase, or BAP—one of the enzymes found in the archaea—to look into its structure and observe how it operates. They found that BAP plays an important role in breaking down proteins and, consequently, the turnover of atmospheric carbon.

The biggest challenge the researchers had was determining BAP's function, because no previously cultured organisms shared a close ancestry. These types of organisms are considered microbial "dark matter" because their physiologies are unknown and they have never been grown in a lab.

"Being able to characterize proteins directly from microbial dark matter, without requiring that they first be grown in a lab, opens up limitless possibilities for discovering novel functions of these strange organisms that control the breakdown of carbon in marine sediments," said Karen Lloyd, assistant professor in the department of microbiology at the University of Tennessee.

According to Karolina Michalska, a protein crystallographer in Argonne's biosciences division, it was originally believed that bacteria were the primary players in the degradation of proteins in marine sediments. But the research shows that archaea are also involved in the process.

"It seems that archaea have a larger role in organic carbon, or protein, degradation than we previously realized," Michalska said.

The research was supported by the DOE's Office of Science, by the U.S. National Institutes of Health and by the Center for Dark Energy Biosphere Investigations led by the University of Southern California. Studies were performed at the 19-Insertion Device Beamline, operated by the Structural Biology Center at the Advanced Photon Source at Argonne, and at Argonne's Advanced Protein Characterization Facility.

The local food movement is booming. Can we do the same for electricity?

PERSONALIZED ENERGY

BY JUSTIN H.S. BREAUX

Being cut off from electricity doesn't just affect whether we can make a phone call or heat dinner; it affects a doctor's ability to perform surgery, a police officer's ability to respond to a 911 call, and a city's ability to provide basic services to its citizens.

For these reasons and more, many experts are increasingly interested in making electricity a local affair. This idea, useful for both cost savings and for backup power, moves the main source of electricity away from remote large-scale plants to smaller local ones. This approach is called distributed energy.

Distributed energy devices can produce enough electricity to power a home, business, or small community, making them ideal backups for power when energy is cut from the main grid in the case of a power outage. They can be solar panels, small wind turbines, batteries, fuel cells or microturbines that connect directly to the home or local electrical grid, but their purpose is to meet the specific power needs of a local population.

"Until maybe about 10 years ago, we never accommodated people's different energy needs—now we can," said George Crabtree, director of Argonne's Joint Center for Energy Storage Research center. "It may be the solar panel on my roof or the battery in my garage, but in the end, these different needs give rise to new technologies that give us a greater amount of choice and, ultimately, control."

Large power plants have several major drawbacks. Firstly, they waste a lot of energy—about two-thirds—when converting fuel to electricity. Secondly, many of them sit idle for a good part of the year (on average about half the time) as they may only be needed to meet peak demand—usually the time of day when the

majority of people come home in the evening. Thirdly, in shipping the power from the large stations to the consumer, we waste another 5-7% in transmission and distribution losses.

On the other hand, distributed systems present smaller, more flexible options. And because they are located close to where the power is needed, less energy is lost in delivery.

Distributed energy devices such as solar panels, fuel cells, microturbines, and batteries come in a variety of types and sizes, from as little as one kilowatt—enough to power ten 100-watt light bulbs—up to as much as 10,000 kilowatts, which might be enough to power a university campus or a neighborhood or community microgrid.

Single homes and small businesses can benefit from rooftop solar panels on sunlit days or portable natural gas generators in the evening. Hospitals and small towns that use considerably more energy can use a mix of microturbines, generators, and industrial-scale batteries.

However, tying these devices together in a way that allows them to communicate with electrical grid operators is a challenge. Each new device connected to the grid becomes another device that operators have to account for when balancing an area's energy demand. As information-sharing between devices gets more complex, and as more consumers install distributed systems in their homes and communities, the next challenge becomes how to share data with local utilities so they can accurately respond to real-time energy demand.

Distributed energy resources are growing rapidly in some parts of the country. At the end of 2014, the U.S. had close to 650,000 solar-powered homes with a new solar project installed every 2.5 minutes, and the grid has managed to handle it fine so far. "But if we're talking about moving from coordinating distributed energy for tens of millions of people, we can't even envision that amount of data," said Argonne energy systems analyst Guenter Conzelmann. "We are talking about a very different scale than the one we are used to, and we just don't have the systems in place to handle that right now."

National grid operators are quite efficient at balancing energy supply and demand, because they can rely on hundreds of power plants to respond instantly each time a device is turned on or off. This type of balance becomes more challenging on smaller neighborhood scales.

"Controlling things on a smaller scale can be more challenging because you have fewer resources," said Jianhui Wang, the head of Argonne's Advanced Power Grid Modeling section. "The solar panels, the wind or gas turbines, the electric cars—all of these things have to communicate with each other to balance out the demand and supply within that community, just as an electrical grid operator has to balance out a region."

Figuring out how distributed energy systems will communicate effectively within a grid the size of a neighborhood is the focus of a new project on Chicago's south side. Argonne and the Illinois Institute of Technology (IIT) are teaming up with electrical utility ComEd to build a microgrid in the Chicago neighborhood of Bronzeville.

A microgrid is a small community that can make and use most or all of its own power using a mix of distributed energy generators and energy storage units.

Argonne is working with ComEd, IIT, and a number of industry partners to develop advanced control system software to help this microgrid balance relatively few resources within a strictly defined area, while matching the energy demand of its community.

Though we'll still rely on remotely-generated power, an increase in the number of distributed systems will decrease this reliance over time, Argonne experts say.

"THAT TRANSITION IS GOING TO HAPPEN, BUT YOU NEED TO TIE IN ALL OF THESE RESOURCES INTO THE GRID TO BE ABLE TO MANAGE IT,"

said Argonne mechanical engineer Sreenath Gupta. "Thankfully, innovation is driving costs down, which is definitely going to help increase the adoption of these types of technologies."

Research described in this article has been funded by the National Energy Technology Laboratory, on behalf of the Office of Electricity Delivery and Energy Reliability, at the U.S. Department of Energy.

UNTIL MAYBE ABOUT 10 YEARS AGO, WE NEVER ACCOMMODATED PEOPLE'S DIFFERENT ENERGY NEEDS—NOW WE CAN.

— GEORGE CRABTREE, JCESR DIRECTOR

TOP 9 TIPS ON HOW TO PREVENT CYBER “BREAK-INS”

BY DIANA ANDERSON

Mike Skwarek, Argonne’s Cyber Security Officer, is an expert on how to protect yourself today in the information age. He’s shared some tips on how to keep personal information protected and hackers at bay.

1 PROTECT PASSWORDS

“They’re just like your toothbrush. Don’t share your password with other people and get a new one every six months.”

2 DO NOT “REMEMBER”

When your computer or mobile device asks if it should “remember” your password, is it safe? “Never allow this!” Skwarek warned. “Do not trust a machine to remember your password. If you okay this, your password is saved on the device and your security can be shattered in one quick hack.”

3 PURCHASE SEPARATELY

“Designate one credit card as your online purchase card and keep that card capped at a certain dollar figure to ensure that fraud is kept at a minimum, just in case it’s compromised,” recommended Skwarek. “That way, you don’t have to cancel and change multiple cards if something happens.”

4 STAY UP-TO-DATE

Version updates and patches block holes that hackers can wiggle in through. "Some of our most used devices are mobile. Just because a device is in your pocket doesn't mean it's safe from attacks," said Skwarek. "Make sure you apply patches and version updates to your mobile devices and home computer regularly."

5 RUN A FIREWALL

A firewall is a protection fence, denying access from the internet into your computer without your permission. "This is how you avoid having someone hack into your machine," advised Skwarek. "However, you still need to patch your computer regularly. Maintain your security network just like you would a real fence. Holes and open gates let anyone in."

6 SOURCE YOUR APPS

How do you know if you can trust an app and how do you know if it's an authentic version? "Consumers should read up on who does a good, or poor, job of vetting apps on their sites and stores for malicious software. A recent study found that the number of malware-infected apps in one major store nearly quadrupled to 42,000 from 2011 to 2013."

7 VERIFY, THEN TRUST

It's good to be suspicious online. "If you get an email from a long-lost loved one asking for money or an email from a company offering you money if you click on a link and provide log-in credentials, be suspicious. Cyber phishing attempts often tug on your heartstrings or present an offer that's too good to pass up."

8 LIMIT PERSONAL INFORMATION

Limit sharing of personal information. "Why does this company, website, or person need my information?" Skwarek said. "I usually ask how they're going to store my information and how they're going to protect it. We don't want to challenge people all the time, but these are things we should be asking in order to protect our interests."

9 SHARE CYBER SOURCES

Help get the word out. "Cyber issues are a global problem, not just a U.S. problem. Young people should talk to their parents and their grandparents about cyber security," suggested Skwarek. "We should all be socializing what the potential threats are and how individuals can protect themselves."

To find out about the secret life of another Argonne cyber security expert, turn to page 46.

WOMEN IN STEM CAREERS

BREAKING DOWN BARRIERS

BY DIANA ANDERSON

Three Argonne researchers share their experiences, why they pursued STEM careers, and how they're continuing to help the next generation of scientists and engineers to flourish.

Growing national attention is focused on increasing the number of women in Science, Technology, Engineering, and Mathematics (STEM) careers.

Even as educational programs ramp up efforts to encourage girls in STEM fields—an effort to close the gender gap—women continue to face challenges as they move forward.

At Argonne's annual Science Careers in Search of Women day, high schoolers talk with Lisa Durham, head of Argonne's Leadership Institute.

NANCY KARIUKI

Chemist

When I was in high school, I wanted to be a pharmacist, so I took lots of chemistry and math classes. Math came easily to me, but I had to work hard in chemistry. It's ironic, because I'm a chemist today. I was born and grew up in Kenya. There, at that time, we didn't get to choose what fields we would go into for college. We took a national exam and based on those results and the number of students who excelled in each area, we were placed, rather than chose, our schools and fields of study. I did not make the cut for pharmacy school. Instead, I was placed in general science courses, where I chose to focus on chemistry. Math, chemistry, and physics were considered more of men's territory at that time, so I was one of two women and 28 men in these courses.

Being brought up in Kenya, where there are certain expectations for women, and having overcome that, I don't feel that I am limited by barriers for women in science. I don't feel that I am limited or that I have been limited because I'm a woman or because I'm African. **I had always wanted to conduct research. It's my passion.** Today, I'm actively involved in encouraging young people to pursue STEM career fields. I mentor postdocs and summer interns at Argonne, and last year I mentored high school students interested in STEM fields. There's a common misconception that math and chemistry are difficult, but I like to show young people that it's possible to succeed, using myself as an example. I'm not exceptional. It just takes hard work. **Set your goals and don't be afraid to ask for help.** I tell them, "Hey, I'm doing it. So you can, too."

57%

WOMEN EARN 57% OF ALL BACHELOR'S DEGREES.

33%

WOMEN EARN 33% MORE WHEN THEY WORK IN STEM CAREERS.

27.5%

WOMEN MADE UP ONLY 27.5% OF THE NATION'S STEM WORKFORCE AS OF 2010.

KATRIN HEITMANN

Theoretical Physicist/ Computational Scientist

I was interested in mathematics and problem solving from a very early age, puzzling out math problems **even in kindergarten.** I grew up in Germany. There, in the last two years of high school, you get to pick a focus of study. I chose mathematics and physics because I enjoyed it. My older brother invited me to sit in on university lectures with him so I could see what the coursework was like. It became a straightforward decision for me—I gravitated to physics.

Thankfully, I've always had people in my life who were supportive, including my family, friends, and instructors. **When I first started studying physics at university, I was the one woman out of 150 men.** It didn't feel bad, though. No one treated me rudely. I know there are women who have other stories, like they weren't taken seriously, but I never had that experience. I received support and respect throughout my career from the very beginning and I hope that encourages more young women to enter the field of physics. **I have had lots of mentors, but the ones who stand out most are the people who have challenged me to think differently and to consider my future in a way that I hadn't up until that point.** Now when I'm hiring staff, I make sure I take a close look at all applicants, digging beyond the surface to find the talent within each individual. I also mentor postdocs and early career scientists so they have the support they need and encouragement to grow.

DIANE GRAZIANO

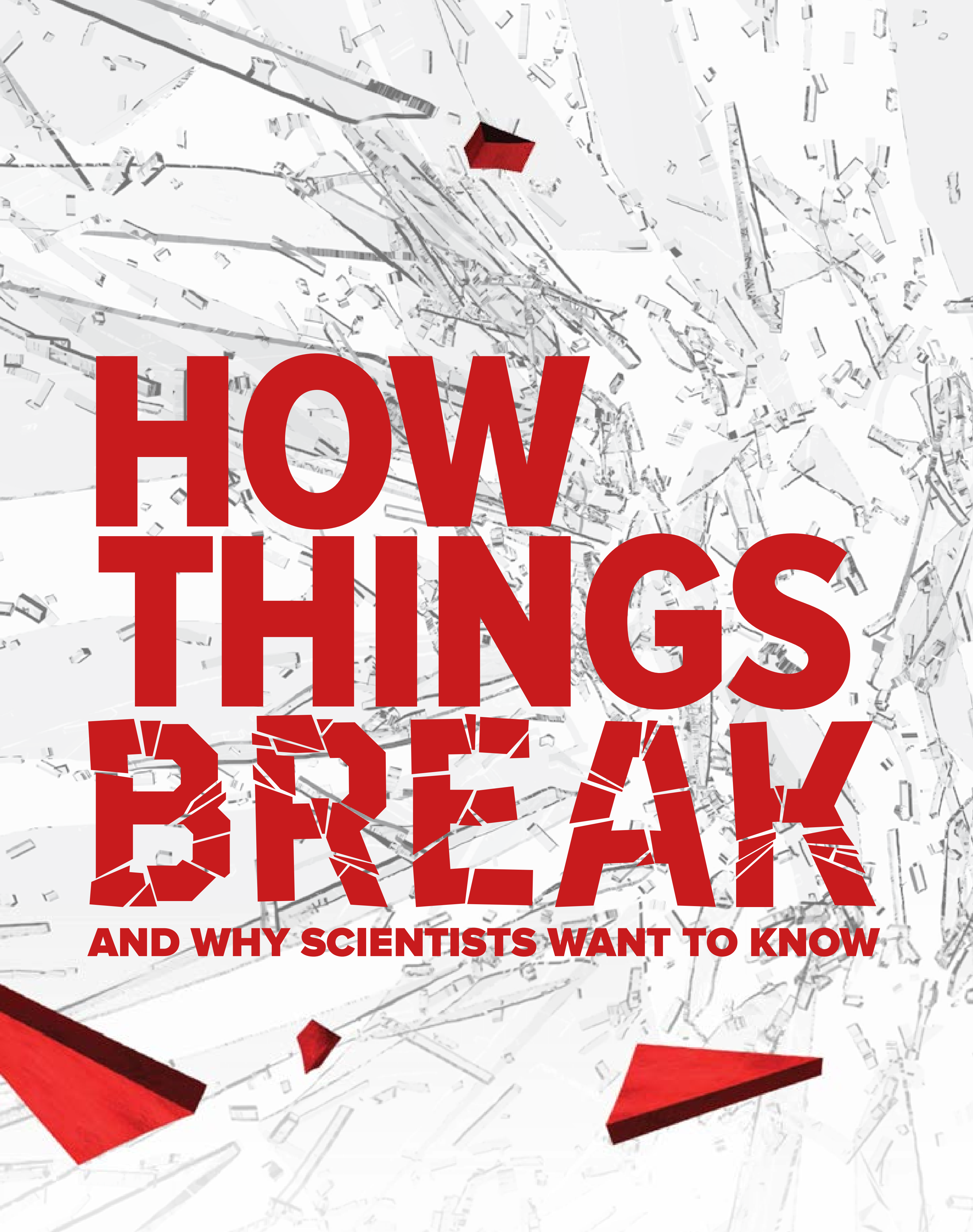
Chemical Engineer

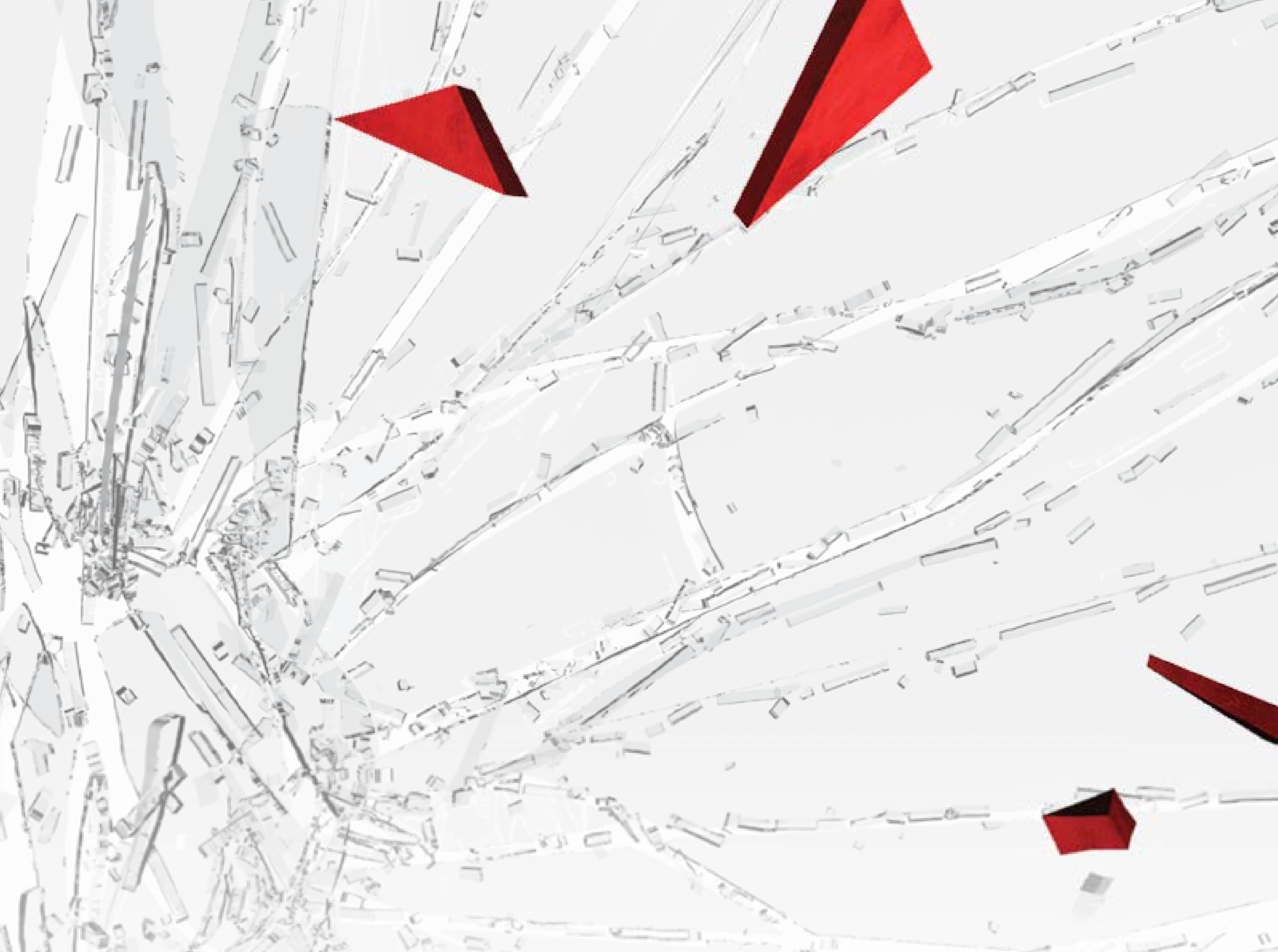
When I graduated with my first chemical engineering degree in the '80s, companies had quotas, so they were hiring women like crazy. I was in the top of my class and was being recruited from all sorts of places, even institutions I'd never heard of before. I found I had more opportunities than barriers. **Later I worked at Amoco Chemicals for a number of years and was promoted to be one of the first two female research supervisors.** After my second child was born, my job required me to work in Belgium for 18 weeks out of the year. It was difficult being away from my family for that amount of time, so I decided to quit. It was a difficult decision, but I felt it was the right one for me and my family. I looked for a job a few months and found something that struck a healthy balance between my work and home life, doing materials recycling for the U.S. Department of Energy.

Today as a senior researcher, I help guide and encourage postdocs and early career researchers by introducing them to others in my network. I'm also involved with the Society of Women Engineers. I run a booth at a local college during their Engineering Week event, encouraging young women and men to pursue careers in science. **I always recommend internships to students**. It's essential to get hands-on experience. It helps students figure out which career direction they may prefer and will also make them more attractive to potential employers.

HOW THINGS BREAK

AND WHY SCIENTISTS WANT TO KNOW





Breaking things can help scientists answer both the most elemental and the most everyday questions.

Humans spend a lot of time creating things—this drives a huge amount of our lives, economically and personally—and we are always in a fight to keep them from breaking down. Houses, roads, cars. Power lines and bridges. Solar cells and computers. Batteries. People.

Then there are the things we want to break down, and are always searching for better ways to do it: Harmful pollutants in the soil. Old buildings. The cellulose in plant fibers, so we can make it into biofuels. Atoms, so we can harness the energy they release as nuclear energy, and find out what makes up the universe.

Much of our lives revolve around either of these categories, and they constantly occupy the minds of scientists and engineers. An entire lab at Argonne is devoted to finding out what goes wrong when batteries stop working. No fewer than five accelerators designed to smash tiny things into one another are running at any given time on the campus.

You break things when you want to know what they're made of, and this is useful for answering both the most fundamental questions—like what the universe is made out of—and the most everyday questions, like why your cell phone battery dies after just a few hours.

To fix a performance problem, researchers want to know what exactly is happening when a device—the battery, a solar cell, an engine—doesn't do what it's supposed to do anymore. If you want to fix the problem, you need to know how it happens.

But finding out what's happening at the molecular level is surprisingly, or maybe unsurprisingly, difficult to do. You can't see atoms except in a very small cross-section, in a very thin sample, with very expensive and bulky instruments (an electron microscope, in case you're wondering.) And real life is a lot messier than that. Lithium-ion batteries, for example, the kind in your cell phone and laptop and possibly your car, are made up of layers and layers of complex molecular machinery with both liquids and solids.

Much of science, in fact, is devoted to finding clever ways to intuit what atoms are doing based on clues they leave behind—the effects they have on things around them. Besides electron microscopes, there are many different types of instruments, each with its own strengths.

One of the most powerful instruments in the world for exploring tiny things is called the Advanced Photon Source, a Department of Energy user facility at Argonne. It's an X-ray synchrotron, so big around a baseball stadium could sit inside its circular ring. Researchers aim extremely powerful X-ray beams at a sample of what they're studying. Once a beam hits the sample and scatters, scientists can piece together information about the sample's molecular and atomic structure.

Another very powerful way to simulate how things might unfold in the real world is to build a computer program to model how it happens. This is very useful in industry, where companies can simulate a hundred different possible versions of their product to narrow it down to a handful of the very best prototypes to actually build in the lab. Supercomputers and scientists like those at the Argonne Leadership Computing Facility can build and run these models.

On any given day at Argonne, scientists and engineers are breaking and building things all around the laboratory using dozens of different methods. We'll follow along as scientists break three things: a **battery**, an **atom**, and a **nuclear reactor**.

BATTERIES

Deep in the Argonne battery-testing facility, rows of humming black towers hold five battery prototypes each. They are charging and draining the batteries over and over to find out how long each lasts before breaking down. Nearby, other machines are cooling and heating batteries to find out how temperature affects their performance.

Established in 1976, the computer-controlled lab has been running 24 hours a day ever since, testing prototype and production batteries from both private and government-funded initiatives. Over 100 batteries can be tested simultaneously in the lab—useful because a thorough testing can take from two months to two years.

"For example, we answer questions such as 'What will happen to my battery if I fly out and leave my car in the airport parking lot for a week in January?'" said manager Ira Bloom, who runs the facility. "Or conversely, July?"

When the batteries have completed their rounds, they go back to developers along with the results of each test. By seeing how the batteries failed—or succeeded—the developers can change the battery's design to improve performance and life.

But if you want to design an entirely new battery from scratch—as scientists are doing elsewhere at Argonne—you have to start further back.

There are hundreds of potential chemistries for the three main parts that make up a lithium battery. These are the two electrodes, the positive cathode and negative anode, and the medium that lets ions swim back and forth between them, the electrolyte.

When scientists have an arrangement that looks promising, they cycle the battery at high temperatures to mimic what happens during years of use, said Lynn Trahey, a materials scientist with the Joint Center for Energy Storage Research, a U.S. Department of Energy Innovation Hub led by Argonne.

"High temperatures accelerate the unwanted side reactions that eventually reduce the battery's performance," she said. "The electrolyte starts to break down, and you start to see changes along the surfaces where it meets the electrodes."

All the while, they're measuring how long the battery still holds a charge, how much power it can put out. Then, when the cell finally dies, they open it up to do a post-mortem.

TO FIX A PERFORMANCE PROBLEM, RESEARCHERS WANT TO KNOW WHAT IS HAPPENING AT THE MOLECULAR LEVEL WHEN A DEVICE—THE BATTERY, A SOLAR CELL, AN ENGINE—DOESN'T DO WHAT IT'S SUPPOSED TO DO ANYMORE.

“WHEN WE SMASH PARTICLES, WE’RE TRYING TO FIND OUT WHAT IS OUT THERE.” — MARCEL DEMARTEAU, HIGH ENERGY PHYSICS DIRECTOR

Researcher John Basco prepares for battery testing at Argonne’s Electrochemical Analysis and Diagnostics Laboratory. With the lab’s state-of-the-art, custom-built equipment, simulations are performed to provide information on battery characteristics such as life cycle and calendar life.

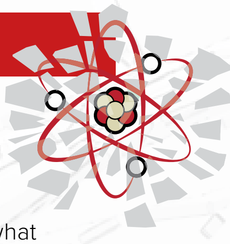
“All the side reactions change the physical landscape inside a cell,” Trahey said. “For example, some of the lithium might have formed dendrites that act like microscopic metal spikes inside of your battery, poking holes through the electrolyte and separator and letting the electrodes touch each other, which short-circuits the battery.”

Researchers can do all this in a special facility at Argonne called the Battery Post-Test Facility, one of the few facilities in the world capable of this kind of research. Inside a giant glovebox filled with inert gas, they can dismantle the battery, analyze it, and take images with an electron microscope to see that physical landscape.

These and other facilities at Argonne help scientists understand how different chemistries work together on the atomic and molecular level.

This background helps scientists design safer, better, and cheaper batteries, which could make your cell phone stay charged longer—and also improve the driving range of electric cars, help our power grid keep electricity flowing smoothly, and make wind and solar easier to use by storing the electricity they generate.

ATOMS



Atoms don’t break very easily (thank goodness, since they’re what you and everything you love is made of). So to break them, and therefore find out what they’re made of and what holds the universe together, you have to build an accelerator.

Accelerators take beams of particles and shoot them at nearly the speed of light until they smash—either into a target, or into one another. “Then you see what comes out,” said Marcel Demarteau, who leads Argonne’s high-energy physics division.

At the heart of any atom is the nucleus. There’s a lot about nuclei we still don’t know; locked inside are the keys to understanding the forces at play in the cosmos and the story of how all of the elements were formed in stars and scattered across the universe.

At the Argonne Tandem Linac Accelerator System (ATLAS), scientists shoot beams of heavy nuclei at different targets. “By calibrating the energy at which the nuclei collide, we can fuse the nuclei, break them apart, or have them rotate together, picking up pieces of the target,” said Robert Janssens, director of the physics division at Argonne. Each interaction creates data that illuminate different pieces of the interactions that govern matter.

If you want to go smaller, into the parts that make up the parts of the atom, you are delving into a realm of physics called high-energy physics—and you need an extremely powerful accelerator, like the Large Hadron Collider in Switzerland.

In high-energy physics, scientists put two different types of particles into accelerators: protons (or anti-protons, their antimatter counterparts) and electrons (or their antimatter counterpart, the positron).

Protons are made up of several sub-particles. “The way it’s often explained is that smashing protons is like throwing two garbage cans at each other. A whole bunch of stuff comes out,” Demarteau said. These are quarks and the things that hold quarks together, called gluons.

LOCKED INSIDE ATOMS ARE THE KEYS TO UNDERSTANDING THE FORCES AT PLAY IN THE COSMOS AND THE STORY OF HOW ALL OF THE ELEMENTS WERE FORMED IN STARS AND SCATTERED ACROSS THE UNIVERSE.

The Large Hadron Collider in Europe helps scientists explore the laws of the universe by smashing particles. Above: Argonne helped design, prototype, and build a key piece called the ATLAS Tile Calorimeter.

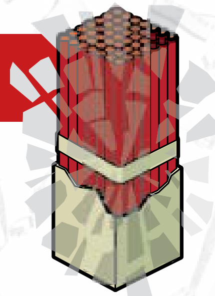
But an electron is a "fundamental" particle, which means it has no substructure. So when electrons and positrons collide, the collisions are much cleaner; the particles annihilate in a flash of light and then rematerialize as entirely different particles.

"When we smash particles, we're trying to find out what is out there," Demarteau said. "What are the fundamental constituents of matter made out of? Are there forms of matter we don't know about?"

And there are a lot of things we don't know. A partial list of physics' current greatest mysteries: Some huge amount of "dark matter" out in the galaxy is causing light to bend oddly around galaxies, but we can't see it directly and don't know where it came from. As you read this trillions of particles called neutrinos are zipping through your body, but they're so difficult to catch or detect that we know there are different kinds, but not how much mass they have or which is the heaviest. And there's a lot more matter than anti-matter out there, which doesn't make sense according to the models we have.

The answers to all of these questions are locked inside particles, waiting to be broken open and teased apart in accelerators.

NUCLEAR REACTORS



While scientists were figuring out how to break an atom, they also discovered that breaking atoms can release energy. A lot of energy; one piece of uranium the size of a tennis ball could generate all the electricity you'll use over the course of a lifetime.

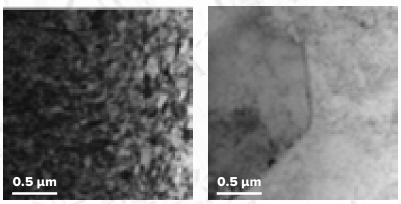
When you split the nucleus of a heavy, unstable atom like uranium, it gives off a burst of energy, some of which is in the form of heat. Nuclear reactors capture this heat to boil water into steam. From then on it's the same as a coal or natural gas plant; the steam turns a turbine that makes electricity.

Inside the heart of a reactor, the pressure, heat, and radiation are intense. Engineers designing the plant to withstand these conditions want to know exactly how the concrete, steel, and fuel rods react over the course of their lifetimes, which are typically several decades.

"Being inside a nuclear reactor changes the microstructure of a material," said Argonne materials scientist Walid Mohamed. The microstructure is what the material looks like if you zoom in very close; it might have long thin rods, or a strict ordered lattice, or big interlocking puzzle pieces.

These different arrangements give the materials very different properties—some bend easily, others are stronger, others conduct heat or electricity well. But being subjected to the harsh environment eventually changes the microstructure, and hence the properties. This is what engineers designing and maintaining reactors want to know.

“For example, nuclear fuels materials will swell and expand when irradiated, but we want to know where and how it will swell,” Mohamed said. Does it crack or form tiny bubbles (called voids)? How big? How quickly? Where?



Microstructures affect a material’s properties. For example, nanocrystalline copper (left) displays much higher strength compared to its conventional counterpart (right).

“Because there’s steam inside a reactor, the materials will also be oxidizing,” Mohamed said. The surface of the metal will react with the steam to form a layer of oxide on top; engineers want to know exactly how thick that will be and how long it will take to form.

To find out, Mohamed and other researchers are using high-brightness, high-energy X-rays from the Advanced Photon Source to peer inside the metals. The APS allows them to gather microstructural data even as they are twisting, pulling, heating, and pressurizing the materials to form cracks and defects.

To simulate the effects of radiation—which tends to make things more brittle—they use ATLAS to shoot xenon ions at the test nuclear fuel material, then take it to the APS.

After you find out how the material performed, then you can modify it to make it do better. “For example, adding nanostructures to a material can make it stronger and resistant to damage, said Argonne nuclear engineer Meimei Li. “Radiation creates defects, but nanostructures increase the amount of surfaces inside a material. This lets it absorb defects, which improves its radiation resistance.”

“The fact that we can gather X-ray data in real time while these materials deform is extremely important,” said Jonathan Almer, an Argonne physicist who works with Li at the APS. “It gives scientists and engineers who used to have as little as one data point—i.e., how long it takes before this material breaks—now up to millions of them.”

They can take all their data to the Argonne Leadership Computing Facility, where they work with computational scientists to produce maps of the evolving materials with unprecedented detail. The data can then be compared to complex simulations of reactors also performed at the computing facility. Together, these studies can help existing reactors safely extend their lifetimes, Li said, or model new, advanced reactor designs that are more efficient, create less waste, and operate more safely.

Research described in this story is conducted at the Advanced Photon Source, a U.S. Department of Energy Office of Science User Facility, at beamlines 1-ID and 32-ID, and is supported by the DOE Office of Science. The Battery Test Facility and Post-Test Facility are supported by the Vehicle Technologies Office at the DOE Office of Energy Efficiency & Renewable Energy. JCESR is a DOE Energy Innovation Hub funded by the Office of Science. Additional research takes place at the Argonne Tandem Linac Accelerator System and the Argonne Leadership Computing Facility, both DOE Office of Science User Facilities. Argonne and other national labs’ work at the Large Hadron Collider, including parts of the detector built at Argonne, is supported by the Office of Science and the National Science Foundation.

ON ANY GIVEN DAY AT ARGONNE, SCIENTISTS AND ENGINEERS ARE BREAKING AND BUILDING THINGS ALL AROUND THE LABORATORY USING DOZENS OF DIFFERENT METHODS.

BY LOUISE LERNER

WEATHER OR NOT WE'RE READY

Are America's cities prepared for the drought, heat, and floods of climate change?

From September 2012 until March 2013, Australia sweltered. And burned.

The worst heat wave recorded in the continent's history sent temperatures soaring well over 100°F for weeks. Fires spread along the coasts and across Tasmania. In the Outback, roads melted.

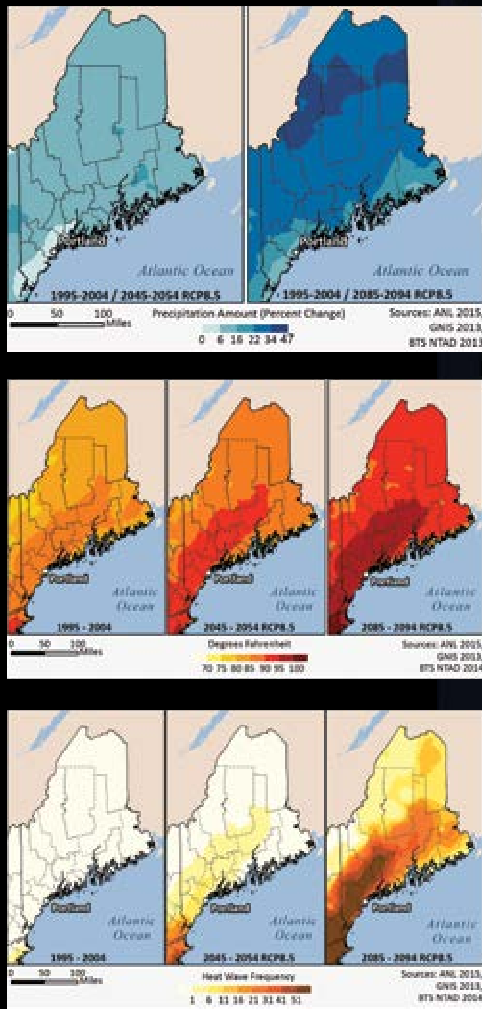
News reports called it the "angry summer." It was so bad that it literally changed the map: meteorologists had to add two new color bands to their maps on the evening weather reports, to go up to 130°.

So Australians turned on the air conditioning. The electric grid suffered in both Melbourne and Sydney. Urban railways were delayed as heat damaged the wiring. A report later that year found the heat wave was almost certainly beyond the bounds of natural climate variation.

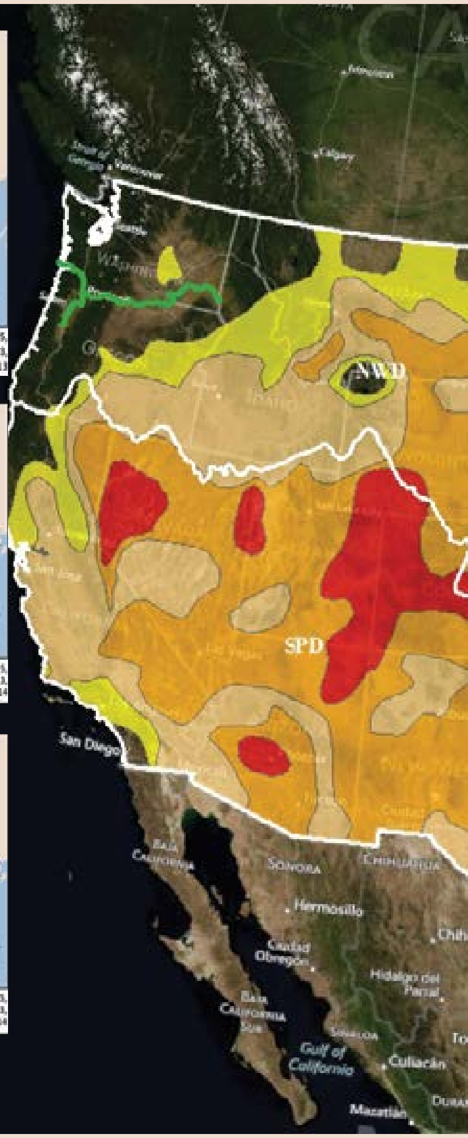
Scientists agree that the future will bring higher temperatures for longer periods of time, higher sea levels, and both more droughts and more storms. "This means that our infrastructure, as it exists today, isn't going to be able to operate at the same level in the future," said Megan Clifford, deputy director of the Risk and Infrastructure Science Center at Argonne.

Infrastructure is, by design, largely unnoticed until it breaks and service fails. It's the water supply, the gas lines, bridges and dams, phone lines and cell towers, roads and culverts, train lines and railways, and the electric grid; all of the complex systems that keep our society and economy running.

IF WE DON'T ADAPT THE SYSTEMS, THEY WILL BREAK.



Argonne teams generated maps to show how Maine's climate would change under a high emissions scenario.



Engineers typically design systems to withstand reasonable worst-case conditions based on historical records; for example, an engineer builds a bridge strong enough to withstand floods based on historical rainfall and flooding. But what happens when the worst case is no longer bad enough?

"If we don't adapt the systems, they will break," said Duane Verner, an urban planner who works with Clifford.

"When you look at cities' long-term plans, which every city has—and they go out decades for planning major infrastructure—they rarely have local climate projections available for their planning assumptions or design criteria," Clifford said.

A major difficulty, she explained, is that it's difficult for city planners to look at a large-scale climate model and understand the impacts to their local area.

That's where Argonne scientists and researchers are bridging the gap. Argonne's infrastructure experts are just a building over from climate scientists in the environmental science division and supercomputing resources at the Argonne Leadership Computing Facility. They can develop and interpret the complex global climate models to predict the effects of climate change by region.

The Risk and Infrastructure Science Center can pull all of these forces together with other subject matter experts, including engineers and analysts with experience in various infrastructure industries. Combining these resources helps them develop practical and comprehensive analyses for planners. These tools not only help city planners analyze risks, but also prioritize them in light of tight budgets.

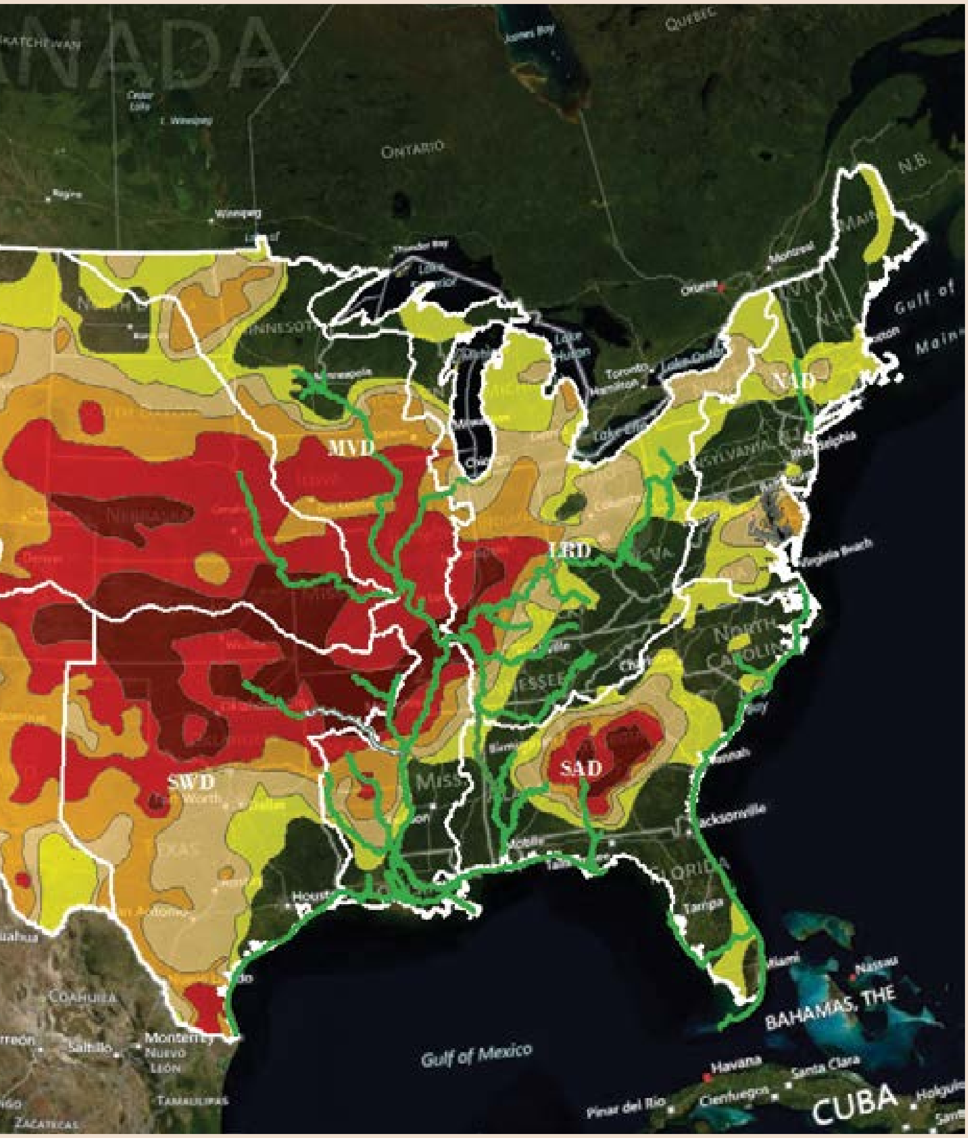
One type of analysis that Argonne frequently conducts is called an RRAP—the Regional Resiliency Assessment Program. Every year, the U.S. Department of Homeland Security funds several assessments that each look at a particular area's vulnerabilities.

Verner is part of a team working on an RRAP for the Casco Bay region of Maine. Like other regions they've studied, they are finding that floods, heat waves, and other changes predicted for Maine could cause trouble for its infrastructure.

For example, in general, power plants don't like heat—their output declines, some types more than others. The same is true for transmission lines; they lose some ability to carry electricity in the heat.

"This change is in the margins, but when you add that together with increased demand for power to run air conditioning, for example, you can cross the thresholds for brownouts," Verner said.

Then there's rain. "The climate models are showing that increases in extreme precipitation events are projected for the entire U.S., because there's more humidity in the atmosphere," Verner said, "and structures like culverts, that are built to standards for past historical rainfall events, won't be able to accommodate this rush of rain." (Culverts are pipes that channel streams and water underneath roads.)



Record drought in 2012 sent the U.S. Army Corps of Engineers scrambling to keep the Mississippi, Ohio, and Missouri Rivers open for shipping. Image by the Army Corps of Engineers.

HEAT

Heat stresses bridge joints, buckles pavement and train tracks, damages wiring, and slows down power plants at the same time as electricity demand ramps up.

RAIN

Heavy rains flood roads and homes, overwhelm sewage systems, and wash out the soil that supports tunnels, roads, and bridges.

DROUGHT

Disruption to normal rain cycles drains aquifers and reservoirs and lowers river and lake levels, which hurts crops, farmers, and agriculture and interrupts shipping lanes.

SEA LEVEL

Rising seas could submerge thousands of miles of roads, not to mention homes, businesses, roads, airports, power plants, and train lines, just as a taste.

A WORST-CASE SCENARIO MISSISSIPPI RIVER DROUGHT COULD PUT THOUSANDS OF JOBS AND BILLIONS IN INCOME AT RISK ACROSS SIX STATES.

Engineers typically design systems to withstand reasonable worst-case conditions based on historical records. For example, an engineer builds a bridge strong enough to withstand floods based on historical rainfall and flooding. But what happens when the worst case is no longer bad enough?

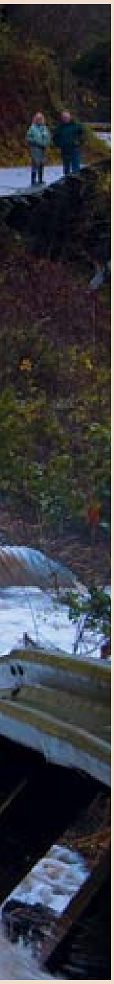
Too much rain all at once causes floods, and floods are devastating to infrastructure. Water is extraordinarily destructive. Hurricane Sandy shut down New York City, one of the largest, most prosperous cities in the world, for days. Floods wash out roads and bridges, damage homes, schools, and buildings, and overwhelm sewer systems, causing sewage dumps into local waterways; the economic impact can be severe. Sandy caused $65 billion worth of damage.

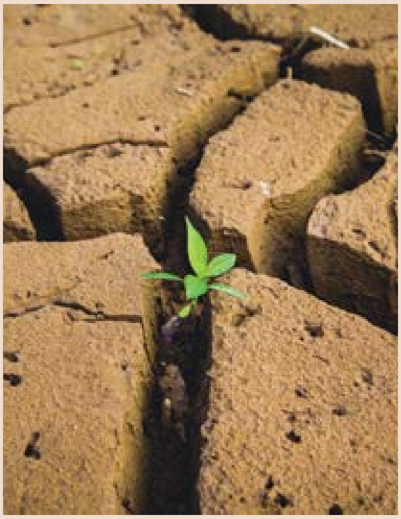
At the same time, we've also seen record droughts in recent years. "Generally, planners are using historical records for droughts in their water resource planning processes, and our climate models show that, in many cases, historical records won't provide an adequate worst-case scenario to plan for," Verner said. "It will be much worse."

"WHEN YOU LOOK AT CITIES' LONG-TERM PLANS, THEY RARELY HAVE LOCAL CLIMATE PROJECTIONS AVAILABLE FOR THEIR PLANNING ASSUMPTIONS OR DESIGN CRITERIA."
— MEGAN CLIFFORD, RISC DEPUTY DIRECTOR

Droughts are financially ruinous for farmers and agriculture; that same year as Sandy, 2012, saw a Midwest/Plains drought that cost $35 billion. That drought saw the mighty Mississippi River drop to such low levels that shipping on the river, which normally carries billions of dollars of cargo every month, was nearly halted. "I have never seen anything like it," Colonel Chris Hall, commander of the Corps of Engineers' St. Louis District, told the *Chicago Tribune*.

In response, Argonne researchers scrambled to analyze the potential economic impacts if water levels dipped below a certain point on the middle Mississippi River. Billions of dollars of cargo are shipped on the river every month; power plants pull cooling water; and local communities draw water, including drinking and irrigation water. The analysis quantified the thousands of jobs





U.S. Department of Homeland Security, Office of Cyber and Infrastructure Analysis, May 2015

24%
OF U.S. BRIDGES ARE STRUCTURALLY DEFICIENT OR OBSOLETE

54%
OF NAVIGATION LOCKS ARE MORE THAN 50 YEARS OLD

70%
OF NATURAL GAS PIPELINES ARE MORE THAN 30 YEARS OLD

and billions in income that could be in jeopardy across six states for a worst-case scenario drought.

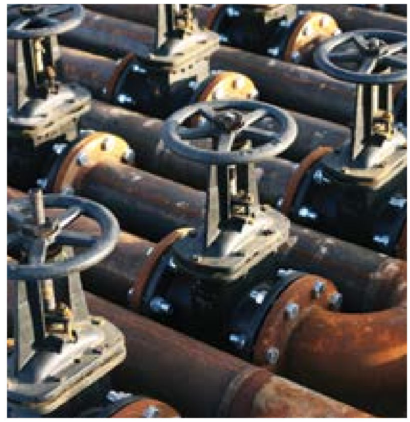
These kinds of analyses help federal, state, and local governments understand stakes and prioritize action. With the help of the Risk and Infrastructure Science Center, as well as resiliency efforts in multiple areas at Argonne, planners can find out the types of stresses their cities and regions will face in the future.

Infrastructure is generally an ounce-of-prevention game; smart changes now can save a region billions of dollars in damages and lost economic productivity in the future. Communities can ration water from aquifers, shore up electric grids, and build roads out of water's reach. New estimates of rainfall help engineers determine what kind of storms their bridges should withstand; power companies can estimate energy demand in upcoming heat waves. They just need to know what they're facing.

"Our goal is to help planners get the information they need to do their jobs, and to drive national efforts for future resilient infrastructure design," Clifford said.

With the ongoing involvement of Argonne and the scientific community, infrastructure can be adapted and designed to withstand the changes ahead—before it breaks.

Funding for the Risk and Infrastructure Science Center comes primarily from the U.S. Department of Energy, the U.S. Department of Homeland Security, and the U.S. Department of Defense.



RESILIENT INFRASTRUCTURE INITIATIVE AT ARGONNE

Climate change is only one risk facing our nation's infrastructure; infrastructure also faces natural and man-made disasters, growing and shifting populations, and deterioration from age. Our nation's infrastructure must be designed and built differently to adapt to these risks. Argonne's Resilient Infrastructure Initiative aims to do just that—advance the science and technology needed to revolutionize the design of future infrastructure systems. Combining multi-disciplinary resources within and outside of the lab, Argonne applies advanced modeling and assessment capabilities to uncover infrastructure vulnerabilities and the cascading impacts among infrastructure systems. This leads to the next generation of resilient infrastructure materials, techniques, and design. For more than 25 years, the U.S government, international entities, and private sector organizations have sought Argonne to address the resiliency of complex infrastructure and systems.
For more information, visit www.anl.gov/egs

THE COMPLEX CHEMISTRY OF COMBUSTION

Your car is powered by a series of tiny explosions. Scientists think they could make them cleaner and more efficient.

BY JO NAPOLITANO

A BILLIONTH OF A SECOND.

That's how quickly some of the most critical chemical reactions of combustion occur.

Argonne chemist Stephen Pratt leads the Gas-Phase Chemical Dynamics Group at Argonne. His team, which includes a dozen Ph.D. scientists, several postdocs, and numerous visiting students and researchers, is trying to gather as much information as they can about something that lasts only an instant.

Their focus: understanding the chemistry of combustion.

Combustion chemistry in the cylinder of an engine takes place in the gas phase. Individual reactions can be considered at the molecular level.

"If you think about combustion in an engine with fuel, it seems like a simple process but it is actually very complex," Pratt said.

This is true of even the simplest process, one in which hydrogen and oxygen combust, he said.

The reaction of oxygen (O_2) with two hydrogen (H_2) molecules results in the production of two water molecules (H_2O). But when they combust in real life, dozens of other things occur.

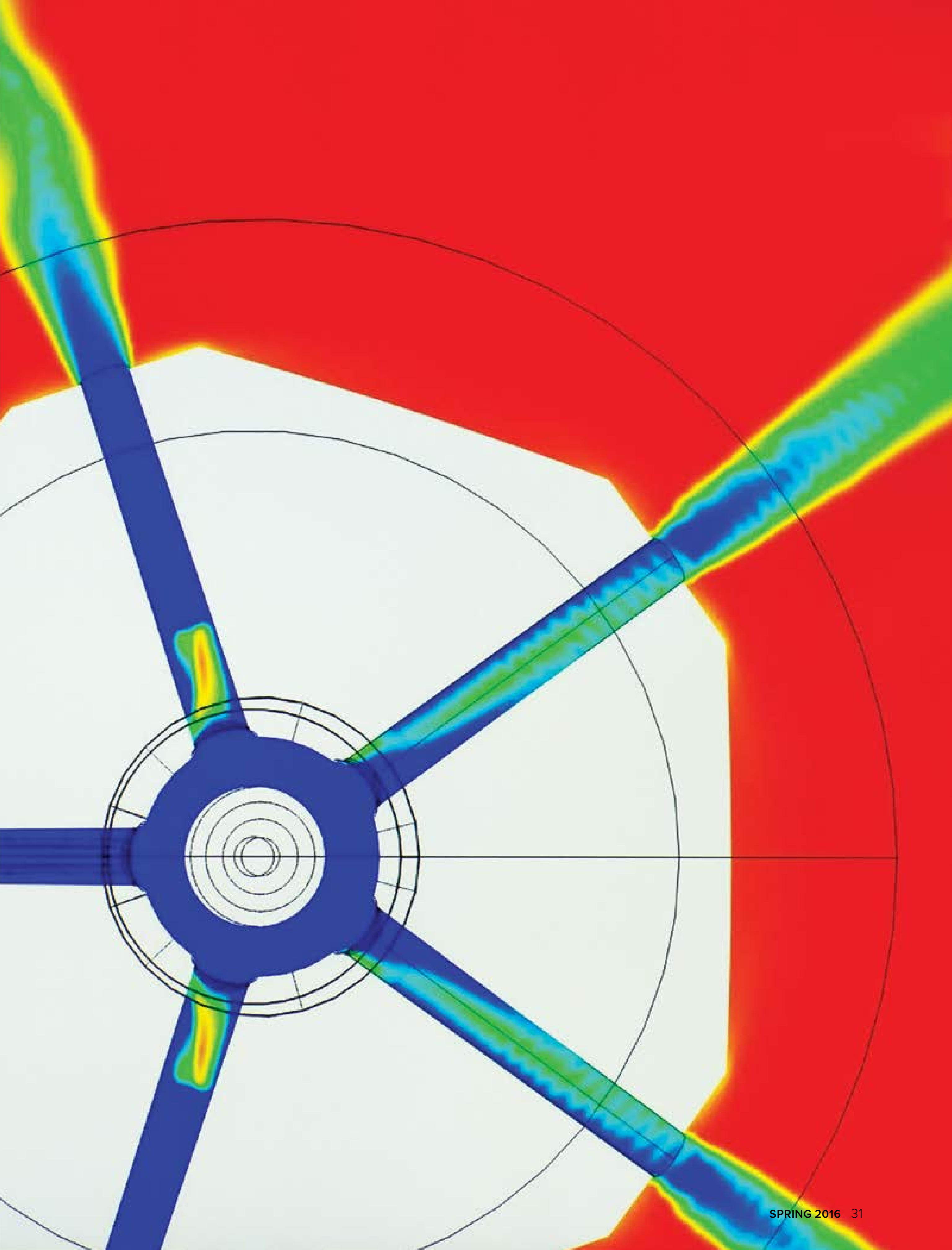
For an accurate description of this process, 25-30 different reactions must be considered, even though only two chemical elements are involved.

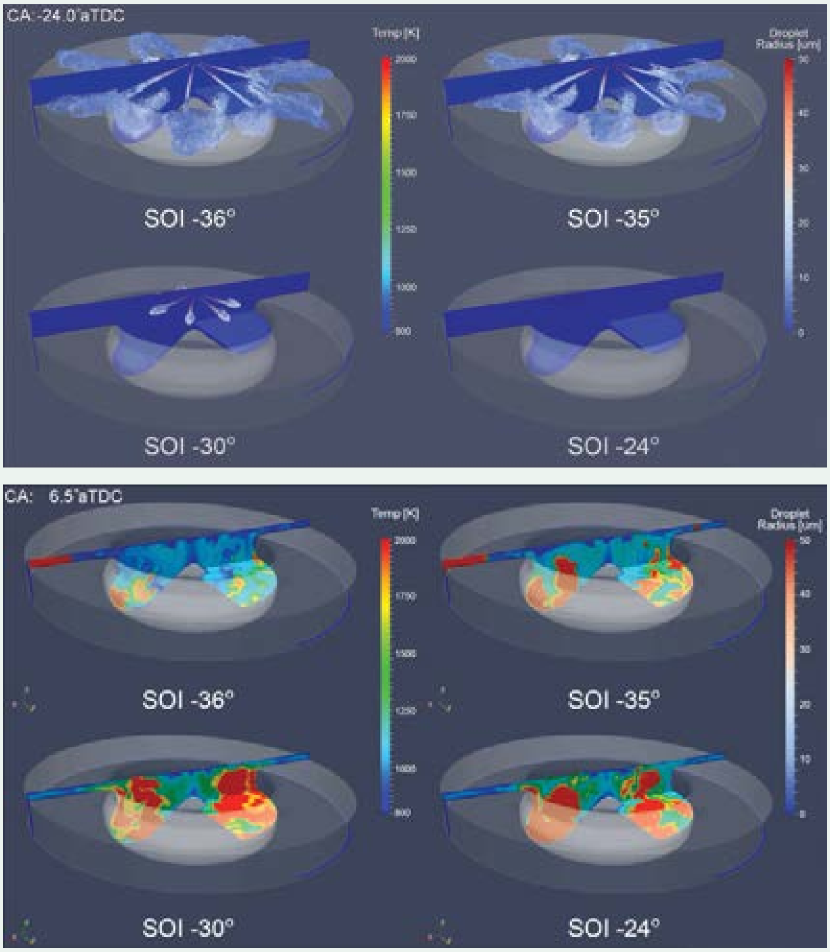
COMPLEXITY, BY THE GALLON

Current fuels, such as those that power our cars, provide an even greater challenge.

The gasoline we use each day on our way to work is actually a mixture of more than 1,000 different chemicals. When it burns, the number of chemical species and reactions multiply dramatically.

"If you try to model something like that, you have to consider the rates of all the reactions and how those rates depend on temperature and pressure, among other factors," Pratt said. "A tremendous amount of information needs to be built into these models to make them sufficiently accurate for quantitative predictions.





Argonne researchers are studying gasoline compression ignition as a way to combine the efficiency of diesel with the cleanliness of gasoline engines. Simulations at the Argonne Leadership Computing Facility model the combustion, above. Images courtesy Ray Bair & Sibendu Som.

"Some of the important reactions involve very reactive fragments of these fuel molecules that live for a very short time," Pratt said. "They are incredibly difficult to study experimentally."

If accurate reaction rates and energetics could be determined by theoretical calculations—rather than through experimentation—it could provide a solution to this problem.

Thom Dunning, now at the University of Washington, initiated Argonne's combustion chemistry effort in the late 1970s. His vision was that theoretical chemistry would one day be good enough to calculate all of the necessary information, allowing the construction of predictive combustion chemistry models from first principles.

"Forty years ago, that seemed far-fetched," Pratt said. "Today, we are closer than ever to making it happen."

Since the beginning of this effort, Pratt said, Argonne has pulled together a balance of experimentalists and theoreticians to study reaction dynamics and rates.

"The constant interplay between these researchers has been invaluable for understanding the chemistry and improving the theoretical methods," Pratt said.

Their research is broad in scope. While some focus on chemical energetics, others study the dynamics and rates of the reactions, as well as the rates of related processes like energy transfer between colliding hot molecules.

Once the individual reactions are characterized, they are assembled into larger chemical models for selected fuels.

Techniques are also being developed to improve the predictivity of these models through improvements of selected rate data.

PREDICTIVE SCIENCE

After decades of research, theory alone can now reproduce experimental results for many classes of reactions, and can also make accurate predictions for some reactions that are not easily amenable to experimentation.

While considerable challenges remain, Pratt said, the goal of predictive chemistry models is almost within reach.

"We are beginning to see a light at the end of the tunnel," Pratt said. "It's really exciting."

THE GASOLINE WE USE EACH DAY ON OUR WAY TO WORK IS ACTUALLY A MIXTURE OF MORE THAN 1,000 DIFFERENT CHEMICALS.

Ultimately, this capability will not only aid the development of improved engines and fuels, but also speed the introduction of alternative renewable fuels into the commercial market.

Argonne's efforts in this area are widely recognized. Three of its scientists—Argonne Distinguished Fellows Lawrence B. Harding and Albert F. Wagner and senior chemist Joe V. Michael—were recently feted by the *Journal of Physical Chemistry A* with a special issue in honor of their 100 years of combined work in combustion kinetics.

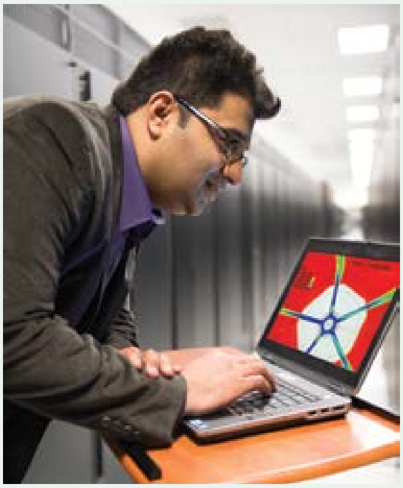
"The three of them are terrific scientists," said Pratt. "This is one of the top journals in our field, and this special issue highlighted the importance of Larry, Al, and Joe's contributions to combustion chemistry."

"IN ORDER TO BURN GASOLINE MORE EFFICIENTLY, WE HAVE TO ANSWER QUESTIONS LIKE 'WHEN SHOULD THE FUELS BE INJECTED? AND AT WHAT ANGLE?' IF IT IS NOT INJECTED AT THE CORRECT ANGLE, IT WILL NOT BURN PROPERLY."
– ARGONNE MECHANICAL ENGINEER SIBENDU SOM

SIMULATIONS

Sibendu Som, a mechanical engineer at Argonne, develops predictive tools to simulate the processes taking place inside internal combustion engines.

"Engines are very forgiving," said Som, who joined the laboratory in 2009. "Burning is not the challenge. You can put in any fuel and it can



Engineer Sibendu Som of Argonne's Virtual Engine Research Institute and Fuels Initiative reviews a five-hole injector diesel engine visualization conducted at the Argonne Leadership Computing Facility.

burn. It's the efficiency of combustion that is the challenge. How do we get better mileage out of our vehicles? And how do we do it cleaner than it's been done before?"

As the principal investigator on the simulation program, Som uses computing clusters and the lab's supercomputer to test theories about combustion that would make the process far more efficient.

"In the past, engine simulations used only very simple models, which were not predictive," he said. "What we are trying to do is use complex models that capture more of the physics in terms of fuel spray and combustion. By using the clusters and the supercomputer, we can run tests and simulations with a 24-48 hour turnaround, which would be impossible otherwise. And this technology allows us to reduce the uncertainties in the simulation so the outcome is far more precise. We can do things now we could not do five years back."

As part of that effort, Argonne has entered a cooperative research and development agreement with a leading company that designs, manufactures, distributes, and services diesel and natural gas engines as well as another company that is a leader in computational fluid dynamics software.

Som's work allows him to test for ignition delay, heat release rate, and emissions, among other essential components of combustion.

"My team is responsible to help and optimize gasoline combustion," he said. "In order to do that, we have to answer several questions, like 'When should the fuels be injected? And at what angle?' If it is not injected at the correct angle, it will not burn properly."

MOLECULE BY MOLECULE

Douglas Longman, a section manager in Engine Combustion Research at Argonne, has been with the laboratory for 17 years. His team is responsible for a broad range of experimental and computer simulation work, including fundamental combustion research—where scientists use a rapid compression machine to mimic the same type of conditions found in an engine, but in a far more controlled fashion—to the study of the basic chemistry behind each explosion.

The mystery, Longman said, lies at least in part with the gasoline itself. The octane rating of 87 or 91 that we see at the service station doesn't tell scientists enough about how the fuel will perform, so they rely on something called a rapid compression machine to fill in the blanks.

"Gasoline is composed of hundreds of different components, and each has its own unique combustion properties," Longman said. "The rapid compression machine shows us the interaction of different types of molecules. The real fuels are then compared to our simplified mixtures to understand their characteristics."

Beyond that, scientists at Argonne also study exhaust emissions and the performance and ignition of different engine configurations.

"We can do imaging inside the combustion chamber, which helps us get a better experimental data set that we can compare to the simulations that other scientists, like Sibendu Som, do on the computers," Longman said. "The imaging allows us to account for temperature, the distribution of fuel and air mixture, whether it is well mixed or has pockets of too much or too little fuel."

DIESEL ENGINE, GASOLINE FUEL

One of the key projects in this area is a new engine combustion concept: gasoline compression ignition.

"It's kind of a combination of a diesel engine and a gasoline spark ignited engine, which is what most U.S. cars have," Longman said. "Those are two different combustion approaches. They each have their own benefits."

A diesel engine combustion system is very fuel-efficient but creates too much pollution, generating nitrogen oxides and soot. Gasoline engines—which are spark-ignited—are cleaner-burning, but are not as efficient. In terms of miles per gallon, you burn more fuel with gasoline than with diesel, Longman said.

"Basically, the gasoline compression ignition is trying to use the gasoline fuel in a diesel-like combustion process," he said. "We are putting gasoline in a diesel engine and are able to operate it by controlling how the fuel is introduced into the combustion chamber."

And by doing that, scientists are hoping to gain the high efficiency of the diesel process and the low emissions of the gasoline fuel.

"We have been working in this area for four to five years," Longman said. "And we've made a lot of progress. We imagine this could be available to consumers in about 15 years."

STATIONARY NATURAL GAS ENGINES

The lab also is studying stationary natural gas engines, which are the same type of engine found in our cars, though much larger and connected to a generator. They would supply electricity to the power grids.

"We have been working for years on how to make those engines more efficient," Longman said. "There are a couple of ways to do it, but both tend to make it more difficult to ignite the natural gas and air mixture. The spark plugs don't work well under some of these conditions. We are using laser igniters to ignite the fuel and air mixture instead of a spark plug."

The lab also is researching locomotive-sized diesel engines.

"As with almost all of our programs, the focus is on better fuel efficiency at lower emissions levels," he said.

VERIFI-ABILITY

Argonne computational scientist Ray Bair has twice worked for the laboratory. During his first tour, he was in the theoretical chemistry group and focused on combustion research. He currently works in the computing, environment and life sciences directorate, where he serves as the chief computational scientist for applications.

"My background is in computational molecular science, but what I do now draws on more than a decade of interactions with computational science and engineering teams," he said. "I work with research teams across the lab to help develop computing strategies and build partnerships to try and solve some of the key computational challenges in energy research."

With a focus on high-performance computing, he manages the lab's internal supercomputer center, where he works with dozens of scientists in varying fields of research.

He is currently part of a multidisciplinary team helping with the plans for the Virtual Engine Research Institute and Fuels Initiative, or VERIFI, which brings together expertise from all four directorates at Argonne.

"If you look at the common practices of the engine industry in terms of the accuracy of their models and how predictive they are, there is an opportunity to do a lot better with supercomputers," he said. "VERIFI is just one example of how an institution like Argonne can work together with industry to solve these problems."

WHAT IS TO COME

Historically, consumers had a narrow selection of fuels, e.g., gas or diesel.

But looking forward, the worldwide fuel mix is becoming ever more varied. As biofuels are introduced—they come from different sources and burn differently—engines will need to accommodate a wider range of fuel properties.

Having accurate models of engine operations gives us a way to accommodate this diversity in the fuel mix—and improve the safety, efficiency, and cleanliness of the combustion engine.

Research described in this story is supported by the U.S. Department of Energy under the Office of Science's Office of Basic Energy Sciences, including the Division of Chemical Sciences, Geosciences, and Biosciences, and the Office of Advanced Scientific Computing Research, as well as the Office of Energy Efficiency & Renewable Energy's Vehicle Technologies and Advanced Manufacturing offices.

ART OF SCIENCE

Thermal Hydraulic Simulation

by Elia Merzari & Justin Walker

This simulation of a rod bundle, a basic component of a nuclear reactor core, was done at the Argonne Leadership Computing Facility. Researchers are using supercomputers to better understand the physics of turbulence within a nuclear reactor.

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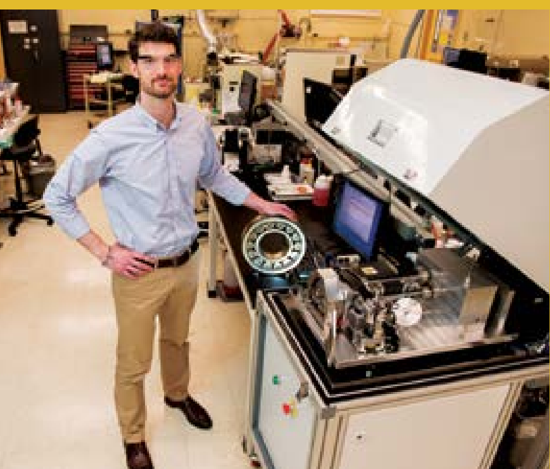
7 THINGS YOU MIGHT NOT KNOW ABOUT TRIBOLOGY

BY JUSTIN H.S. BREAUX

1. TRIBOLOGY STUDIES THE WEAR AND TEAR OF THINGS

Objects rubbing together cause friction, which eventually wears down one or the other surface. Finding ways to reduce this friction—in your knees, in an engine, or in factory machinery—can help scientists develop stronger materials that last longer and slide easier, which increases efficiency.



Argonne engineer Aaron Greco works to improve the reliability of wind turbines using tribology.

2. YOUR CAR WASTES ABOUT 13% OF THE GAS YOU BUY

Gas engines waste about 13% of their fuel overcoming friction created by all the mechanical sliding and rotating parts within the car. Increasing this efficiency by just 10% for cars would mean importing 100,000 fewer barrels of oil every day.

3. IT'S NOT ME, IT'S YOU

When your artificial knee or hip hurts, it's not the gadget, but the body's natural defenses that wear you down. The act of walking, bending, or stretching rubs off molecule-sized pieces of metal or plastic, which the body sees as foreign objects. Irritation results as the body tries to repair itself, causing the joint to loosen or cause pain.

4. WIND TURBINES DO THE WOBBLE

With an average height of 370 feet, wind turbine blades cover a lot of area. Because of this, blades at the top experience faster wind speeds than blades at the bottom, causing a wobble as the blades spin. This back and forth vibration can cause increased wear on the bearing and gears within the wind turbine's gearbox.

5. NO WD-40 ALLOWED IN SPACE

Lubricants like oil used for our machines here on the ground won't work in space. In a vacuum, oil quickly evaporates, increasing the amount of friction on moving parts and causing gears to grind to a halt.

6. AN OIL'S CHEMICAL ADDITIVES, NECESSARILY, PAVE THE WAY

About 15% of the oil we use in cars and other machines consists of a chemical cocktail that helps prevent foam, slow corrosion, prevent oxidation or rust, and allow you to pour oil in sub-zero temperatures.

7. THE FAULT IS THAT THERE IS NO FRICTION IN THE FAULT

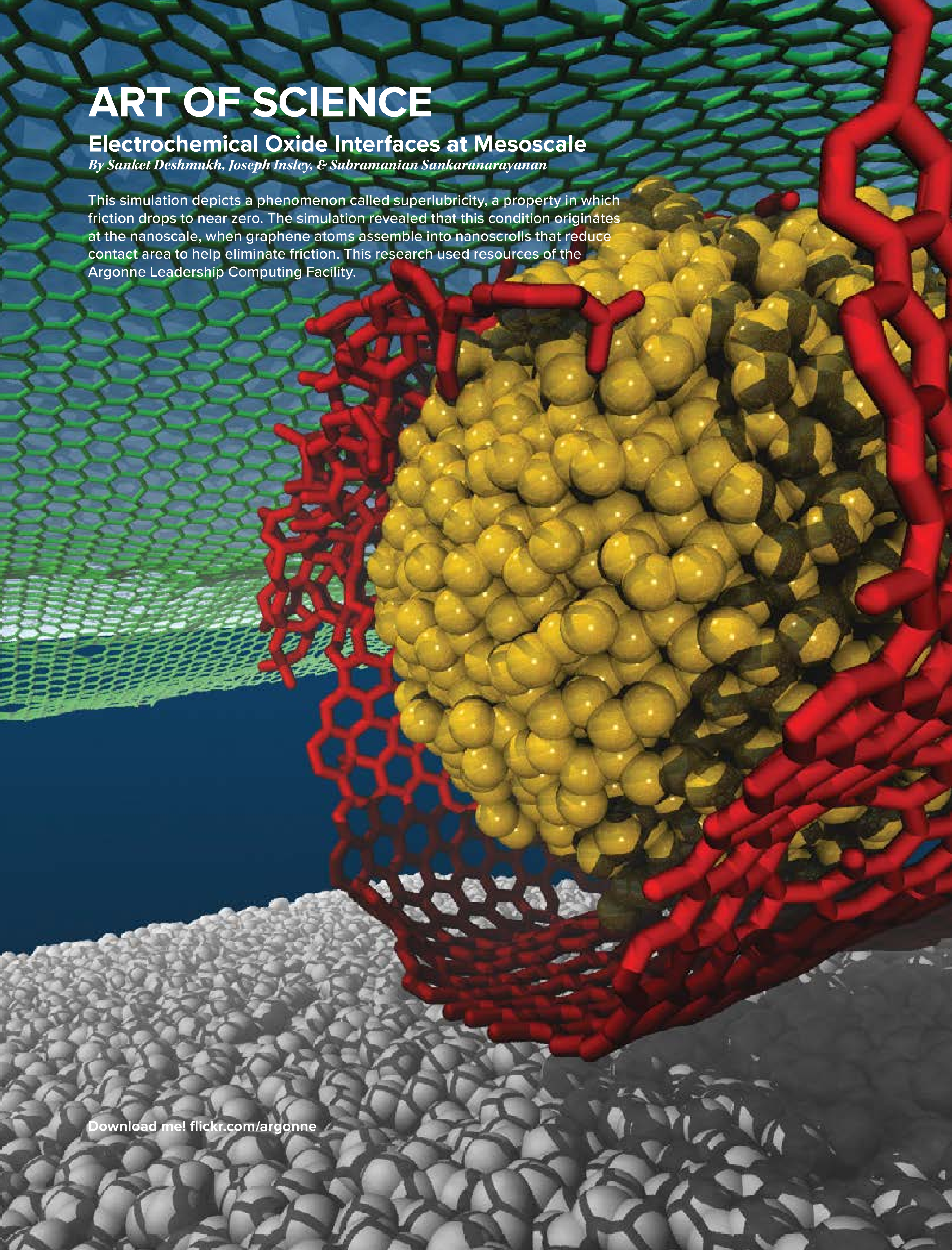
The earth's surface is a 3-D jigsaw puzzle with large sections that move, very slowly, all the time. Sections that stick together at the fault line store up energy as other sections move. When the force of the moving sections overcomes the friction of the sections that are stuck together, they slip, releasing energy like a ripple in a pond. In other words, an earthquake.

ART OF SCIENCE

Electrochemical Oxide Interfaces at Mesoscale

By Sanket Deshmukh, Joseph Insley, & Subramanian Sankaranarayanan

This simulation depicts a phenomenon called superlubricity, a property in which friction drops to near zero. The simulation revealed that this condition originates at the nanoscale, when graphene atoms assemble into nanoscrolls that reduce contact area to help eliminate friction. This research used resources of the Argonne Leadership Computing Facility.



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"HOW DO WE MAKE COMPUTERS FASTER?"

Argonne scientists from different disciplines each provide a perspective on a complex question facing society.

Marc Snir
Director, Mathematics & Computer Science division

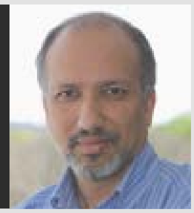
"We have a couple of more generations with current silicon transistor technology where devices continue to shrink. I'd say 8-10 years.

Today's supercomputers are massively parallel; they are so fast because they string many processors together. When you keep adding more processors, the problem becomes software. Can you split your task into 10 million smaller tasks? 100 million? Then power becomes a problem. So does resilience; how do you build a system that keeps functioning if some individual gates are misfiring?

One interesting area is called approximate computing. We're spending a lot of power to reduce the frequency of error. What if you built a system that makes mistakes much more frequently but uses much less energy?

We can also explore specialized computers; we've known for a long time you can build specialized computers that can be faster than general-purpose computers for a particular problem. As silicon gets to its limits and general-purpose computing starts slowing down, perhaps specialized systems get more attractive."

Supratik Guha
Director, Center for Nanoscale Materials

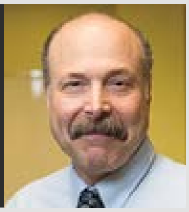


"The basic architecture of the computer hasn't changed in 60, 70 years. But as we go forward, the kinds of computing workloads we need are increasingly different and it's driving a feeling that we need new architectures.

It's not a question of figuring out a new device. I think it has to come from the other way around. It's got to be a new architecture that may demand a new type of device—not the way we do it now, where physicists come up with a new device and then try to figure out how to use it for computing. We need to come up with new architectures to solve problems more efficiently, both in terms of computing time and power, and then find the circuits, devices, processes, and materials in order to build that architecture.

To get there, one of my goals at the Center for Nanoscale Materials is to increase the interaction between physicists, chemists, and materials scientists with computer scientists."

David Awschalom
Deputy Director, Institute for Molecular Engineering

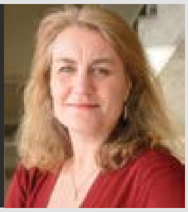


"In the past 15 years we've made enormous strides in using quantum systems to store and manipulate information. In a classical computer, information is encoded in binary (1 or 0). But the quantum state of an atom can exist in an arbitrarily large number of states, and this can be used to store and process information in a fundamentally different way. In a quantum system, a single computational cycle could perform highly complex calculations and could solve certain problems which are difficult for even the fastest supercomputers.

In addition, as the act of measurement can change the state of a quantum system, it could offer inherently secure communication. If anyone tries to eavesdrop, they will end up destroying the message.

Quantum technology is rapidly progressing and may soon have an impact on many parts of society. If you told someone 10 years ago you wanted to control the quantum states of atomic nuclei at room temperature, they would think you were crazy. Now we do that routinely."

Suzanne G.E. te Velthuis
Physicist



"Memory is a serious bottleneck for better, faster computers. One approach we're studying is to base memory on skyrmions, tiny bubbles of magnetism that form in certain materials.

In current hard disk memory drives, the read-and-write head measures changes in magnetism as it goes across a drive. But in an alternative system called "racetrack" memory, you move the data, not the head. That data could be a ribbon of skyrmions, encoding the 1s and 0s. This system could be more efficient and use much less power.

Just recently our team discovered a way to make skyrmions at room temperature that can be controlled with a relatively small current of electricity. The field has made a lot of progress in the last three to five years, but we still need to shrink the skyrmion bubbles, and understand more about their behavior and motion at different scales."

Anand Bhattacharya
Physicist

"I think the greatest challenge of the age may be how to process information in a way that mimics the elegance of the human brain. The brain does incredibly power-efficient computing. It runs on about 20 watts; supercomputers run on many megawatts. It's something like a million times more efficient. Google and these other big companies that use huge computer banks spend a lot of energy cooling them.

And the thing is, the 'clock cycle' is very slow in the brain compared to computers. A neuron can only fire 5 times per second. Transistors can switch billions of times. But computers are very linear; one operation and then another. Human brains are wired very differently. So maybe when we look for the "next transistor," we don't actually need a faster version of silicon, but something with new properties that inspires us to build computers with some entirely different architecture."

WORKING WITH ARGONNE

5 QUESTIONS with the new director of Argonne's technology development and commercialization division, Suresh Sunderrajan.

Suresh Sunderrajan joined Argonne in April 2015, bringing with him a wealth of experience in all aspects of technology commercialization and business growth at large corporations and start-ups. He took a few minutes out of his schedule to sit down with us and talk business development, Argonne's role in spurring U.S. innovation, and regional cuisine.

Q: What was your path prior to joining Argonne?

A: My path to Argonne was, to put it mildly, non-linear. I came to the United States in 1991 to do my Ph.D. in chemical engineering. While working at the Eastman Kodak Company, one of my early projects made it through the stage-gate development process, giving me an opportunity to lead the commercialization effort. This was my first exposure to the multidisciplinary, multifunctional challenge that is product commercialization and I found that this was just incredibly fun.

While at Kodak, I was lucky to be sponsored for a business degree at MIT (Sloan School). I was also offered opportunities working in the Kodak New Business Ventures organization and in the Kodak Venture Capital group. As a corporate venture capitalist, while I enjoyed my job, I couldn't help but feel that the start-up teams that I met with regularly were accomplishing great things, while I was little more than an informed bystander. I took the plunge, and over the next eight years co-founded/ran four different start-ups.

While I didn't set out to either work at a national lab or to focus on technology commercialization, my experiences have actually prepared me very well for my current role.

Q: What is the role of Argonne's technology development and commercialization (TDC) division?

A: Whereas the mission of the Lab is to address vital national challenges in clean energy, environment, technology, and national security, TDC exists to assist the researchers in executing their work and in delivering the solutions they develop to real-world use. We work with large companies, small to medium enterprises, and start-ups, as well as with other organizational entities in this ecosystem, to facilitate the development, transfer, and use of Argonne technology for public benefit.

Q: Given that you are new to Argonne, what do you view as a 'hidden' strength of the lab?

A: The ability to be a one-stop-shop solutions provider for the organizations we work with. For example, if you are a company that has a tough R&D challenge that requires work in materials science, computer modeling, and nanoscience, rather than work with three different partners on the individual pieces, you can call on Argonne to assemble a cross-functional team of people here at the lab to tackle that problem in a coordinated and efficient way, using tools and facilities that are cutting-edge and in some cases truly one-of-a-kind. A good analogy would be if you want to build a house, rather than hiring a plumber, a carpenter, a concrete crew, and so on, all separately, it's more efficient and easier for you to hire a general contractor to assemble the team and ensure everyone is working together. Argonne acts as that general contractor for our partners, making their lives easier and delivering superior results.

To this end, there are two new centers Argonne has just opened—one focused on energy storage and the other on nanotechnology (see sidebar)—that take this idea and build upon it.

Q: What is the rationale behind national laboratories getting involved in this type of activity? Can't the private sector handle this?

A: Large companies are investing less and less in basic scientific research, and basic scientific research is the foundation of commercial products and processes that improve our lives, make us healthier, help us take better care of our environment, etc. Given the highly competitive nature of private industry, companies feel compelled to ensure that they perform well in the near term, because if they don't, there might not be a long term. The national labs are filling a critical hole by taking a longer-term view and bridging the gap between basic research and real-world products and solutions.

Q: Seeing as you are new to the Chicago area, we have to ask: Chicago-style hot dog or deep-dish pizza?

A: I haven't been in town long enough, so I'll need some guidance on this, but my guess would be both?

(Ed. note: That was actually a trick question, and you nailed it: the correct answer is in fact "both." Now, as far as which pizzeria or hot dog stand is the best, you'll have to ask your new neighbors, and you'll likely get five different answers in each category.)

SCIENCE TO SOLUTIONS

Two new centers poised to work with industry

ACCESS

ACCESS helps companies that are developing energy storage technology easily tap into the massive basic and applied science resources of a national lab to perform research and analysis to bring their products to market. Argonne's unique combination of resources offers scalable process research and development: battery technology can be tested at the commercial level and analyzed at the molecular level. With ACCESS, companies have access to the breadth of Argonne's resources in one place.

Argonne's all-encompassing battery program spans the continuum from basic materials research and diagnostics to scale-up processes and ultimate deployment by industry. The lab's multidisciplinary teams are working to develop advanced energy storage technologies to aid the growth of the U.S. battery manufacturing industry, transition the automotive fleet to plug-in hybrid and electric vehicles, and enable greater use of renewable energy.

access.anl.gov

NANO DESIGN WORKS

Nano Design Works is a new center that puts the laboratory's vast resources at the fingertips of the nano industry by allowing American companies, particularly small- and medium-sized businesses, access to Argonne's expertise in fundamental and applied research as well as its world-class facilities. Nano Design Works will help ensure that fundamental nanoscience finds its way to the market and that American small businesses can compete in the global marketplace.

The barrier to nanoscience R&D has always been prohibitively expensive; the complexity of the instrumentation alone prevents widespread entry. Nano Design Works dismantles that barrier by providing access to thought leaders and some of the world's most sophisticated scientific facilities. Nano is also unique in that it spans the scientific spectrum; with expertise in nanomaterials, computing, chemistry, materials, and energy systems, Argonne is a perfect match for companies looking to make a big impact with tiny materials.

nanoworks.anl.gov

SCIENCE IN THE **1000 MOST COMMON WORDS**

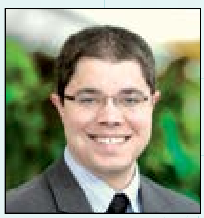
The webcomic XKCD published a diagram of a rocket using only the 1,000 most commonly used words in the English language.

So we asked two of our postdoctoral researchers to try a hand at explaining their research the same way.

JESSICA LINVILLE
Engineer

People throw away a lot of food and other things that makes a lot of stuff that makes the world get warmer. There are tiny life forms that grow without air that break down the food and other things we throw away. These tiny life forms make air type stuff that is made of stuff able to make power, bad stuff that makes our world get warmer, and a small bit of other stuff. The way we now take out the bad stuff that makes the world get warmer and other stuff takes a lot of money.

In our group, we focus on finding a way to take out the bad stuff that makes our world get warmer and the other stuff using very little money. We do this by causing the bad stuff to get caught in heavy things so that only the stuff able to make power is left. The heavy things have lots and lots of little pockets and the bad stuff that makes our world get warmer gets stuck inside of those pockets. The heavy things that our group uses is also made of things that people throw away so it takes very little money to buy. What is left is the stuff able to make power, which can be used to power homes, cars, or to make food.



JOSHUA BERGERSON
Building Scientist

Every building in the world uses power for things like making the air inside a building cool when the air outside is really hot, running the computers in the office, and to light rooms at night. This power usually makes a lot of the bad air that causes the world to get hotter. As people around the world try to make less bad air and use less power, the question becomes how quickly will change happen and what things are stopping change from happening right now. Many people have guessed answers to this question, but we need a better way to know what to expect in the years ahead.

My work studies how a person who owns a building decides to spend money to make their building use less power over time. When we track how many people change their building over several years, we have a good idea of how much power will be saved over time. We can also see how much power saving is possible in different areas of the world or in different building types to figure out where the biggest changes will happen and to help figure out what to do in different areas and building types slow to change. Finally, we can save even more power by making the things an owner can buy save more power or buy them for less money. This helps those people who lead know which changes they need to make to realize a greener world in the years to come.

aurora.alcf.anl.gov

INTRODUCING AURORA

The U.S. Department of Energy announced a $200 million investment to deliver a next-generation supercomputer, known as Aurora, to Argonne. The new machine will be based on an Intel system framework and built by Cray. Scientists and researchers are awarded time on the supercomputer to model and explore everything from engines and nuclear reactors to brain science and supernovas via a peer-reviewed allocation process.

TO BE COMMISSIONED IN 2018

FULLY OPERATIONAL IN 2019

18 TIMES FASTER THAN PREDECESSOR

180 PETAFLOPS

MORE THAN 50,000 CORES

Run by the Argonne Leadership Computing Facility
Funded by the U.S. Department of Energy

SUMMER CAMPS INSPIRE CURIOSITY IN HIGH SCHOOL STUDENTS

BY PAYAL MARATHE & ROBYN HENDERSON

Kids today grow up surrounded by technology, from computers to laptops to smartphones. Despite this exposure, they aren't always taught how that technology works.

Argonne held two different special events for high school students last summer, both designed to get students thinking more deeply about the tech they use every day and what it's like to be a scientist or engineer that produces it.

42 Chicago-area students came to a summer computer coding camp where they took four days of lessons that included an introduction to the Python programming language, emphasized problem-solving skills, and showed students what it's like to be a professional in a science, tech, math, or engineering career.

"Programming boils down to problem-solving," said Ti Leggett, a researcher in Argonne's computing, environment and life sciences directorate who led curriculum design and teaching for the camp.

"It's all logical thinking—breaking down problems and attacking them in parts. We wanted to help students develop this way of thinking," he said.

For example, on day one, the kids instructed each other on how to navigate an obstacle course, where each step involved moving a certain distance in a specific direction. The exercise was meant to illustrate how a coder thinks.

Maria Curry-Nkansah, chief operations officer for Argonne's physical sciences and engineering directorate, works with the DuPage County chapter of the Afro-Academic, Cultural, Technological and Scientific Olympics (ACT-SO) and helped organize this camp. To increase the number of African Americans who pursue college degrees in STEM, she said it's important to expose them to science at a young age, "before they start thinking 'I can't.'"

ACT-SO is coordinating a weekly code-writing club that will meet Saturdays at a local high school so that students can continue building upon what they learned at camp.

Meridith Bruozas, manager of Argonne's educational programs and outreach, said there are ideas in the works to do even more in the realm of computer science. In September, Leggett's team held a workshop to train STEM educators on how to best teach computer programming skills. The goal is to extend the reach of this curriculum—train 30 teachers, and each will transfer these lessons to at least 30 students.

Earlier in the summer, 80 students went to an event called "Charging up the Classroom" to learn more about at a different part that makes their cell phones run: the battery.

Students attended workshops where Argonne scientists explained how batteries work and discussed their research on new battery concepts. The presentations helped to show

High schoolers learned about coding and batteries with Argonne researchers in two different summer camps.

students that energy science can solve practical problems that will affect everyone in the future by increasing electric car mileage, reducing energy emissions, and stabilizing the electric grid.

Lei Cheng, a scientist with the Joint Center for Energy Storage Research, led a workshop that not only showed the students how batteries work in a way that they can relate to, but also showed why the world needs better energy storage technology. She introduced students to uses for batteries that are not necessarily intuitive.

"Before I joined JCESR, I didn't think of applying energy storage technology to the electric grid," said Cheng. "For example, we're trying to switch to more renewable resources like wind or solar power. But the sun doesn't shine all the time and the wind doesn't blow all of the time. When everybody's off work and it gets dark, they start to use electricity more. Because the demand is higher than the energy input at that time, we need to have a higher level of grid storage, so that when demand is high, we can still send energy to the grid."

The event also focused on the business aspects of battery science: Chicago business owners Anna Stork and Andrea Sreshta led a workshop on entrepreneurship.

Stork and Sreshta are the co-founders of LuminAID, a company that makes inflatable solar-powered lights. The two developed the product in response to the earthquake in Haiti after realizing that one of the greatest dangers after a disaster is not having light. Their lights are sold to disaster relief organizations in locations around the world.

"It all starts with an idea," said Sreshta. "Science is where it begins, and businesses work to make the idea viable and accessible for the public. When you start off, you might not have all the resources or the funding, but if you have an idea that could help people, you shouldn't let that get in your way."

For more information about education at Argonne, **visit www.anl.gov/education.**

"Charging up the Classroom" was sponsored by the Joint Center for Energy Storage Research (JCESR), Argonne's educational programs department, the Chicago Innovation Exchange, and Clean Energy Trust. The summer coding camp was a partnership with the ACT-SO; Deputy Associate Lab Director Mike Papka, who directs the Argonne Leadership Computing Facility, and other computer scientists teamed up with Argonne's educational programs department to design the curriculum.

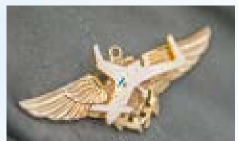
MATT KWIATKOWSKI
CYBER SECURITY MANAGER & PILOT

THE SECRET LIVES OF SCIENTISTS

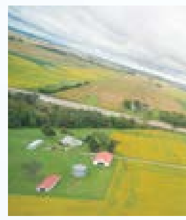
Meet researchers and employees from Argonne with unusual hobbies and interests.

Kwiatkowski takes a member of the Young Eagles program up in a plane he built by hand.

The cockpit and captain's seat



Matt's homemade experimental aircraft wings



ARGONNE NOW: WHAT DO YOU DO AT ARGONNE?

MK: 95% of my job is cyber security. I manage the team that does intrusion detection for malicious actors, firewalls, cyber forensics, and incident response. The other 5%, believe it or not, is that I'm officially the Argonne aviation safety officer. Every government agency has to have one.

AND WHAT'S YOUR HOBBY?

MK: I'm a pilot! I've been a pilot since January of 2000, so about 16 years. I'm certified as a private pilot single engine on land. So I can fly any aircraft that's under 12,000 pounds. I'm also a certified airframe and power plant mechanic.

HOW DID YOU GET STARTED?

MK: I've always wanted to fly, ever since I could remember. It was just in my blood, just in my soul for whatever reason. Nobody in my family flies, which is unusual—usually you have generations of pilots—but my dad was an electrical engineer, so what was also in my blood was the engineering stuff. And when you're building remote control models, like I did as a kid as soon as I could, you learn about how wings are built, the structure of an airplane, center of gravity, Bernoulli's principle, all the math behind building an airplane that will fly correctly.

Kwiatkowski monitors live cyber threats.

I HEARD YOU BUILT YOUR OWN PLANE.

MK: Once you have a license you say to yourself, "Okay, how do I get an airplane?" It turns out the cheapest way to get an airplane is just to build your own. I bought a half-finished project and finished it myself. It took me about another five years. The model is called a Rutan Long EZ. Its race team name is the Special K.

WHAT DOES IT LOOK LIKE?

MK: It's tandem seating, pilot and passenger. Its engine is in the back; it doesn't have a traditional tail. A small wing in front, a large wing in the back.

NOT WHAT YOU SEE EVERY DAY!

MK: It's technically classified as an experimental design. Standard aircraft certification restricts what you can and can't do with it, even if it's to add extra safety or efficiency features. My same engine in a Cessna, a more standard engine-in-front plane, it has a top speed about 115 mph. I can go 220 mph—almost twice as fast on the same horsepower. So mine has an anti-stall configuration, it's faster, and it's cooler-looking. I always draw a crowd wherever I bring it. I'll land at an airport and 10 people come over to say "Where do I get one?"

HOW HIGH CAN YOU GO?

MK: The highest I've been is about 16,000 feet. You need oxygen over 12,500. Other people have taken this model up to 22,000. That's almost as high as a commercial flight—the big boys, as we call it. You can go faster at higher altitudes. So if you're going somewhere, like my sister lives in Dallas, Texas, so I go up to about 10, 11,000 feet—

WAIT, SO YOU FLY YOURSELF TO TEXAS?

MK: Oh yeah, the beauty about this is that I can pop over to Texas for a weekend. It takes about five hours from here, including one stop for 30 minutes to refuel. The world gets smaller.

HOW OFTEN DO YOU FLY?

MK: I try to fly every weekend. I have about 400 flight-hours—that's a lot for a recreational pilot. 500 hours is when you get cheaper insurance [laughs].

EVEN IN THE WINTER?

MK: Oh yeah. Since the engine is in the back my airplane doesn't have traditional heat, so I have an electric heating system. Just like people who are hardcore motorcyclists—they have electric heated clothing: socks, long johns, and vests with heating elements built in. You just plug into the airplane and it's actually quite comfortable.

ARE YOU STILL MAKING CHANGES TO THE PLANE?

MK: Oh yeah. Mostly small. I just got a set of glasses that superimpose an image from the instrument panel, so it projects the artificial horizon, airspeed, altitude, so you don't have to look down. It's helpful because I just started getting into air racing, so I've been modifying the plane to make it iteratively faster. Some of these guys go really crazy though, they'll be out there waxing the airplane to make it go faster. A clean airplane goes faster than a dirty airplane.

REALLY?

MK: Bugs hit the airplane, you know, and if you have a lot on there it'll slow you down by a couple miles an hour. And if you're racing, over a 150-mile course that means they're gonna be 30 seconds in front of you.

WHAT DOES YOUR AVIATION SAFETY JOB AT ARGONNE ENTAIL?

MK: Well, one big part of it was when the president visited Argonne. The Secret Service called my house on a Sunday morning—I thought it was a joke. I worked with them for a week, choosing the landing site, making sure the airspace and landing zone were clear. That was a blast. I got to chat with the Marine One pilots. Definitely something you don't get to do every day.

DO YOU SEE ANY PARALLELS BETWEEN PILOTING AND CYBER SECURITY?

MK: Yes, actually! It's risk management. When you've done the ultimate risk management—balancing my life based on decisions I've made on the engine and modifications—those kinds of thought processes translate directly into making sane cyber security risk decisions. What allows the lab to do its mission, but mitigates bad guys breaking into the system? So those complement each other.

Kwiatkowski takes his hand-built plane for a spin at 200 miles per hour and 4,000 feet.

ASK A SCIENTIST

ARGONNE'S NEW BATTERY CENTER

Jeff Chamberlain, director of the Argonne Collaborative Center for Energy Storage Science and external integration officer of the Joint Center for Energy Storage, took to Reddit to answer questions from users on that site's "Ask Me Anything" feature. He dishes on the next generation of batteries, why new inventions take so long to get to market, and clean room suits for dogs (they exist!).

From user TrueBlueShteve: Is the next gen going to be lithium-ion, or something else?

JC: We scientists have been debating this question for many years. I personally realized a couple years ago the question itself is flawed in its implied assumption that there will be a single winner amongst the possible technologies.

The answer to your question is yes and no. Next gen will be lithium-ion, and next gen will be other than lithium-ion. Depending on the application.

Lithium-ion is going to improve at least 2x (maybe 2.5 or 3x) in performance, and decrease in cost by 50% or 60% in the coming years. As such, it's going to be around as a successful technology for a long, long time. Remember that lead-acid has been around for over a hundred years, improving all the time. It's actually a great technology. Same thing will happen with lithium-ion. And then new technologies like those we are working on in JCESR will also emerge and be adopted, because they will improve in performance beyond the theoretical limits of Li-ion.

Also, note that lithium-ion is not like alkaline or nickel-metal-hydride batteries. In the latter two cases, the chemistry set, so to speak, is fairly constant. Lithium-ion, on the other hand, can be changed significantly and still fall under the umbrella name "lithium-ion." Cathode materials can be changed from cobalt oxide to iron phosphate, and the anode can change from carbon to titanium dioxide, and it's still called lithium-ion, because that is the ion that shuttles a charge back and forth. So, one battery can be used for laptops, and the other for power tools. Point is, lithium-ion has room to evolve substantially in the near future.

Inthenameofscience: About how long does it usually take to go from mulling over an idea to research, experimentation, and eventually production?

JC: It takes a long, long time. Most folks outside of science and engineering don't have a good feel for this, so I am glad you asked. For reference, I suggest reading *The Idea Factory*, by Gertner, about Bell Labs.

To go from an idea for something physically new to implementation commercially, it usually takes a low number of decades. The Manhattan Project and the Apollo Missions are exceptions, but in my view there are two variables: time and effort (effort = money + person-years). In these cases, the effort variable was WAY larger in the Manhattan Project and the Apollo Missions than for typical science and technology projects.

The reason we fool ourselves into thinking it only takes a short time is because of the rapid evolution of technology once the basis is there. An example is the advance in personal computing (up to and including smart phones) through the 80s, 90s, and 2000s. But it took decades to understand and perfect the microchip before this series of rapid advances. (Remember, all integrated circuits are silicon, so advances have been incrementally based on this one material.)

In batteries, we are trying to go to a completely different set of materials. We incorporate industry in our research to try to compress this long time scale.

hwalsh01: Do you have any research/designs working toward large grid-level storage?

JC: Yes. The problem of energy storage for vehicles is tangible to the average person, because the average person uses a cell phone and a laptop, and gets the importance of portable energy storage. (E.g., Ahhhhh!!! My phone charge is 1%!!) Less obviously tangible is the grid problem. As the grids around the world adopt more and more renewables (wind and solar), we need to store the energy produced by them.

Here's why: electricity is an on-demand production cycle for the consumer. The power knob in a coal-fired power plant gets turned up for every light switch turned on, basically. As it is produced, electricity is consumed. Well, we can't turn up the wind or the sun as needed. Not yet, anyway!

So, as the percentage of electricity production goes up from renewables, we need to find a way to take electricity being produced when we don't need it and store it. It is one of the two main missions of our JCESR research to identify through scientific research how to develop a battery from the materials up that can efficiently store energy from the grid. For an overview see here: **www.jcesr.org.**

Researchers test new battery electrodes with special cell testing equipment.

David_D_Montes: I understand that after JCESR became the U.S.'s battery hub, President Obama visited Argonne to survey the energy storage research facilities and talk with staff. Did you meet him?

JC: Yes, President Obama visited Argonne in March 2013. He wanted to learn about our battery work, as well as our work in advanced vehicles in general. The visit was crazy—the day before the visit I watched from my office as three Marine Force helicopters landed in the parking lot of my building for practice. A favorite story was the Secret Service wanted to bring a bomb-sniffing dog into the clean room…Turns out there is such a thing as a clean room suit for dogs. Why?? *(Ed. note: see page 57 for more about the clean room).* Day of his visit was great. His speech was inspiring—he was preaching to the choir about the importance of science! I sat in the second row, and shook his hand; others in the battery team actually toured him through our facility.

Lithium-ion battery cells are prepped for testing.

Entries and questions have been lightly edited for length.

SCIENCE BEHIND THE FICTION

BY ROBYN HENDERSON

Science Behind the Fiction critiques the science and engineering portrayed in popular films and literature. In honor of reaching the "future" of Back to the Future Part II, we're taking a look at the technology its creators predicted for 2015.

Imagine a future full of impossibly amazing technology: holographic movie trailers, self-drying jackets, and a weather service that actually controls weather patterns. Welcome to 2015—as perceived in 1989.

In Back to the Future Part II, Marty McFly time-travels 30 years into the future to find that his hometown is like a completely different world, complete with flying cars and hoverboards. Looking back from the reality of 2015 on the opening scene of the movie, we might laugh at the things they thought possible.

But commercial flying cars and hoverboards aren't impossible. They're just completely improbable.

If flying cars or hoverboards ever became available to the everyday person, one way to build them would be using magnetic levitation based on a special kind of material called a superconductor. Here's how it works:

"The simplest way to generate magnetic levitation is with several magnets pointing in different directions," said Argonne scientist Axel Hoffmann. "When you put a superconductor above these and cool it, it traps the magnetic field, and therefore is held in its original position. It can be pushed and pulled, and even turned upside down, but it is always strongly attracted back to where it was."

The vehicles could hover about four inches off of the ground, Hoffmann said—as long as the superconductor is cooled to -320° Fahrenheit and there is a magnet underneath.

But if maglev cars were made, they would not be able to "fly" as shown in Back to the Future Part II. In one of the scenes in the movie, the cars ride up a ramp and fly about 30 feet above the ground, which would require an extremely powerful magnet.

There are two major problems, though. A maglev vehicle levitates as long as the superconductor stays cold and there is a magnet underneath. Without either of these factors, it stays on the ground.

The magnets are the hardest part to deal with. For maglev cars and hoverboards to work, entire towns would need magnets underneath the streets and sidewalks. Even then, it would be difficult to drive freely without a track. The superconductor would try to follow a definite path, so roaming around in a hoverboard—or something as simple as changing lanes in a flying car—would be very difficult.

Another factor is the cooling system. All superconductors need to be kept cold, and the most common coolants for this are liquid helium for conventional superconductors and liquid nitrogen for high-temperature superconductors. The second the coolant is gone, the levitating superconductor drops back down to the ground. Maglev cars and hoverboards would need cooling units and regularly available liquid helium or nitrogen, all of which are, for the moment, too expensive for widespread use.

This is not to say that companies aren't working on them—just this year Lexus released a working prototype hoverboard that uses superconductors, and Hendo Hover is making its own with a different system. Meanwhile, Argonne scientists are working on superconductors and ways to make them easier to use for practical purposes.

So give it another 30 years—we might yet be hovering to school.

THE UNIVERSITY OF CHICAGO
Metallurgical Laboratory

June 12, 1946

To: All Employees

Effective July 1, 1946 Argonne National Laboratory will officially commence operations succeeding the Metallurgical Laboratory, which was created as a war time emergency organization. The Argonne National Laboratory is being established to foster scientific investigation and discovery and to undertake research programs in the field of Atomic Energy on a cooperative basis with Participating Institutions within the Midwestern Area. The Argonne National Laboratory will be operated by The University of Chicago under a Government contract. The University is delegating the operation of the Laboratory, under necessary procedural regulations, to the Director of the Laboratory.

The Argonne National Laboratory will continue to use buildings now occupied by the Metallurgical Laboratory until new facilities are available at the Argonne and will be staffed by the present Metallurgical Laboratory personnel together with such additional individuals as may be necessary. The contractual conditions between the Government and The University of Chicago, for the operation of the Laboratory, permits accrued benefits earned with the Metallurgical Laboratory to be credited to each employee at the time of the transfer of operations to the Argonne National Laboratory.

Dr. W. H. Zinn has been appointed Director and Dr. Norman Hilberry has been appointed Associated Director of Argonne National Laboratory. Mr. W. M. Branch will be in charge of administrative matters as Business Manager of the Laboratory.

Farrington Daniels
Laboratory Director

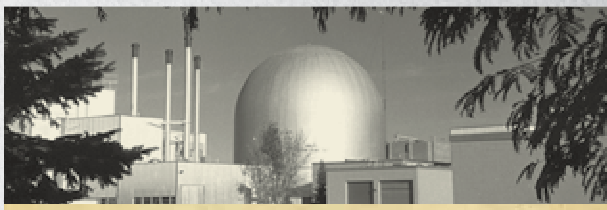
W B Harrell
Business Manager
The University of Chicago

70 YEARS OF DISCOVERY AT ARGONNE

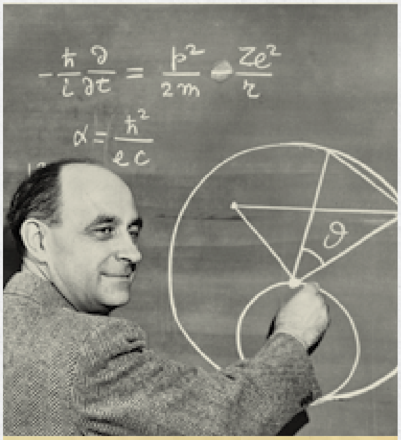
July 1, 2016 is Argonne's 70th birthday.

After World War II ended, Argonne was designated a national laboratory to continue the groundbreaking scientific work of the Manhattan Project for peaceful purposes.

In the years since, the lab has expanded its mission and made strides in nearly every scientific field. As the lab looks forward to its next 70 years of discovery, here's a look back at where we've come from.



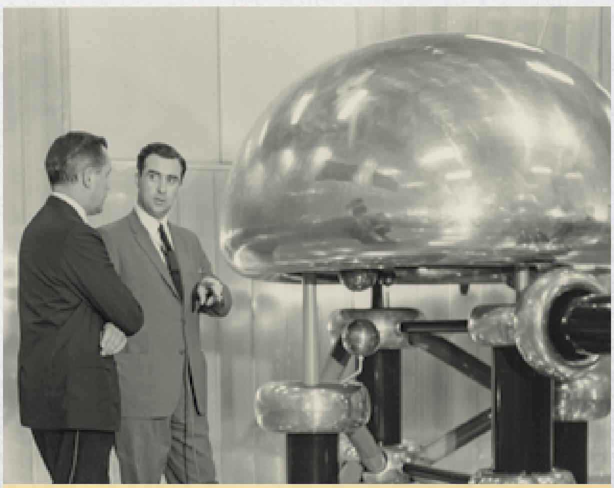
The Experimental Breeder Reactor-II was a pioneering fast reactor which operated for more than 30 years, providing data that influenced reactors built around the world.



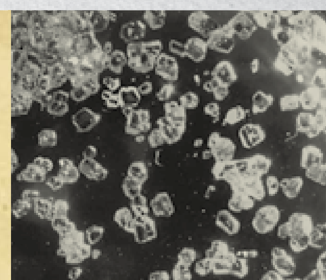
Enrico Fermi led a group of 49 scientists to the world's first man-made sustained nuclear chain reaction—an experiment that would later lead to the founding of Argonne.

This string of 100-watt light bulbs is powered by the first useful electricity ever produced by nuclear power, generated on Dec. 20, 1951, by Argonne's Experimental Breeder Reactor 1.

Argonne computer scientist Jean F. Hall works with AVIDAC, Argonne's first digital computer, which began operation in January 1953.



Argonne director Albert Crewe stands next to the Cockcroft-Walton preaccelerator that fed the lab's Zero Gradient Synchrotron—the nation's first high energy physics user facility. Ca. 1962.



In 1962 Argonne announced the creation of xenon tetrafluoride, the first simple compound of xenon, a noble gas widely thought to be chemically inert. The creation opened a new era for the study of chemical bonds.

On June 4, 1990, leadership broke ground for the Advanced Photon Source at Argonne. Completed in 1996, the APS provides some of the world's brightest X-rays for breakthroughs in many fields.

ART OF SCIENCE

Ancient Helium

By Wei Jiang

Butterflies are drawn to water from the deep Guarani aquifer as scientists sample it to determine how long the water has been underground. The study found that helium filters from the Earth's crust into aquifers, where it is carried to the surface and released.

Download me! flickr.com/argonne

BY THE NUMBERS

THE CLEANEST ROOM

Argonne's Center for Nanoscale Materials has a special facility called the Nanofabrication Clean Room, where scientists can build and study extremely tiny materials—so sensitive that they can be thrown off by the normal dust particles in indoor air. The Clean Room controls the air quality, temperature, and humidity, and filters dust and particles to prevent contamination.

CLEAN ROOM AIR CONTAINS NO MORE THAN **100 PARTICLES** LARGER THAN 0.5 MICRONS IN ONE CUBIC FOOT. A NORMAL ROOM HAS **1,000,000**

VALENTINA KUTEPOVA
ARGONNE CLEAN ROOM MANAGER

MORE THAN **200 RESEARCHERS** A YEAR FROM **24 STATES** AND **13 COUNTRIES** USE THE CLEAN ROOM

STAFF HAS MORE THAN **100 YEARS** OF COMBINED EXPERIENCE IN NANOMATERIALS

MACHINES CAN DETECT **1 PARTICLE** OF METHANE PER **1,000,000 PARTICLES**

13 BAYS

11,500 SQUARE FEET

SPECIAL INSTRUMENTS CAN CARVE FEATURES JUST 10 NANOMETERS WIDE

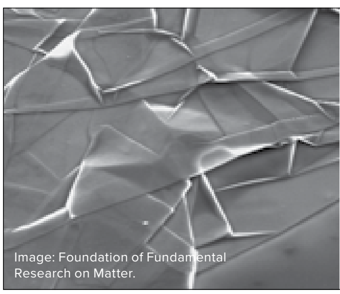
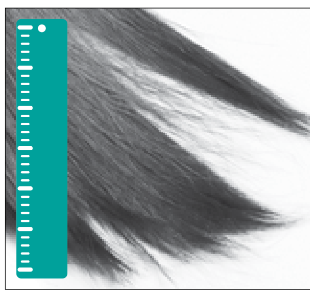


Image: Foundation of Fundamental Research on Matter.

OR LAY A 1-ATOM-THICK LAYER OF GRAPHENE



A HUMAN HAIR IS ABOUT 60,000 NANOMETERS WIDE

The Center for Nanoscale Materials is a U.S. Department of Energy Office of Science User Facility.

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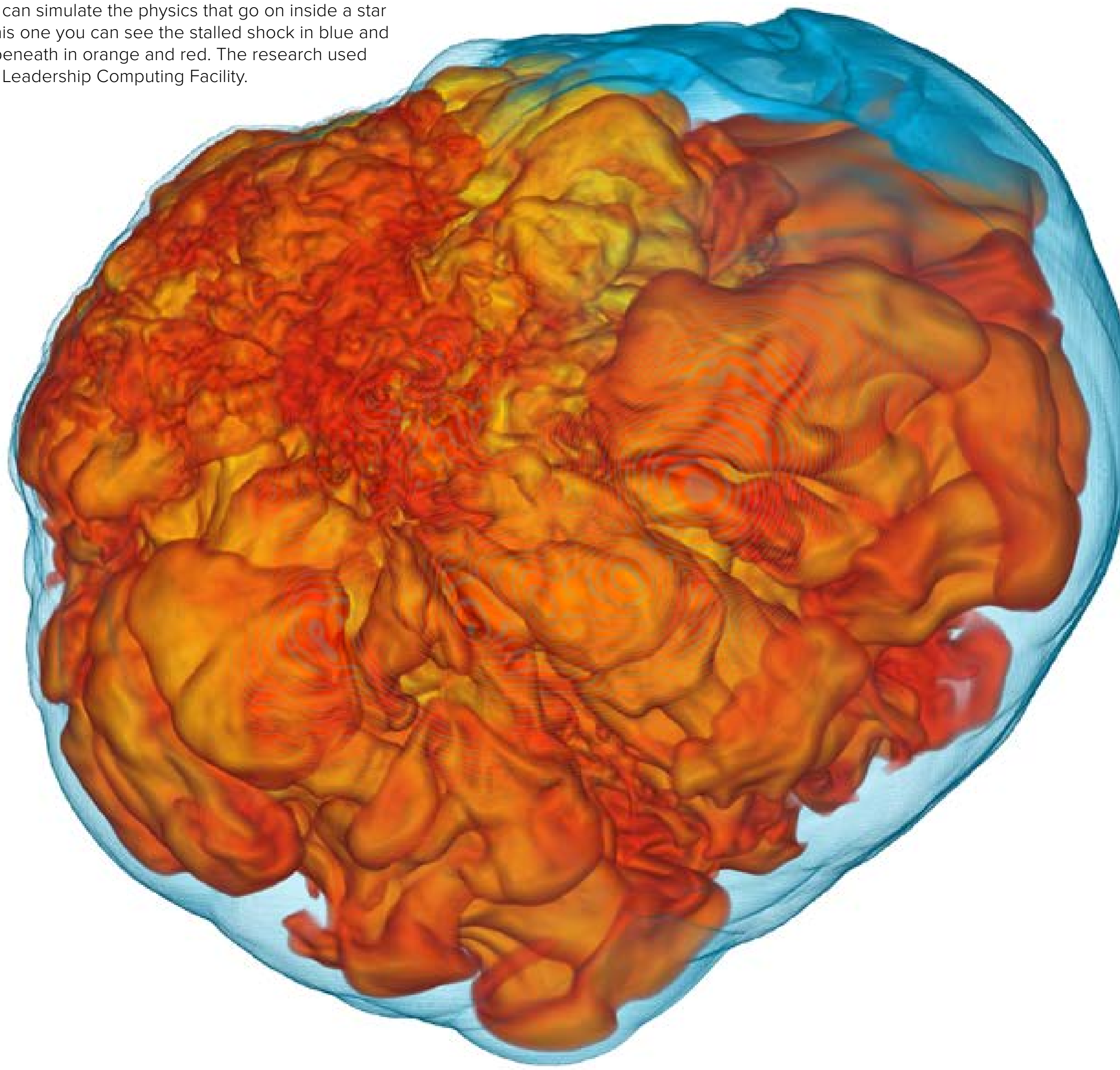
ART OF SCIENCE

Core-Collapse Supernovae

By Sean Couch, Michigan State University

Powerful supercomputers can simulate the physics that go on inside a star as it goes supernova. In this one you can see the stalled shock in blue and the turbulent convection beneath in orange and red. The research used resources of the Argonne Leadership Computing Facility.



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