Oak Ridge National Laboratory
REVIEW
• MANAGED BY UT-BATTELLE FOR THE US DEPARTMENT OF ENERGY •

Vol. 47 • No. 2 • 2014
www.ornl.gov/ornlreview

ORNL's research institutes

Focusing on critical challenges

OAK RIDGE NATIONAL LABORATORY
REVIEW
• MANAGED BY UT-BATTELLE FOR THE US DEPARTMENT OF ENERGY •
Vol. 47, No. 2, 2014

contents

editorial
1 Institutes provide a new avenue for research collaborations

features
2 Capitalizing on a new research model
4 Climate Change Science Institute breaks research barriers to build options for a changing world
8 Imaging institute examines materials atom by atom
12 ORNL institute will transform Big Data into sustainable solutions for urban living
14 Understanding big data: New partnerships support health care innovation
16 Going off grid : Integrated energy systems research rethinks reliance on traditional electric grid
18 Sharing scientific vision: The Joint Institutes

Wigner Distinguished Lecture Series
22 Craig Barrett
24 Venkatraman Ramakrishnan

research horizons
26 ORNL study reveals new characteristics of complex oxide surfaces
27 ORNL, UTGSM study compares structures of Huntington's disease protein
28 Data gathered with high-energy X-ray telescope support the SASI model—a decade later

Institutes provide a new avenue for research collaborations

The nation's most pressing scientific challenges do not typically fit into neat categories. They are complex and subtle, and a useful understanding of them must span multiple scientific disciplines. As the country's largest multiprogram science and energy laboratory, ORNL is uniquely qualified to tackle many of these challenges, but to do so we must be able to work together in ways that transcend traditional organizational boundaries.

This is why we have created institutes to address specific problems. Institutes attract collaborators from different directorates and divisions, harnessing the talents and expertise of researchers looking at the same problem from different points of view. They also couple us to partners in industry and academia and provide a focus for building programs and leveraging investments from multiple sources.

Consider the following:

- Climate change is a grand challenge for Earth system modelers who must help us look into the future, but we also need the expertise of scientists who can tell us what will happen to carbon currently locked into soil and vegetation, coordinate existing data sources so that they are universally accessible, and evaluate strategies for adapting to changing conditions.
- Realizing the promise of exciting new materials envisioned by the federal government's Materials Genome Initiative will require coordinated efforts among experts in materials design and synthesis, imaging and neutron scattering, theory, and data modeling and analytics, as well as new partnerships with industry to accelerate the deployment of innovative materials.
- Alternative technologies for generating, storing and distributing energy will help us mitigate the risks inherent in our reliance on the traditional power grid, but genuine progress in this area will also require a variety of specialists working together.
- The United States generates an enormous amount of health-related information each year, including imaging data, genomics data, and clinical records. This information can be a data gold mine that helps improve our health and lower the cost of health care, as long as we can learn to manage it responsibly and develop the new systems and software needed to extract knowledge from this massive array of heterogeneous data.
- In the urban environments where most of us live, new sensor-based, data-driven tools can help individuals and communities make the best choices for healthy and sustainable living, as well as supporting our response to disasters or emerging threats.

Each of these areas lends itself to a broadly collaborative effort, and each is a natural target for ORNL's strengths as a multidisciplinary laboratory. We have also found this collaborative approach to be profitable as we work with our colleagues at the University of Tennessee. Over the years we have created several joint institutes to focus our collective attention on challenges in advanced materials, computational sciences, neutron sciences, biological sciences, and nuclear physics and applications.

Finally, we are delighted to work with our UT colleagues to educate the next generation of energy researchers. The Bredesen Center for Interdisciplinary Research and Graduate Education gives Ph.D. candidates a chance to participate in ORNL's research programs and take advantage of our one-of-a-kind research facilities while they learn from scientists and engineers at both institutions. We are confident that Bredesen Center alumni will play a substantial role in addressing the next set of compelling problems that we will face in the future.

Thomas Mason

Thomas Mason
Laboratory Director

Capitalizing on a new research model

In many ways ORNL is organized like any other large research facility, with scientists and engineers working together according to specialty—physicists with physicists, chemists with chemists, and so on.

What has always distinguished ORNL is the breadth of its research, the diversity of its workforce, and the power of its facilities. The research here varies from the most basic (e.g., the workings of subatomic particles or the dynamics of the Big Bang) to the most practical (e.g., advanced manufacturing techniques and the strategies for coping with a changing climate). The people here come from literally all over the world. And the facilities are highly advanced and often unique, including the world's strongest pulsed neutron source and the nation's most powerful supercomputer.

But some of our most pressing scientific challenges don't lend themselves to a traditional, discipline-by-discipline approach. Instead, they call out for a collaboration among diverse specialists working toward a common goal. In response, researchers and managers at ORNL have created several institutes—focused, interdisciplinary teams dedicated to a large common problem.

Consider the challenges posed by our warming climate. We know that change is coming, but there are a lot of details to be worked out, from how fast it's coming, to how specific environments will react, to how we can best mitigate and prepare for the change. The challenges cut across disciplines and skill sets.

Or look at the materials genome effort, which promises to accelerate the process that has brought us seemingly miraculous materials, from life-saving Kevlar to high-capacity computer storage. Scientists have the ability now to understand materials atom by atom, deduce why they behave as they do, and create new materials that behave as we want them to. But the effort must include a range of imaging specialists, theorists, and computer scientists.

"Institutes bring scientists and engineers with different expertise and perspectives together to tackle an important issue," explained Michelle Buchanan, associate laboratory director for physical sciences. "This ability to bring teams together to work on large projects that are of high national importance is a hallmark of national labs, especially ORNL."

"The idea is to bring people together to share insights and thereby solve problems that are not necessarily solvable by a disciplinary approach," agreed Ramamoorthy Ramesh, ORNL's deputy director for science and technology.

Institutes at ORNL are a relatively recent initiative, with the first being the five-year-old Climate Change Science Institute. But they are not ORNL's only examples of collaboration among specialties. The lab serves as headquarters to both the BioEnergy Science Center—created in 2007 to improve biofuels production—and the Consortium for Advanced Simulation of Light Water Reactors—which conducts advanced modeling

Some of our most pressing scientific challenges don't lend themselves to a traditional, discipline-by-discipline approach. Instead, they call out for a collaboration among diverse specialists working toward a common goal.

Institutes help keep research collaborative, flexible, and focused

The idea is to bring people together to share insights and thereby solve problems that are not necessarily solvable by a disciplinary approach.

Ramamoorthy Ramesh
ORNL deputy director for science and technology

and simulation for commercial nuclear reactors. BESC comprises biologists, chemists, physicists, mathematicians, and engineers, while CASL brings together specialists in nuclear science, computational science, and engineering. Both pull together collaborators from national laboratories, universities, and private business.

ORNL is especially well positioned to take advantage of this diverse and flexible model because it houses researchers from across the spectrum of science and engineering, according to Martin Keller, associate laboratory director for energy and environmental sciences.

"This is the beauty of what we have," Keller explained. "When you look at a single-purpose laboratory, it doesn't need to create an institute for a specific problem because that's the whole laboratory.

"But look at ORNL. We go all the way from hard-core fundamental science in all these different disciplines—from biology to chemistry to physics to neutrons—all the way to a 25-ton carbon fiber facility in the Manufacturing Demonstration Facility. This is a tremendous benefit if we use the diversity in our science to bring these different groups together to work on a common problem."

One common thread among the institutes is the ability to collect and analyze more data than ever before. It's no coincidence that interdisciplinary institutes are finding a home at the same institution that houses the country's leading supercomputing organization. Not only is ORNL able now to collect, collate, integrate, and analyze large and disparate datasets, but it is also able to perform digital experiments that guide physical data collection.

"Compared to 30 years ago, we've got nine orders of magnitude more capability on the floor," noted Jeff Nichols, associate laboratory director for computing and computational sciences. "Oh, and by the way, the computational methods and theories and algorithms have also adapted to these hardware processes and have generated nine orders of magnitude more capability. So compared to the hardware and software of 30 years ago, we've got 18 orders of magnitude more capability today than when I was a graduate student."

By the way, 18 orders of magnitude is a million trillion.

"What does that mean?" Nichols continued. "It means we are no longer just trying to get close to experiment. We're now trying to design new materials and predict the properties of these new materials with some known confidence. With CASL, for example, we want to build a virtual reactor and tell you the answer you're looking for without having to do experiments. Modeling and simulation are leading the effort as opposed to trying to explain what we're seeing from experiment."

The lab is also in a strong position because it has a solid traditional organization. The institutes provide an avenue for collaboration among research directorates, but the directorates themselves are home to the researchers. In other words, the traditional organizations provide stability while institutes provide flexibility, a means to focus on research challenges and opportunities as they arise.

"I think it's critical that we not act as though the institutes are there forever," Keller said. "They can be there 20 or 50 years, perhaps, but they don't have to be. If you institutionalize them then they lose a lot of the flexibility and benefits from making modifications." —*Leo Williams*

Climate Change Science Institute breaks research barriers to build options for a changing world

Richard Norby, right, leads environmental journalists on a tour of a prototype site at Oak Ridge National Laboratory for the Spruce and Peatland Responses Under Climatic and Environmental Change experiment, which is currently being carried out in northern Minnesota. Image credit: Genevieve Martin

In May, atmospheric carbon dioxide concentrations were recorded at 400 parts per million for the first time in history. According to the 2014 National Climate Assessment report, this is a 43 percent increase since the 1800s and has resulted in the Earth warming 1.5 degrees Fahrenheit since then. That warming is evident from melting sea ice and glaciers, plant and animal migrations, ocean and atmospheric temperature increases, and sea level rise. The National Climate Assessment tells us that over the next few decades, we will likely experience a climate that is three to five degrees Fahrenheit warmer than today.

"Atmospheric carbon dioxide concentration continues to grow, and there is concern about what this will mean for weather extremes like hurricanes, tornadoes, floods, droughts, and their impact on energy and water availability," said Jack Fellows, director of Oak Ridge National Laboratory's Climate Change Science Institute.

Since 2009, CCSI's 130 researchers in high-performance computing, terrestrial ecology and carbon cycling, data and informatics, and climate adaptation have been collocated in the same research space and are working together to better understand climate change and how to mitigate or adapt to its effects.

"CCSI wants to provide actionable climate science and tools that can help users understand and build climate resilience and economic strength for their communities," Fellows said.

Measurements are compiled for the PACIFICA database, which collects data from more than 306 scientific cruises on research vessels. Sampling equipment lowered into the ocean includes detectors that measure conductivity, sea-water temperature, and depth. Samples are also brought back to the surface for measuring pH, salinity, oxygen, and more. Image credit: Alex Kozyr

Four parts, one machine

CCSI works on actionable climate science through four groups—Earth System Modeling; Data Integration, Dissemination, and Informatics; Terrestrial Ecosystem and Carbon Cycle Science; and Impacts, Adaptation, and Vulnerability Science.

The Earth System Modeling group is using ORNL's high-performance computing resources, including the world's second-most powerful supercomputer, Titan, to advance global Earth modeling techniques and run these models at resolutions that are in demand by decision makers. Earth science datasets that inform complex climate models are the domain of the Data Integration, Dissemination, and Informatics group, which hosts a number of projects that merge data from separate archives into single portals for model developers, scientists, and stakeholders.

Experts estimate 50 percent of the world's carbon is stored in soil and vegetation, and warming threatens to release this carbon, impacting both human activities and natural ecosystems. The Terrestrial Ecosystem and Carbon Cycle Science group studies carbon cycle processes and feedbacks to understand how these huge stores of carbon contribute to the climate system. The Impacts, Adaptation, and Vulnerability Science group develops analysis tools and methods for predicting the consequences of climate change to society and assessing adaptation strategies that span local to global scales.

Gary Jacobs, former director of the ORNL Environmental Sciences Division and CCSI business and operations manager until he retired in 2012, was one of a handful of lab leaders who conceived of CCSI.

"We thought if we could find a construct that would allow information gathering, sharing, and collaboration, the lab would be successful in the field of climate change science in multiple ways: increased funding, publications, and communication across disparate groups," Jacobs said.

Jacobs and James Hack, director of ORNL's National Center for Computational Sciences and co-director of CCSI until Fellows came on in 2013, created the themes by identifying the lab's strengths in climate change science.

"The themes helped frame how we talked about the institute and addressed ORNL's approach to climate change science," said Benjamin Preston, CCSI deputy director.

The MODEX approach

Hack, a computational climate scientist, and Jacobs, a geochemist, helped develop the CCSI "MODEX" approach, which links models, observations, data, and experiments to solve expansive problems. Understanding climate change means tackling a slew of large-scale problems: ecosystems like the tropics can span continents; the atmosphere is a complex matrix of gases and solid particulates; and the oceans are vast and have tremendous impact on coasts, sea ice, and the atmosphere. It simply isn't feasible to study climate change with just sensors and measurements or to model climate systems without experimental or observational data.

Laboratory Director Thom Mason addressed this emphasis on interdisciplinary research in his 2009 CCSI organizational announcement: "Through the fusion of modeling, data, and observations, the Institute will explore complex questions such as the analysis of vulnerability and adaptability to climate change impacts and the effectiveness of options to mitigate future climate change."

For CCSI this integrated approach required a bolder move than one might imagine—putting modelers and experimentalists in the same office space.

Earlier this year the institute moved from rented office space to its permanent location on the main campus, where the four groups share an open office environment with multiple conference rooms and seating areas to accommodate collaboration.

"After moving into the same space, we began to learn each other's language," Jacobs said. "I think you'd find that has really accelerated research."

Exchanging dirt for data

Five years in, CCSI is leading and supporting major projects that are successfully bridging the communication gap between fieldwork and modeling.

"I think it's clear we're seeing the powerful immediacy in interdisciplinary research. The integration of CCSI's large-scale environmental experiments and advanced climate modeling is not only helping us understand how climate change will affect us directly but also is equipping with us with the means to prepare for these complex changes," said Martin Keller, associate lab director for energy and environmental sciences.

These projects, which range from developing next-generation climate models to setting up research stations in some of Earth's most sensitive ecosystems, are guided by the President's Climate Action Plan and the Department of Energy's strategic objectives. Both aim to protect the US economy and its natural resources through such measures as conserving water, managing drought and wildfires, and preparing for floods.

"CCSI has more than 50 national to local priorities that help guide our activities," Fellows said. "When we look at projects, we look for those that encompass all four topics of modeling, data, ecosystems, and impacts."

CCSI projects are funded primarily by the DOE Office of Science's Biological and Environmental Research program and by external organizations including the National Aeronautics and Space Administration, the United States Geological Survey, and the Environmental Protection Agency.

SPRUCE (for the Spruce and Peatland Responses Under Climatic and Environmental Change) project is an ORNL-led, decade-long experiment in the peatlands of northern Minnesota where vast accumulations of carbon are stored in undecomposed plant material. Experimentalists will impose increased temperature and carbon dioxide concentrations on designated forest plots and, by closely working with computer modelers, observe and quantify future conditions.

Further north in Alaska, the Next-Generation Ecosystem Experiments (NGEE-Arctic) project, also led by ORNL, has established research sites where scientists are studying the relationships among permafrost dynamics, hydrology, vegetation, microbial activity, and carbon uptake and release. The Arctic permafrost also contains enormous amounts of stored carbon that may be released in a warming climate as carbon dioxide or methane, both potent greenhouse gases.

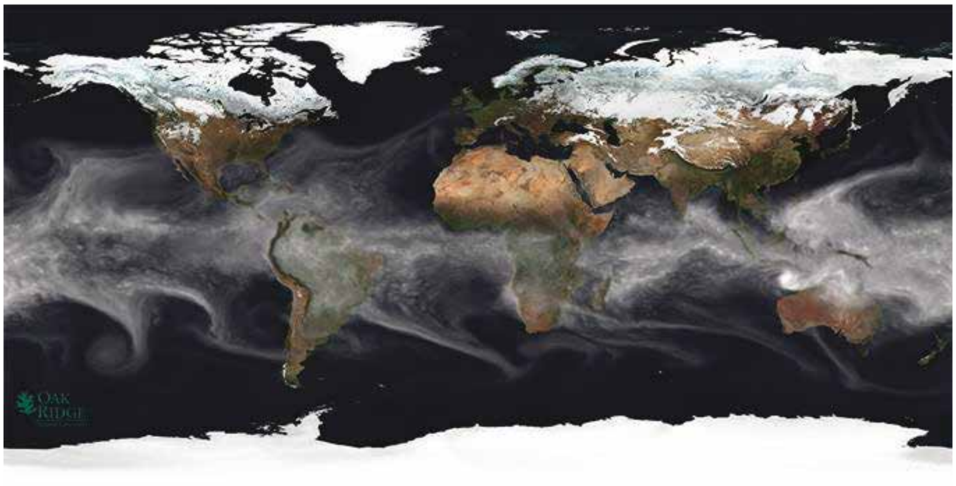
Going tropical

More recently, the NGEE model has been extended to the tropics. CCSI is collaborating with Lawrence Berkeley National Laboratory in a pancontinental study of tropical forests. Still in development, NGEE-Tropics is designed to study the carbon cycle in forests in Central America, South America, Africa, and Asia.

"The tropics are a tough place to work so not a great deal of experimental work has been done there, yet Earth system models are very sensitive to how the tropics are represented. So we need good measurements," said Richard Norby, corporate fellow in ORNL's Ecosystems Observations and Experiments group.

CCSI scientists will venture into the uncomfortable tropical heat and humidity to directly measure root growth, nutrient interactions, and other below-ground activities that impact the carbon cycle.

Colleen Iversen takes a soil core sample from an Alaska field plot for Next-Generation Ecosystem Experiments–Arctic.



Snapshot of water vapor generated as part of a multi-laboratory, next-generation climate modeling project known as ACME, or Accelerated Climate Model for Energy. Climate Change Science Institute researchers Katherine Evans, Patrick Worley, and Forrest Hoffman are helping to lead ORNL efforts in this project. Image credit: Jamison Daniel

All three ecosystem projects rely on the MODEX method, directly linking field experimentation with computer models and data analysis.

Meanwhile, CCSI climate modelers are working with several national laboratories to build the next-generation Earth system model. The Accelerated Climate Model for Energy project is tasked with providing a modeling tool to address science questions that focus on the hydrological cycle, biogeochemical cycles, and cryosphere (surface ice and snow). While global models have been used primarily for predicting average changes, new models must be able to resolve regional details and extreme weather statistics to inform small-scale decision-making.

Managing the data collected from modeling and experimental work would not be possible without the tools and expertise of CCSI's Data Integration, Dissemination, and Informatics group, including the Carbon Dioxide Information Analysis Center, the Atmospheric Radiative Measurements Data Archive program, and NASA's Distributed Active Archive Center. These archives, which are made available to the public, include hundreds of terabytes of cloud properties, aerosols, and precipitation data from around the world; fossil fuel emissions estimates dating back to the eighteenth century; and a broad range of ecosystem products that examine soil, vegetative, hydrologic, and weather parameters and changes. The powerful data management tools produced by these centers and programs are being incorporated into all major CCSI projects so data is properly formatted, archived, and disseminated.

Smart tools for big decisions

Informing decision makers is an ultimate goal of conducting research and developing better models. Understanding climate change is especially valuable if people can adapt to negative impacts or take advantage of new opportunities.

Researchers predict increased storm surges, hurricanes, and sea level rise will affect coastal areas in the Southeast; drought will affect water availability in the Great Plains; wildfires will threaten forest health in the Southwest; and warming temperatures across the country will impact farms and fisheries, energy prices, and human health.

Impact, Adaptation, and Vulnerability Science researchers quantify the potential risks of climate change on regional and local scales. In Global Environmental Change, Preston predicts US economic losses from extreme weather could double by 2050, requiring fast solutions. To prevent monetary and physical damages, CCSI researchers across themes are looking to the future of scientist–stakeholder collaboration on local to national scales. For example, CCSI's Esther Parish and co-investigators teamed up with Olufemi Omitaomu of ORNL's Urban Dynamics Institute to develop the Urban Climate Adaptation Tool (Urban-CAT) for the City of Knoxville with expectations that the tool will be applicable in other mid-sized cities. Urban-CAT will help the City of Knoxville determine how to use green infrastructure, such as permeable pavement and green roofs, to naturally collect runoff water to reduce flooding and lessen impacts on water treatment facilities.

"CCSI has massive amounts of projected climate data, so we want to bridge the gap between local decision makers and scientists," said Omitaomu. "By working with Knoxville, we will learn how they use information and what their resources are, so we can develop our models and the Urban-CAT tool accordingly."

The future of CCSI is one desk over

Now that the institute is out of its infancy, Fellows recruited input for a 2014–2020 strategic plan, and many of those recruits were early-career scientists.

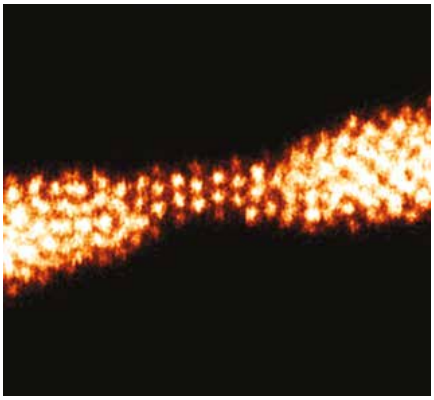
Colleen Iversen, who studies root interactions in soil and joined CCSI as a staff scientist in 2010, said the institute has many senior staff and early-career scientists, which encourages informal mentorships and fosters collaboration.

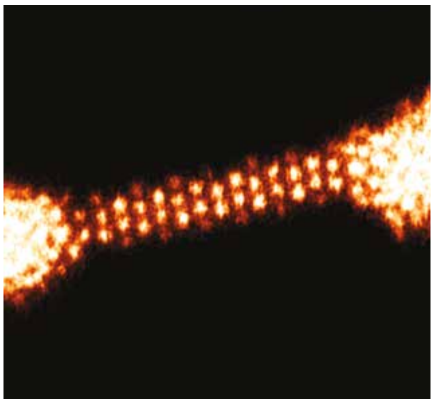
"Early-career scientists are enthusiastic about collaboration and using new technology to solve problems, and that's the foundation of CCSI as an institute," Iversen said.

Other measurements of CCSI's success are evident as its researchers produced 139 publications and shared the immediacy of climate change science at nearly 300 presentations and seminars in 2013.

"The earth's climate stabilized enough to sustain life roughly 10,000 years ago. It is our responsibility to ensure that stability for future generations. I see that commitment in each and every CCSI staff member, and I believe everyone in CCSI is proud to be part of this effort," Fellows said.

—*Katie Elyce Jones*





Atomic-level view of an ultrathin nanowire seen through a scanning transmission electron microscope. Image credit: Wu Zhou and Junhao Lin

Imaging institute examines materials atom by atom

ORNL is uniquely qualified to uncover the mysteries of matter at the level of atoms and molecules.

The lab has the talent and technology to map individual atoms, observe materials under a wide range of conditions, make sense of the data produced by these examinations, and deduce both what makes the material behave as it does and how we can make it behave as we want.

This wide range of skills is the driving force behind the Institute for Functional Imaging of Materials, created this summer to coordinate ORNL's strengths in imaging, theory, and data analysis.

"The institute is formed to respond to the new opportunities that are now being opened in imaging, but also in materials and Big Data," said its director, Sergei V. Kalinin of ORNL's Center for Nanophase Materials Science. "ORNL has a tremendous strength in all these areas."

ORNL has the tools

Consider just a few examples.

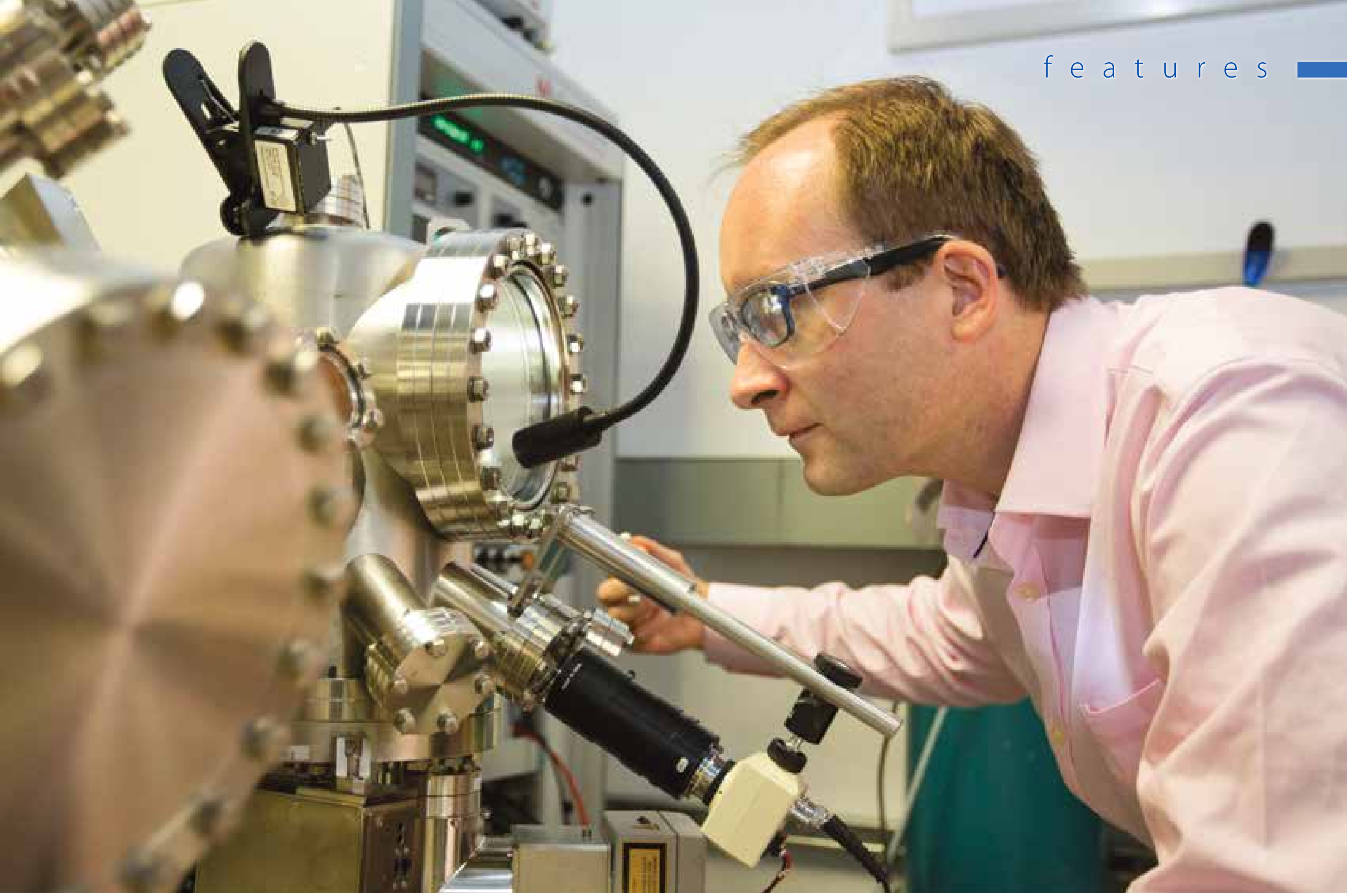
CNMS houses 16 scanning probe microscopes ranging in size from desktop appliances to hulks that cannot fit into a room unless a hole has been dug in the floor.

The tip of a probe can get as narrow as a single silicon atom, making it roughly 3,000 times sharper than a razor blade. By touching a sample one atom at a time, the instrument not only maps the surface but also tells how far apart the atoms are and how they are arranged. The microscope can analyze electronic behavior by running voltage through the tip. And with the larger instruments, the microscope can take samples down to a third of a degree above absolute zero (far colder than deep space), allowing for analysis of material properties—such as superconductivity—under extreme conditions. Many of these instruments are equipped with advanced controls that allow them to explore single-atom electrochemistry, polarization switching, and electrochemical reactions at the level of a single defect—such as a dislocation or grain boundary—as a function of bias, temperature, and time.

These microscopes produce a mountain of data.

ORNL has other types of high-tech microscopes as well. The lab's Advanced Microscopy Laboratory hosts several scanning transmission electron microscopes, each of which occupies a well-shielded room, with control equipment set up in an adjoining room. The microscopes focus an electron beam to half an angstrom (roughly half the width of an atom), shining it through samples that are only tens to hundreds of angstroms thick. Detectors on the other side register electrons from the beam as they bounce off the electrons and nuclei of atoms within the sample.

When all is said and done, the microscopes get not only an atom-by-atom view of the material, but also information on aspects such as bonding of the atoms, electron



orbitals, and magnetic spin contained in the intricate details of energy loss spectra. They are used to explore a wide variety of materials, including catalysts, batteries, thermoelectrics, and superconductors.

The electron microscopes also produce a mountain of data.

These are just isolated examples. Across the lab are dozens of state-of-the-art microscopes customized to provide valuable, unique insights into promising materials. These materials may advance DOE's goals in energy production or energy storage, or they may meet a wide range of other pressing needs.

But ORNL's imaging talents don't end there. The lab's most ambitious imaging effort is the Spallation Neutron Source, a unique facility that produces the world's most intense neutron beams.

Very fast and very quick

SNS does its job by hurling protons at 90 percent of the speed of light into a mercury target, which spits protons into a ring that releases them in bursts of less than a millionth of a second.

The neutrons are routed into 17 beam lines, each containing a unique instrument. These instruments allow scientists to explore questions as fundamental as how light elements were produced in the Big Bang and why the universe has more matter than antimatter, as practical as the effects of solvents on nanoscale structures and the workings of materials used in catalytic converters, and as promising as the structure of materials for storing hydrogen and the workings of high-temperature superconductors.

Institute Director Sergei Kalinin examines a sample with a scanning probe microscope at ORNL's Center for Nanophase Materials Science. Image credit: Jason Richards

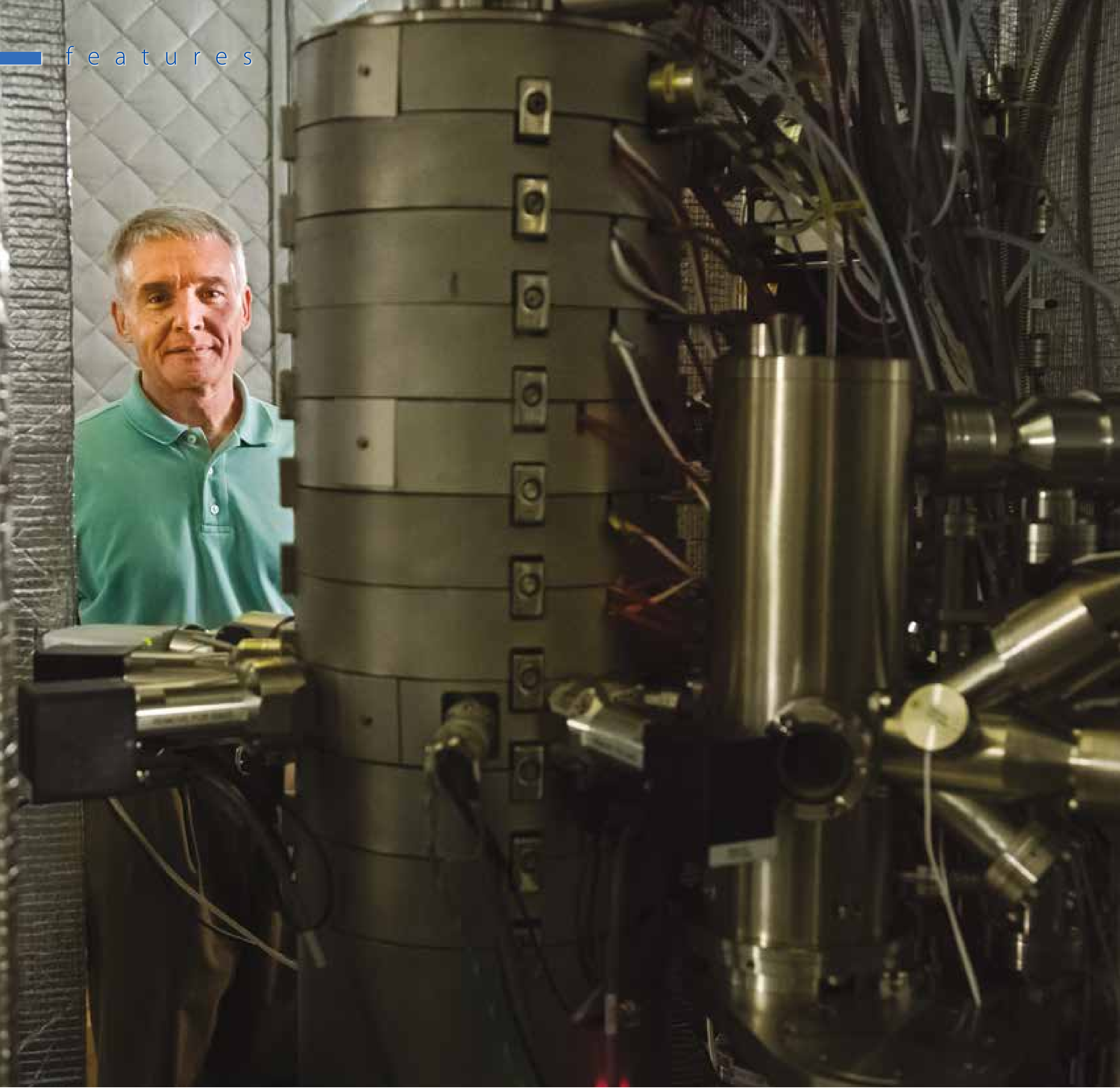
SNS lets researchers study iron under conditions the same as those found at the Earth's core and ice under conditions similar to those found in comets and far-off moons. It lets them study processes under timescales as fleeting as trillionths of a second.

Saying that SNS produces a mountain of data would be an understatement.

Fortunately, ORNL is also uniquely qualified to handle mountains of data. Located at the Oak Ridge Leadership Computing Facility on the ORNL campus, Titan is the world's second most powerful supercomputer, capable of up to 27 thousand trillion calculations each second.

ORNL has long valued high-performance computing and has stayed at or near the top of the field even as the field rapidly changes. While the world's top supercomputer today is nearly 500 times faster than the top

The principles of physics, as far as I can see, do not speak against the possibility of maneuvering things atom by atom.—Richard Feynman, 1959



ORNL researcher Matt Chisholm works with scanning transmission electron microscopes located at ORNL's Advanced Microscopy Laboratory. Image credit: Genevieve Martin

system a decade ago, ORNL has remained at the forefront, with a top 10 system included in all but two of the 20 "Top 500" lists published during that time.

Researchers have been using Titan and its predecessors for years for materials research on topics ranging from high-temperature superconductors to organic photovoltaics to thin films to exotic magnetic properties.

Bringing strengths together

ORNL has all of these skills, but they are spread among different organizations and directorates—Physical Sciences, Neutron Sciences, and Computing and Computational Sciences. While scientists need close collaboration within their individual disciplines, researchers with different specialties face the danger that they might work on different aspects of the same problem and not know it.

"I see people doing research over here in electron microscopy, here in scanning probes, over here in mass spectrometry, over here in neutrons, and over here in something else," said Michelle Buchanan, associate laboratory director for physical sciences, "and they're just working by themselves, as scientists do, diving down deep and doing their science."

The outstanding experimental capabilities and advances, when tied to theory and simulations, can enable intimate understanding of how a material works and what controls its properties.
—Bobby Sumpter, ORNL researcher

"Many of these developments resulted from long-term—in many cases, decades—investment in instrumentation and people," Kalinin said. "However, the last decade has seen a revolution in the capability to analyze and process large volumes of data, as exemplified by Google, Facebook, and myriad other web applications. Now is the time to learn how to utilize it in physics."

Nanoscale imaging comes of age

Recent advances in imaging have made an effort like the Institute for Functional Imaging of Materials both more promising and more necessary. It is just in the last decade that microscopes have become so powerful that they not only can identify individual atoms but also can accurately measure the distance between them. By knowing these distances and angles, researchers can gain insight into the electronic, magnetic, and chemical functionalities of materials and predict how they will behave under various conditions.

"The outstanding experimental capabilities and advances, when tied to theory and simulations, can enable intimate understanding of how a material works and what controls its properties," said Bobby Sumpter, also a researcher at CNMS.

"For example, using theory and large-scale simulations, we can easily monitor individual atoms and follow their dynamics," Sumpter said. "This can be used to make direct correlations to highly resolved experiments. This integration and feedback provides a validation of the model/simulation that can then subsequently enable not only a detailed understanding of the material and underlying processes but also the potential to rapidly probe other scenarios such as introducing defects, dopants, etc. This brings things from observations toward materials discovery and design."

Indeed, if we glance back a half century, to 1959, we get a better idea of how exciting recent progress is. In that year, Nobel Prize winner Richard Feynman foreshadowed the rise of nanosciences with a talk delivered to an American Physical Society meeting at Caltech. The talk was titled "There's Plenty of Room at the Bottom."

"The principles of physics, as far as I can see, do not speak against the possibility of maneuvering things atom by atom," Feynman said. "It is not an attempt to violate any laws; it is something, in principle, that can be done; but in practice, it has not been done because we are too big."

As Sumpter points out, Feynman's vision is not just theoretically possible; many of the things he discussed are taking place.

"Now we're in the sweet spot that we dreamed of within nanosciences," Sumpter said. "What would happen if we could actually do that? Well, we can do that to a large extent now."

The value of real-time analysis

Much of the progress anticipated by the institute will rely on the number-crunching powers of Titan and its successors, as well as the ability of researchers to make the best use of this computing power.

"These are multidimensional datasets," noted Hans Christen, CNMS director. "They contain complex information for each point, at each temperature, as a function of time. They very quickly become too complex for the eye to visualize and, in many cases, for the brain to process. And so we now need to use computational approaches to get the most out of imaging data and use these approaches to tell us how and where we need to measure and image. Those are the things that we are really after."

As it moves forward, the institute will also push the limits of real-time data analysis, feeding measurements as they are taken to Titan or another supercomputer, getting results back almost immediately, and guiding the experiment as it proceeds.

In other words, rather than doing an experiment, doing the computational analysis, and using those results to guide the next experiment or computer simulation, researchers will be able to analyze the data while they're still doing the experiment and make appropriate modifications suggested by that analysis.

"So you can start pushing the advances in materials understanding and discovery much more quickly," Sumpter said. "The concept is to reduce the time scale from ideas to discoveries." ®—*Leo Williams*

ORNL institute will transform Big Data into sustainable solutions for urban living

Across the United States, abandoned strip malls and half-empty high-rises coexist with the noise of new construction to tell a story about the dynamics of cities and towns.

Our environment changes with our needs—neighborhoods go in and out of style; new freeways are built, followed by power lines and sewer systems; the latest technologies shutter outdated businesses; and the shifting demographics of a city's population can mean the difference between building a new clinic or a new school.

But one thing doesn't change: "Once the concrete or asphalt is laid, that land has been irreversibly used, and now we have to work around that," said Budhendra Bhaduri, founding director of the Urban Dynamics Institute at ORNL.

Understanding the complex relationship among changes in our environment, population growth, and population movement is critical for designing urban infrastructures for a sustainable future. Through data collection and analysis as well as advanced computer modeling and simulation, ORNL's new Urban Dynamics Institute will study the interaction between humans and their energy and urban infrastructures, with the goal of providing analysis and planning tools that can help citizens understand the complexities of urban lifestyles and help cities make the best development and policy choices for sustainable living.

Nearly 80 percent of the US population lives in urban areas. In this context "urban" doesn't necessarily mean huge metropolitan areas like New York City or Atlanta.

"Defining urban areas has traditionally been perceived as population density," Bhaduri said. "But we look at it based on access to infrastructure and services like electricity, water, and societal services, so in this way, suburban areas are just as important as dense cities."

As population growth continues to crowd large cities and further suburban sprawl, the institute wants to ensure that decision makers are maximizing the use of energy, natural resources, and space in the built environment. These include local governments, businesses, and residents, along with large industries and developers. This investment in conscientious planning can be particularly important in smaller cities.

"If we just look at big cities, we will miss out on the real problem. Income, home size, and how much you travel determine your environmental footprint, so, in the United States, suburban areas tend to contribute a larger environmental footprint. However, small cities and suburbs don't have the resources big cities have to study how they use their infrastructure," Bhaduri said.

"Landscape and infrastructure decisions made by emerging cities of population 100,000–250,000—and there are many more of those than the megacities—are extremely important and will profoundly impact the future of our planet. We want to ensure they have access to the data, analytical tools, and expertise so they can make the optimal decision for sustainability."

DOE laboratories already employ world-class scientists and engineers to invent clean, energy-saving materials and technologies,

but informing decision makers how to best deploy these products can accelerate solutions for large-scale problems such as greenhouse gas emissions and water scarcity.

"As a national laboratory, we have an opportunity to not only solve problems that big, urban areas have but to go out and provide small areas with the information to make insightful decisions," Bhaduri said.

The institute provides such information and analysis through Big Data and advanced computing capabilities; leadership in the management of unique datasets; and the development of cyber tools and transportation and energy technologies.

"With the arrival of Big Data, we have increasing access to information compiled by local, state, and federal governments. We also have unprecedented levels of observations and measurement of our planet. From satellites to the sensors in our smartphones, we can generate detailed depictions of the built environment—the movement of trains and cars or the flow of electricity and water," Bhaduri said. "But with data generated by the crowd, a phenomenon buoyed by social media, we can capture the behaviors and preferences of individuals living in a society as well. That is what makes urban dynamics an exciting, emerging field."

Under the institute's Lab-directed Research and Development initiative, Science and Informatics for Energy and Urban Infrastructures, the institute will focus on four key areas: population and land use, sustainable transportation, energy and water use, and urban resiliency (or urban disaster management).

Big Data at the core

More than 100 scientists and engineers in the institute will be drawn from several ORNL research areas, including the Computing and Computational Sciences and the Energy and Environmental Sciences directorates.

"At our core is a focus on Big Data, computing, and cyber communication and security. We will bridge these strengths with groups across the lab to conduct interdisciplinary research," Bhaduri said.

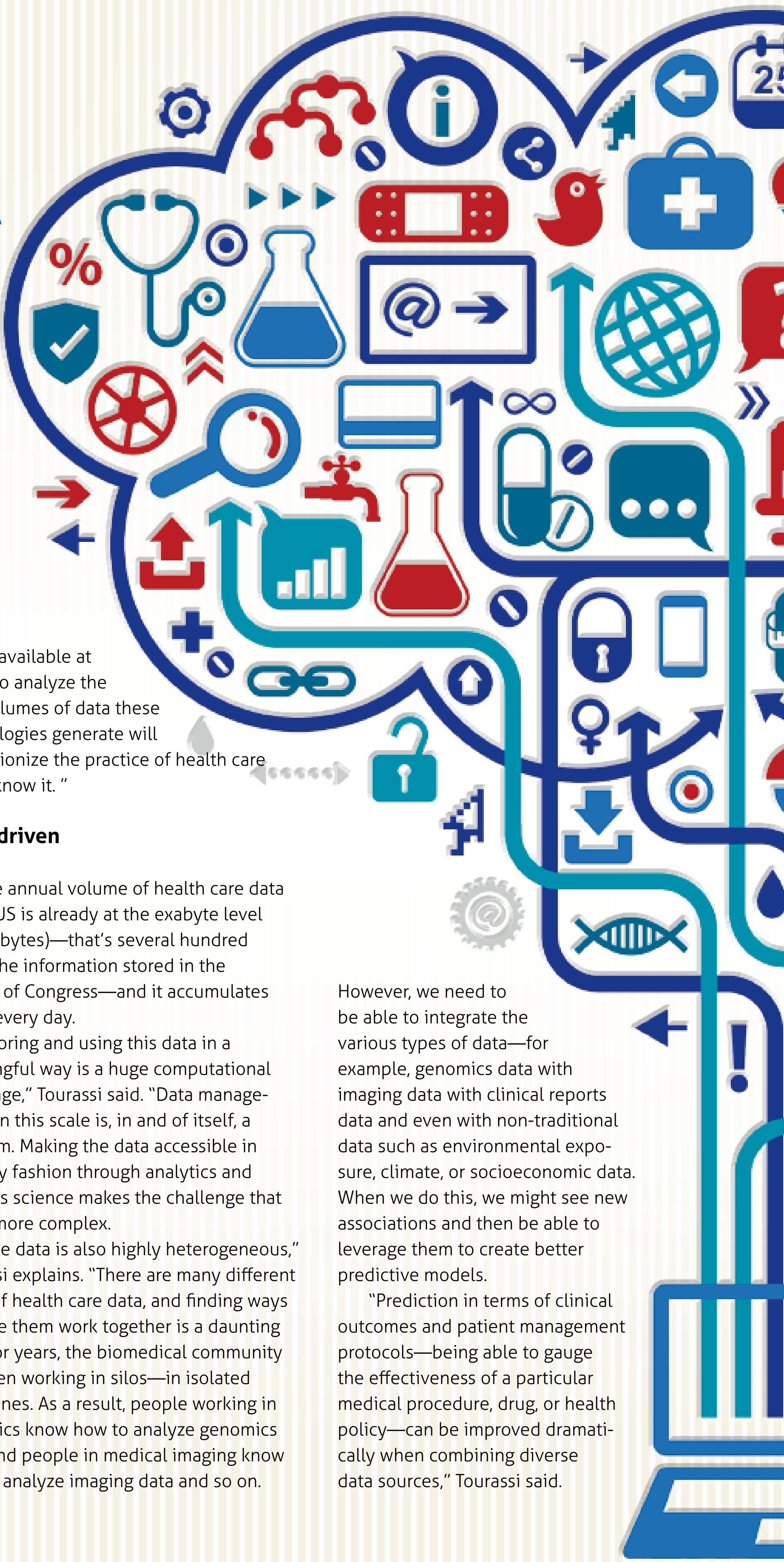
The Urban Dynamics Institute will collaborate with ORNL research teams that are reducing the energy consumption of buildings, improving manufacturing methods for new materials and clean technologies, upgrading the US electric grid and integrating renewable power sources, engineering environmentally friendly vehicle fuels and engines, and identifying key climate change vulnerabilities on the local and regional scale.

Outside the lab, the institute will collaborate with leading research organizations across the world, foundations, city governments, and federal partners including the Department of Energy, Department of Transportation, Environmental Protection Agency, and US Census Bureau to access and appropriate large datasets for urban analysis and planning.

"At the end of the day, individual decisions lead to society's choice for sustainable living," Bhaduri said. "We have to think about the way we want to shape a society with accelerating population growth. We have to balance energy, environment, and mobility to keep our urban populations healthy and productive." Ⓡ—*Katie Elyce Jones*

Understanding BIG DATA

New partnerships support health care innovation



"Big Data," the burgeoning collection of facts and figures created by our information-driven society, presents big challenges for scientists trying to wring insights out of the digital detritus of our daily lives. In areas as diverse as business, crime, and health care, researchers are developing new ways to collect, store, and analyze this information whose quantity, quality, and complexity overwhelm traditional number-crunching methods.

Some of the most useful tools and techniques for handling data of this magnitude were developed by ORNL scientists working with the federal government. The intent of this three-year partnership was to explore how data analysis could be used to optimize health care business practices.

This effort, along with several smaller, data-driven collaborations between ORNL and a number of biomedical centers, was so successful that it played a key role in establishing the laboratory's year-old Health Data Sciences Institute.

"The institute is working with the broader health care community to apply high-performance computing, in the form of advanced data analytics and systems science, to advance biomedical discoveries and health care delivery," said HDSI Director Gina Tourassi. "The explosive growth of digital technology in health care that began with imaging data and electronic medical records now includes telemedicine and data from implantable or wearable medical devices like heart pacemakers and insulin pumps.

"Health care delivery is undergoing major changes as technological changes are put into practice, and even more changes are in the pipeline. The massive computing power available at ORNL to analyze the vast volumes of data these technologies generate will revolutionize the practice of health care as we know it. "

Data-driven

The annual volume of health care data in the US is already at the exabyte level (1,018 bytes)—that's several hundred times the information stored in the Library of Congress—and it accumulates faster every day.

"Storing and using this data in a meaningful way is a huge computational challenge," Tourassi said. "Data management on this scale is, in and of itself, a problem. Making the data accessible in a timely fashion through analytics and systems science makes the challenge that much more complex.

"The data is also highly heterogeneous," Tourassi explains. "There are many different kinds of health care data, and finding ways to make them work together is a daunting task. For years, the biomedical community has been working in silos—in isolated disciplines. As a result, people working in genomics know how to analyze genomics data, and people in medical imaging know how to analyze imaging data and so on. However, we need to be able to integrate the various types of data—for example, genomics data with imaging data with clinical reports data and even with non-traditional data such as environmental exposure, climate, or socioeconomic data. When we do this, we might see new associations and then be able to leverage them to create better predictive models.

"Prediction in terms of clinical outcomes and patient management protocols—being able to gauge the effectiveness of a particular medical procedure, drug, or health policy—can be improved dramatically when combining diverse data sources," Tourassi said.

"However, integrating such data is a work in progress. It is a very complex problem. This is where high-performance computing and a deep understanding of scalable data analytics are critical. That's what our institute brings to the table."

Strategic partnerships

To help promote data-driven advances in health care, HDSI has been pursuing collaborations with key health care stakeholders. For example, HDSI recently established a memorandum of understanding with the Health Data Consortium, a collaboration among government, non-profit, and private sector organizations.

"The biomedical community is notoriously secretive," Tourassi said. "The Health Data Consortium was established to foster the availability and innovative use of open health data. A fundamental need of the community is a national data enclave where interested partners can contribute data to enable health and health care-related research and development."

Tourassi notes that the success of building such an enclave depends on technical capabilities as well as being viewed as a credible and trustworthy entity.

"The community needs an honest broker, a neutral entity that doesn't have a stake in the game for profit or other business purposes," Tourassi said. "A national laboratory, such as ORNL, with internationally recognized data and computing infrastructure and expertise is ideally suited to play that role."

A health data enclave would be particularly useful for researchers interested in knowledge discovery—the process of searching datasets for patterns of information—as well as for researchers doing more traditional health care research and development. A central data repository would also give researchers a place to test how well their algorithms work against real-world data that they don't have the ability to manipulate, as well as to compare them with other algorithms. The key benefit is encouraging innovation while preserving a high level of transparency and scientific rigor.

Another key collaboration is the partnership with the Summit Accountable Care Organization (ACO), the largest ACO in East Tennessee. ACOs are voluntary alliances of health care organization that work together to improve care for Medicare patients. Summit ACO and ORNL have partnered for exploratory Big Data analytics and systems science engagement. Working with data provided by Summit, ORNL will apply advanced data analytics and predictive modeling tools to help Summit improve both its business practices and patient care.

Catalyst for transformation

The biggest obstacle for national labs in the field of health care research is the lack of national presence and credibility in the health care domain. Health care is not something that's usually associated with the US Department of Energy national laboratories. However, six federal agencies, including DOE, are now involved in an effort to determine how to make the best use of Big Data. At the same time, ORNL is also engaged with Big Data analytics from a number of other domains, like earth sciences, material sciences, and neutron sciences.

"Because health and health care transformation in the 21st century is data-driven, these two paths have converged," Tourassi said. "The timing is perfect for ORNL to get involved and be a catalyst for this transformation. We can provide our data expertise and forward thinking, along with the computing infrastructure DOE has invested in over the past several years, to help accelerate knowledge discovery and translation of data-driven solutions into practice. HDSI's vision is to enable our partners from federal and state agencies, industry, and academia to use big health data to produce better health outcomes at lower cost." R—*Jim Pearce*

Going off grid

Integrated energy systems research rethinks reliance on traditional electric grid

The electric power grid—the network of transmission lines and substations that delivers electricity to homes and businesses—is vulnerable to extreme natural events such as heat waves and storms and even to human threats. It's also under continuous pressure to provide reliable service in the most cost-effective manner.

"We're getting more and more dependent on the grid," said ORNL senior research engineer Roderick Jackson. "A large number of people don't have a landline anymore. When your power goes out, you're totally without communications once your cell phone battery dies. As we get more into the technology age, we're more dependent on electricity being there and being reliable."

To ensure access to reliable electric power despite extreme weather or attempted cyberattacks, ORNL researchers are examining alternatives to the traditional centralized grid. One potential solution is distributed energy generation, which relies on more localized and smaller-scale production from sources such as solar arrays.

"Distributed energy helps with resiliency," said Tom King, director of ORNL's Sustainable Electricity Program. "We are seeing more 100-year storms than ever, and this puts a tremendous burden on the energy infrastructure of distribution lines and transmission towers. During some of these storms, people have been without power for weeks. Resiliency is needed to ensure continued power to the country."

The dropping cost of photovoltaic technologies, combined with renewable energy mandates and other economic incentives, has added to growing interest in distributed energy. But despite ongoing technological improvements, solar can rarely go it alone—when the sun isn't shining, another source of power must meet a building's energy needs.

And that's exactly where ORNL researchers are hoping to fill the gaps.

Holistic approach

Jackson, King, and a multidisciplinary team across ORNL are establishing a proof-of-concept building system to demonstrate how new technologies can supplement and support solar generation. The project's larger goal is to establish the foundation for an ORNL institute focused on integrated energy systems.

"The whole idea of an institute is doing something big," King said. "One division, one group can't do this alone, especially when you start to look at what the needs are—materials, buildings, vehicles, advanced manufacturing, power systems, and microgrid expertise. If you have silos, it's not going to work."

The team plans to start with a laboratory-directed research and development project that looks at the intersecting aspects of energy generation, storage, and building demand.

ORNL's flexible research platforms, part of DOE's Building Technologies Research Integration Center, will serve as home for the team's research project over the next two years. The lab's 50-kilowatt solar array and Distributed Energy Communications and Controls facility will help the research team create a holistic test bed.

"We have unique technologies and control approaches, so we can isolate and separate from our distribution systems and be our own microgrid," King said.

To tackle the issue of irregular solar power generation, the ORNL research team is looking at a diverse and complementary set of energy generation and storage approaches. One technology under development is called Ground-Level Integrated Diverse Energy Storage (GLIDES), which stores energy by compressing gas in high-pressure tanks. The team's initial analysis indicates that the GLIDES approach could outperform lead-acid batteries in terms of round-trip efficiency and storage costs.

A second tactic is a heat engine generator, commonly known as a Stirling engine, which could bridge the energy needs of transportation and buildings. Unlike internal combustion engines, heat engine generators can run on a wide variety of fuels or external heat sources but are comparatively inefficient. The researchers plan to apply ORNL expertise in vehicle technologies and advanced manufacturing processes toward understanding and improving an existing Stirling engine. Recovering waste heat from the generator for use in the GLIDES storage technology, for instance, could raise the engine's efficiency.

"Instead of using a battery, the Stirling engine runs on whatever fuel you want it to run on. It could be stationary or mobile as part of a vehicle. You could potentially hook this engine up to help balance the solar variability," King said.

Looking farther ahead, the team is also exploring basic research in ultracapacitors by drawing on ORNL strengths in materials science. The current generation of capacitor devices boasts a high power density but low energy density, which limits their use in energy storage applications. By fabricating atom-thin layers of graphene and boron nitride, the researchers will investigate ways to increase the performance of next-generation electrostatic capacitors.

To tie together the pilot project's different approaches to energy generation and storage, the ORNL team is developing building management system software to control the individual building environment and integrate distributed energy sources into the existing grid.

"From the grid perspective, being able to manage buildings where we can more optimally run the system is an advantage," Jackson said. "This system we're developing can really help balance things from the generation standpoint, as well as from the utility side. It helps the grid operate more efficiently."

Finding balance

At first glance the idea of a solar panel on every rooftop and generator in every basement might seem farfetched, but ORNL researchers point to lessons from the introduction of the automobile.

"With cars, transportation became much more distributed, more flexible," King said. "We still have the main arteries for rail and freight, but the distributed nature of vehicles allowed for more flexibility. The same could be said for energy; we're still likely to have major arteries of bulk power transmission, but we're going to see more distributed approaches."

In addition to growing interest in distributed approaches in the United States and other industrialized countries, the team's research could be particularly applicable in areas where a centralized electric infrastructure does not yet exist.

"Maybe there's no need to develop a grid in developing countries," Jackson said. "The integrated energy systems or microgrid approach could work in villages where it might not make sense to build bulk transmission lines. When you look at international areas, there are more opportunities for these concepts."

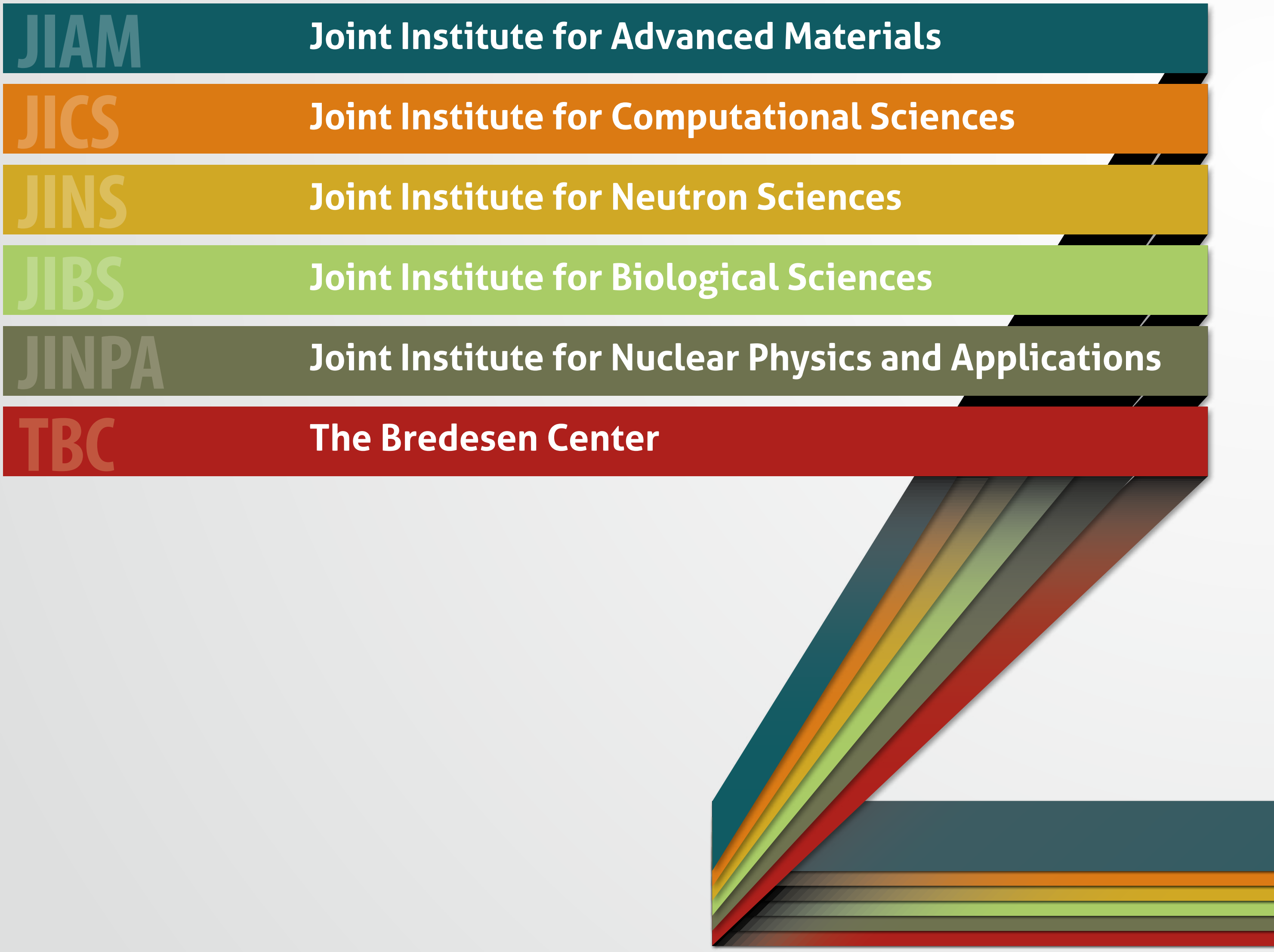
No matter if it's applied locally or abroad, taking an integrated systems approach offers new options for reliable and affordable energy, King said.

"We're looking at ways to balance the whole energy system from an economic perspective and ensure the reliability that's needed in the most cost-effective way possible," he stated. R—*Morgan McCorkle*

Sharing scientific vision

The Joint Institutes

Only 25 miles apart, ORNL and the University of Tennessee's Knoxville campus have a long relationship that has yielded many cooperative research programs, including five joint institutes and a higher education center.



JIAM Joint Institute for Advanced Materials

Growing to make materials smaller

Materials science at ORNL traces its roots to the Manhattan Project effort to develop the first nuclear weapons. More than seven decades later, ORNL's advanced materials sector has expanded far beyond its nuclear beginning.

The Joint Institute for Advanced Materials focuses recent advances in microscopy and other technologies on the need for advanced materials in applications such as computers and fuel cells. The institute's scientists are also uncovering material properties with ever-finer definition.

"Things started off at the millimeter scale, and now we're on the atomic scale," said the institute's director, George Pharr.

JIAM has three main research focuses: advanced structural materials, functional materials and devices, and soft and hybrid materials, which include composite materials, superconductors, synthetic polymers, and more. To better understand these areas, researchers explore material properties such as strength and weight beginning at the nanoscale—the level of atoms and molecules.

Gleaning details at the nanoscale can lead to breakthroughs. For instance, silicon is one of the primary materials in rechargeable lithium-ion batteries, but silicon is extremely brittle. In a lithium-ion battery, the silicon components attract and engulf lithium, which eventually causes the silicon to swell to the point of fracture and renders the battery nonfunctioning.

By studying nanoscale properties, however, JIAM researchers look to increase the strength of materials such as silicon while also reducing their size. That's because strength and size go hand-in-hand.

"The smaller the fibers are, the stronger they get," Pharr said.

As for silicon, Pharr said, researchers aren't far from reducing size and increasing strength enough to create a hardier lithium-ion battery.

JIAM researchers also investigate optical and magnetic material properties and test polymers. Applications include use in thermoelectric materials, thin films, flexible solar cells, and water purification.

"Making the materials that have these special properties—whether it be high strength and low weight, superconductivity, or semiconductors—it's all driven by advances in our understanding of materials and the way they behave," Pharr said.

While JIAM research often focuses on making materials smaller, the institute itself is getting bigger. JIAM is in the process of finishing construction of its new home on the University of Tennessee's Cherokee Farm campus in Knoxville. The building's exterior and some of the interior is due for completion in October, while the final touches are anticipated for the end of the 2015 calendar year.

"It will bring together part of the material efforts at UT under one roof and integrate them more directly with ORNL activities," Pharr said. "It's the first building on UT's satellite campus. We're the first kids on the block."

JICS Joint Institute for Computational Sciences

Real world problems, cyber solutions

The conditions simulated by researchers at the Joint Institute for Computational Sciences can be downright frightening: severe weather tearing through the Midwest, high-magnitude earthquakes rocking California, even black holes ripping stars apart and devouring them.

But the virtual havoc has a purpose. Researchers run these simulations to predict severe weather or better understand other natural phenomena.

The cyber circumstances aren't always so destructive. The computer processors at JICS also track millions of pollutant molecules, helping to uncover air pollution patterns, and investigate the biophysics of the spleen, helping us understand diseases such as anemia and malaria.

Bringing together computing resources at ORNL and UT, JICS attracts researchers from far and wide. Facilities accessible through JICS include the world's second-highest-performing supercomputer, ORNL's Titan, and four other ORNL supercomputers. JICS is also home to the National Science Foundation's National Institute for Computational Sciences, one of the five NSF supercomputing centers.

"Not only is ORNL a leader in national computing because of its DOE center, the University of Tennessee is a national leader in computing because of its NSF center," said Anthony Mezzacappa, JICS director.

For instance, meteorological scientists from the University of Oklahoma's Center for Analysis and Prediction of Storms come to ORNL for six weeks each spring with the goal of improving hazardous weather forecast predictions for the continental United States.

Based on real-time Doppler radar data, the researchers use supercomputing to run 1,000–2,000 simulations per night, five days a week. Each forecast job looks 60 hours ahead of the time that baseline weather data was obtained. Following the tests, the information is sent back to the region of concern as an early warning and planning system.

"The research can save lives," Mezzacappa said.

This year, the researchers used ORNL's Darter supercomputer. In the past, however, the work was done on Kraken, which was the most powerful computer in academia when it was first installed. Kraken was decommissioned earlier this year to make room for a new and increasingly versatile machine. That future supercomputer could play a significant part in JICS' future mission, too.

Mezzacappa said JICS is interested in bringing advanced computing to a wider scope of research, such as the social sciences. High-level computing, he said, could open doors for understanding health related issues or the origin and evolution of poverty.

"More and more science is relying on computing, and that's only going to continue," Mezzacappa said.

JINS Joint Institute for Neutron Sciences

Scattering neutrons but combining efforts

Sitting in the shadow of the Spallation Neutron Source and minutes from the High Flux Isotope Reactor, the Joint Institute for Neutron Sciences welcomes a diverse array of neutron scientists from around the world.

JINS is all about neutron scattering, whereby a beam of neutrons is fired at a sample, with some neutrons passing through and others bouncing or scattering. Researchers measure the amount of scattering to examine the dynamics and structure of materials such as proteins, liquid crystals, metals, and more.

Director Takeshi Egami sees JINS as a way to combine the work of ORNL researchers with those from other institutions. In fact, with only about 1,500 users in the United States, many of them students, neutron scattering is a small and specialized research area.

"We have a very targeted focus compared to the other joint institutes," Egami said.

Yet neutron scattering, especially when combined with computing, is a unique tool for solving difficult problems such as the nature of viscosity. Viscosity is one characteristic that differentiates a liquid from a solid, yet its origins were hidden until recently.

Egami points to water. Stick your finger slowly into a pool of water, and there is almost no resistance. But jump into the water and the resistance is substantial. If the time scale of your motion is shorter than the time scale of a water molecule, the water acts more like a solid than a liquid.

JINS researchers discovered through computer simulation that the important time scale here is the time it takes an atom to lose or gain a nearest neighbor. This is an important finding, and researchers are using neutron scattering experiments to prove it directly.

ORNL is perfectly situated for this type of research and provides the institute with world-class facilities. "SNS is by far the biggest and best accelerator-based neutron facility in the world," Egami said. HFIR, on the other hand, produces a steady beam of neutrons using a nuclear reactor, allowing researchers to conduct experiments in different modes.

JINS brings neutron researchers and graduate students alike to the ORNL campus. Researchers come for sabbatical or on fellowships, and JINS often helps fund travel expenses for graduate students. The institute also offers online open-access classes that discuss the use of neutron scattering in the study of condensed and soft matter sciences.

Still, Egami stresses, "Education is not a file transfer. It's an experience. That's why students have to come here and experience."

JIBS Joint Institute for Biological Sciences

Synthesizing new directions

The Joint Institute for Biological Sciences is yielding new understanding of plants and microbes at the cellular level, or as researchers there say, "the omics."

The omics family includes proteomics, metabolomics, genomics, and transcriptomics, which are biology branches related to proteins, metabolism, genome mapping, and gene functionality, respectively. Studying these biological foundations helps researchers further understand organism relationships from the population and community level up to the ecosystem stage—a systems biology framework.

"We do all this work at the omics level to predict higher-order outcomes," said JIBS director Gary Sayler.

For instance, researchers at JIBS examine how warming temperatures affect microbe communities in permafrost and how microbes in water bodies respond to pollutant chemicals such as mercury and chlorine. While the permafrost microbes could serve as indicators of a changing climate, the aquatic microbes may be able to aid researchers seeking to degrade or control pollutants.

JIBS is also expanding into synthetic biology, which is essentially a controlled and predictable form of genetic engineering. Armed with the knowledge gleaned from this type of research, researchers can design biological systems that carry out specific functional changes in organisms.

"It's almost like the Lego concept. If you want to make changes, you use building blocks to make those changes," Sayler said.

For example, modified yeast is being used at JIBS to convert cellulose-derived sugars directly into a hydrocarbon compatible with diesel and jet fuels. Normally, yeast fermentation yields ethanol, which can't be mixed with diesel and jet fuels. The modified yeast opens new avenues for nonethanol-based fuel in aviation, the maritime industry, and long-haul trucking.

JIBS is also exploring new directions, especially collaboration opportunities with ORNL computer scientists and SNS researchers.

Computer simulation of biological processes such as protein interaction would save researchers significant time and allow them to more easily determine molecular characteristics responsible for specific cellular roles. SNS, on the other hand, could provide vital information on the structure, vibrational nature, and molecular function of proteins.

In addition, JIBS' strength in cellulose conversion technology is encouraging researchers to think beyond bioenergy, as cellulose has potential in making biomaterials such as thermoplastics or nanomaterials.

To enhance the collaboration between the University of Tennessee and ORNL, the institute is also discussing a graduate and postdoc program similar to the Bredesen Center.

"There's an expectation and a need that the institution as it moves forward will change its character," Sayler said. "We're in a major transition."

JINPA Joint Institute for Nuclear Physics and Applications

A nod to the past in new style

When the Holifield Radioactive Ion Beam Facility closed in 2012, the joint institute created to support it steamed ahead, undeterred.

Holifield began operations in the mid-1970s with the goal of broadening collaborations within nuclear physics. Never before had a facility built at a national laboratory been intended for off-site researchers as much as for in-house scientists. This mission inspired ORNL, the University of Tennessee, and Vanderbilt University to create the Joint Institute for Heavy Ion Research.

With Holifield's closing, JIHIR moved forward with only a slight research shift and a name change, revamping its research goals under the banner of the Joint Institute for Nuclear Physics and Applications.

Now, JINPA focuses its efforts on promoting and supporting basic nuclear physics research and nuclear and radiological applications. One focus is exotic nuclei, which are inherently unstable because they are overloaded with either protons or neutrons.

Exotic nuclei are produced by stars and supernovas, and most are not found naturally on Earth. But cosmological distances don't prevent JINPA researchers from investigating them. In the laboratory, scientists use accelerators and fast digital electronics to create and study exotic nuclei to glean further understanding of natural systems.

"We don't know in detail how nature produces these elements in supernovae or stars, and to understand those details, we really need to have more precise information about nuclear reactions and the decay properties of these nuclei," said Carrol Bingham, recently retired JINPA director and University of Tennessee physics professor emeritus.

The research could prove useful to the famed "island of stability" theory in nuclear physics, which suggests that some as-yet undiscovered heavy isotopes may be relatively stable because they have balanced numbers of protons and neutrons. In addition, nuclear reactors produce radioactive isotopes, and exotic nuclei research could contribute to better reactor design.

The nuclear physics theory effort at ORNL and UT is also well represented in JINPA, enhanced by capabilities available on supercomputers such as ORNL's Titan. Last year, JINPA housed the US headquarters for both the Japan–US and France–US Theory Institute for Physics with Exotic Nuclei.

Throughout the year, JINPA hosts conferences and workshops, too. The institute has two conference rooms in its streamside building at ORNL that provide an intimate setting for nuclear physicists to meet or students to mingle. For instance, this summer JINPA provided support for the "Exotic Beam Summer School 2014."

TBC The Bredesen Center

Educating the next generation of energy scientists

The Bredesen Center is the latest collaboration between Oak Ridge National Laboratory and the University of Tennessee, providing a doctoral path to students interested in energy science.

"It's another indication of expanding the partnership to benefit both institutions," said Lee Riedinger, the center's director since it was created in September 2010.

Joining research teams at both ORNL and UT, graduate students come to the Bredesen Center from across the nation to work toward a Ph.D. in energy science and engineering. The students, drawn by ORNL's reputation in energy science, work on projects as diverse as biofuels, nuclear energy, batteries and fuel cells, transportation, and climate change.

And interest is growing.

"With 25 new Ph.D. students in August, we're over 100 Ph.D. students," Riedinger said. "It's remarkable how this program has grown so rapidly."

The August cohort is the fourth class to enjoy city life at UT in Knoxville, a more rural ambience in Oak Ridge, and, of course, the interdisciplinary research focus brought by the doctorate program. But while the center welcomes its new students, it also celebrates those it has already graduated.

"Our first two Ph.D. degrees were awarded in early May at UT. So, the pipeline is starting to flow," Riedinger said.

One of those graduates was Scott Curran, who is working in combustion research at the lab.

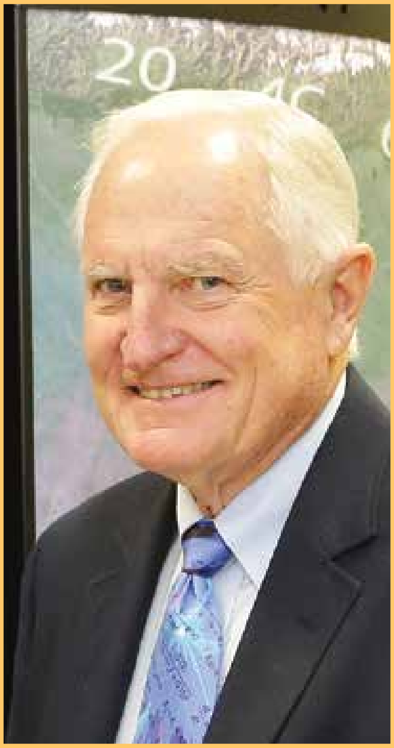
"The interdisciplinary aspect of the Bredesen program was very attractive in terms of broadening my field of knowledge and bridging my interests in mechanical and environmental engineering," Curran said. "The doctoral degree has already opened doors for discussions about gaining adjunct status with the University of Tennessee."

The program is also unique because it requires students to take credits in energy policy or entrepreneurship. Students focusing on energy policy work with a faculty member to develop a report on some aspect of energy policy. In the entrepreneurial classes, students learn about the business side of science, and the lab serves as a complement to the entrepreneurial attitude.

"These are special students. Not only do they want to get a Ph.D., but some of them want to go out and start a company," Riedinger said.

Although the Bredesen Center isn't a joint institute in the traditional sense, it has roots in the joint institute vision and reflects the efforts of a rich partnership between UT and ORNL. By nurturing the next generation of scientists, the center advances scientific research and promotes higher education.

Building on the success of the Bredesen Center, the extended Graduate Opportunities program will reach out to bring high-quality graduate students to ORNL from other universities. The program will promote a vibrant graduate student community at the lab and provide a mechanism for collaborating with key university faculty. —*Chris Samoray*



Craig Barrett

Craig Barrett worked in various capacities at Intel Corp., including president, chief executive officer, and chairman of the board. He has also applied his talents to improve science, technology, engineering, and mathematics education in the United States and economic development globally. He holds a Ph.D. in materials science from Stanford and cochairs the Lawrence Berkeley National Laboratory Advisory Board. His April 8, 2014, Wigner lecture was titled "Economic Competitiveness in the 21st Century."

We asked him about technology's role in addressing society's problems.

How can technology solve (or help solve) our most serious problems?

Technology is already doing a good job of helping to solve problems. It gives us better information, better problem definition. Any scientific problem, engineering problem you want to solve, you really need to first understand the problem and collect the data, and then go after it—whether it's pollution, whether it's mining, whether it's climate change.

What role do the national laboratories play in facing these challenges?

If you look at the problems we're facing today, the national labs play a very key role, in conjunction with their sister institutions, the Tier 1 research universities. Corporations do a lot of applied research and development, but not basic research. You've got literally tens of thousands of researchers in universities, typically working on relatively small projects and trying to move science, engineering, and technology forward. And we have the national labs, who have great capability for those researchers in the universities, plus researchers in the labs, to solve problems using the big research tools, whether they're huge supercomputers, the next generation light sources, or X-ray free electron lasers. These are facilities that no university can afford by itself.

What role do companies like Intel play?

Big corporations like IBM, Intel, Cisco, Microsoft, many others, have huge R&D budgets. That's greatly important for the economic development of that company, but that research is primarily applied research. It's turning something we already know into products: the next-generation microprocessor, router, software package. Companies are involved real time—by real time I mean from zero to a couple of years out—applying R&D to create products. But they depend on what comes out of the universities and the labs for what happens five to 10 to 15 years out.

It's that combination that has been unique to the US, the fact that the labs increasingly are working with industry. The universities historically have had a very close association with industry. You don't find that in many other countries. And, in fact, most other countries now are looking very jealously at the United States to see how to get their universities and their laboratories to work more closely with industry.

Your field is materials science. How are materials important?

I got interested in materials in the post-Sputnik era. I was old enough to have been at the university when Gagarin went up, the first human in space. One of the key things associated with the entire space program was new materials needed for space applications. There was a new push, and I was educated as a metallurgical engineer. While I was an undergraduate at Stanford, they changed the department's name to Materials Science because the government was now funding materials research, not just metals research. I think that was a great application, for materials in space, but the applications today are just across the board. Whether it's composite materials for airplanes or cars or nanomaterials that act at the atomic or molecular level—what materials can you make and what properties do they have? Semiconductors, photonics, all of these things have their roots in the basic materials that the devices are made out of.

You were Chairman of the UN Global Alliance for Information and Communication Technologies and Development. What is the potential value of bringing computers and other tech to the developing world?

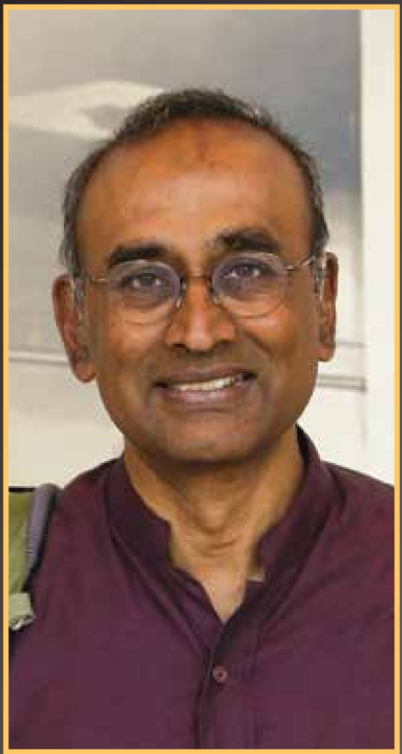
We were trying to apply technology to developing countries in a few very specific areas. One was education, another was health care, and another was good government services. And we were also looking at the impact of technology on economic growth and development. If you went to those countries and showed them by example what could be done, you got a great welcome.

You are also involved in promoting STEM education. How is this important?

STEM education is terribly important. Not everyone is going to work in one of the science, technology, engineering, and mathematics fields, but having a certain fraction of your population not only conversant in but expert in those areas allows you to have an economy that is driven off of technology and technology innovation. Everyone agrees the 21st century is the century of innovation and technology. And unless you have a portion of your workforce that's expert in the STEM areas, you're not going to effectively participate in that 21st century economy. In the United States, we do pretty well in that area today, but if you look at STEM majors, especially master's and Ph.D. candidates, they are increasingly non-US citizens. Increasingly the US is not growing its own workforce, but we're importing that workforce from foreign countries to come to our schools.

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

Coming to Oak Ridge is informative and fun. I actually deal with one of the other national labs—Lawrence Berkeley National Lab. I'm co-chair of their advisory committee, so I get to visit there three or four times a year and see what's going on. But it's great to come out and see one of the other national labs, to see the complementary work that goes on here. And then, as we were talking earlier, to see increasingly how the national labs interplay with the universities. Obviously, Lawrence Berkeley National Lab shares a campus with UC Berkeley. Here you have some schools in the Tennessee area that you interface closely with. But to see that interaction between the national lab, the university structure, and then increasingly in the economic structure. How do you spin ideas out of the labs, out of the universities, commercialize those ideas, create wealth? We're making this investment in the US in basic research, not just because we all love basic research, but ultimately it should benefit society. Ⓡ



Venkatraman Ramakrishnan

Venkatraman Ramakrishnan was awarded the 2009 Nobel Prize in Chemistry for studies of the structure and function of the ribosome. He works at the United Kingdom's Medical Research Council Laboratory of Molecular Biology in Cambridge, England. Other positions included a 15-month stint at ORNL in the early 1980s. His July 28, 2014, Wigner lecture was titled "How Antibiotics Block the Ribosome, the Cell's Protein Factory."

We asked him how we will benefit from an improved understanding of the ribosome.

You won the 2009 Nobel Prize in Chemistry for your work bringing to light the workings of the ribosome. Why is this understanding important?

Many people think that the ribosome is perhaps the single most important molecule in the cell. Almost every molecule in the cell is either made by the ribosome or it's made by enzymes which themselves are made by the ribosome. The ribosome does this by taking information that's present in our genes and translating that information into a protein. And there are thousands of proteins; there are thousands of genes. Each gene specifies a particular protein, and it's the ribosome that makes that particular protein corresponding to the gene.

There are thousands of these in every cell, and they carry out all the thousands of functions in the cell, as well as give cells structure and so on. In a sense the ribosome is fundamental to biology, to all life forms. So studying it is a fundamental problem in biology. It's also a problem that has to do with the origin of life. Many people believe that life began as an RNA world and that the ribosome itself is made of RNA and came out of that RNA world and helped to transform life into the protein–RNA–DNA world that we know today.

How can an improved understanding of the ribosome lead to improved health care?

The most obvious way is that many antibiotics work by blocking the bacterial ribosome, which is slightly different from ours. By doing so, it allows us to kill bacteria without killing our own cells. Some of these have been used for the last 50 years, but resistance is developing to these antibiotics. By knowing the structure of the ribosome and knowing how antibiotics bind to them, it is possible to design better compounds that might overcome resistance.

There are also other ramifications. For instance, you could use the ribosome to make new kinds of proteins. People have used the structures to try to change the ribosome to make proteins that aren't possible to make in nature, which might have interesting properties or useful properties. So that's another example.

There are many viruses that work by preventing the ribosome from doing its normal thing, and getting it to just make viral proteins. By understanding how these viruses interact with the ribosome, you might be able to help try to prevent some of these viral infections.

Then, often the way that ribosomes work and how they're regulated is different in cells—for instance, cancer cells or possibly in other diseases—and so that's again a way to try to approach our understanding of these diseases. So although the ribosome is fundamental, and we're really interested in it for fundamental reasons, it does have a lot of potential spinoffs in terms of future applications.

Your work has made use of advanced imaging techniques such as neutron and X-ray scattering. How are high-tech imaging techniques important to biology specifically and science in general?

There are now three really big imaging techniques that have come up in the last few years. At the cellular level, people have come up with optical microscopy techniques, which are pushing the normal resolution limits of light. At the other end, you have X-ray crystallography, which can produce very detailed structures of molecules, and you also have electron microscopy, which until about a year or two ago couldn't produce sufficiently high resolution for biological molecules. All of these are combining to allow us to look at a whole spectrum from individual molecules all the way to an entire cell and how a cell is organized in molecular terms. It's the first time in history that we've been able to try to start bridging that gap between molecular structure, which you can see by X-ray crystallography, to cells, which you could see under a light microscopy, but you couldn't see enough detail to see where the molecules were inside the cell.

What is the most pressing question currently for you and others in your field?

I'm a structural biologist, and I think what I would like to understand is how basic processes work, like DNA replication, which is what has to happen when cells have to divide. You have to make two copies of a DNA when there was only one. Or transcription, which is when DNA is copied into RNA so that it can be made into a protein, or translation, where the ribosome looks at an RNA molecule and makes a protein. All of these involve very large molecular machines. And at the other end when RNA or proteins happen to be degraded, that's also done by very large complexes. All these fundamental processes in the cell, or many of them, are done by these large machines.

Why was it important to participate in the Wigner Lecture Series?

It was an honor, given the stature of the past speakers. But really the reason was I did work in Oak Ridge for about 15 months, and I wanted to come back and visit. When I was in Oak Ridge, it was slightly unsatisfactory, because I was a biologist working in a physics division, and there was a cultural problem. And I actually told the person who invited me that, and he said, well, we would like you to come back and talk about these issues so that we can get some feedback on how to integrate large facilities with what biologists actually want. I thought this was an interesting challenge. Ⓡ

ORNL study reveals new characteristics of complex oxide surfaces

A novel combination of microscopy and data processing has given researchers at the Department of Energy's Oak Ridge National Laboratory an unprecedented look at the surface of a material known for its unusual physical and electrochemical properties.

The research team led by ORNL's Zheng Gai examined how oxygen affects the surface of a perovskite manganite, a complex material that exhibits dramatic magnetic and electronic behavior. The new avenue to understand surface behavior could benefit researchers who are interested in using a wide range of correlated oxide materials for applications such as solid fuel cells or oxygen sensors.

"Surface properties are key for any sensitive application, because the surface controls the interaction with the outside world," said coauthor Art Baddorf.

The team's results, published in *Nature Communications*, underscore why the materials are called "strongly correlated." Because the chemical and physical functionalities are coupled, any minor change can influence the entire system.

"It's like the material has many knobs, and if you turn one, all the properties change," Gai said. "You turn a different knob and the whole thing changes again. It turns out the surface is another knob—you can use it to change the properties."

The researchers used high-resolution scanning tunneling microscopy to generate images of the manganite surface—down to the level of 30 picometers. A picometer is one trillionth of a meter. They then processed the imaging data to determine the position of each atom and calculate the angles between the atoms.

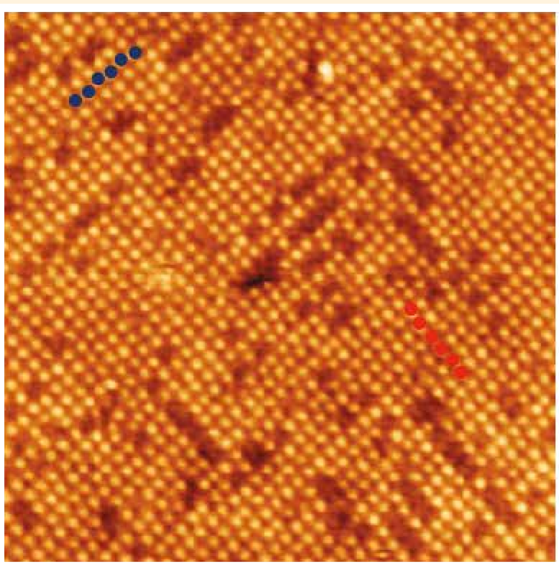
"Knowing where the atoms are positioned shows how they are interacting," Baddorf said.

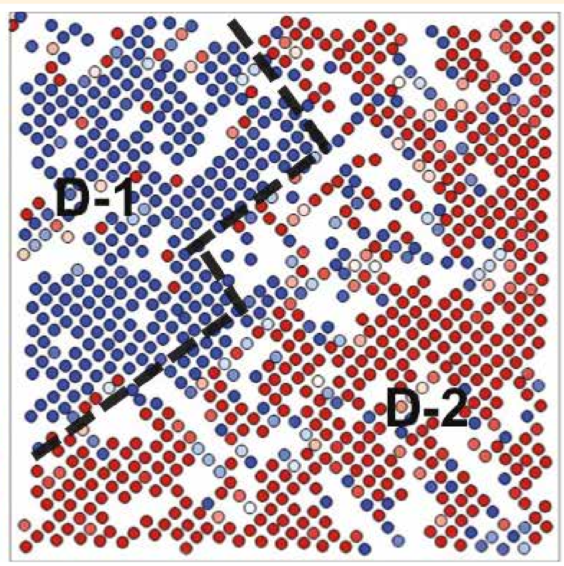
The resulting "distortion maps" brought into view structural areas called domains that were not easily identified in the raw images. The maps clearly showed how the presence of oxygen atoms forced the atoms into a checkerboard pattern known as a Jahn-Teller distortion. Gai says the team's study is the first time the phenomenon has been observed on a material's surface.

"The oxygen totally changes the surface energy," Gai said. "Once you introduce oxygen, the electrons don't like to form a straight line; they zigzag to get to a lower energy state. This distortion is a very common concept in bulk materials, but nobody has been able to show this effect on the surface before."

The study is published as "Chemically induced Jahn–Teller ordering on manganite surfaces." Coauthors are ORNL's Wenzhi Lin, Paul Snijders, Thomas Ward, J. Shen, Stephen Jesse, Sergei Kalinin, and Arthur Baddorf; University of Nebraska's J.D. Burton and Evgeny Tsymbal; and IHI Corporation's K. Fuchigami.

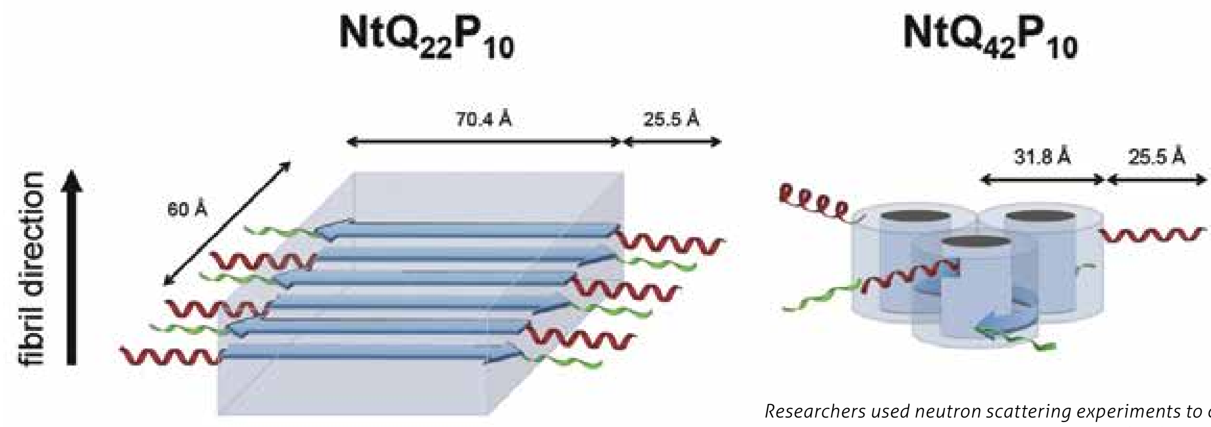
This research was conducted in part at the Center for Nanophase Materials Sciences, a DOE Office of Science user facility. DOE's Office of Science supported the research. Work at the University of Nebraska-Lincoln was supported by the National Science Foundation. Ⓡ





An Oak Ridge National Laboratory study combined microscopy and data processing to provide an unprecedented look at the surface of a manganite material known for its unusual properties. The resulting "distortion maps" (right) brought into view structural areas called domains that were not easily identified in the raw images (left).

ORNL, UTGSM study compares structures of Huntington's disease protein



Researchers used neutron scattering experiments to clarify structural differences between the normal (left) and pathological (right) forms of huntingtin protein aggregates. The pathological form of this protein is implicated in Huntington's disease.

Neutron scattering research at the Department of Energy's Oak Ridge National Laboratory has revealed clear structural differences in the normal and pathological forms of a protein involved in Huntington's disease.

Huntington's disease, an incurable neurodegenerative disorder, starts as a genetic mutation that leads to an overabundance of "huntingtin" protein fragments, which form clumps in the brain.

Valerie Berthelier of the University of Tennessee Graduate School of Medicine, who co-led the study published in Biophysical Journal with ORNL's Chris Stanley, said the goal was to establish a baseline understanding of huntingtin's structure in order to eventually determine the true structural basis of Huntington's disease.

"This is a very first step—the hope is that we do this basic research to shed light on the structures of the protein," Berthelier said. "If we can start identifying any of these structures as toxic or potentially toxic, and then think about how drugs could interact with them, then we might be getting to the point of rationally designing therapeutics that would target those specific structures."

The researchers conducted a side-by-side study of model protein systems in solution using a time-resolved small-angle neutron scattering technique at ORNL's High Flux Isotope Reactor. The use of neutrons, a non-damaging but highly penetrating particle, allowed the team to study the biological materials over time without degrading the samples' structural integrity.

"We compared the normal and disease versions of the protein to see how they change over time," Stanley said. "You can see there's a discrepancy all the way from the early stages to the end-state fibrils."

The study's results showed key differences in the ways mutant and normal huntingtin proteins take shape. The disease protein, for instance, initially forms aggregates of one to two peptides, whereas the normal version makes bigger aggregates, gathering seven or eight peptides together.

These data on the very early stages of protein aggregate formation support a growing focus of the research in the amyloid field. Amyloid disorders, such as Parkinson's, Alzheimer's, and Huntington's, all involve protein aggregation phenomena leading to a disease.

"There is no strong correlation between neuronal cell loss and the amount of protein aggregates found in the brain," Stanley said. "You could have a case with a lot of aggregates but minimal symptoms—and you can find the converse. Researchers think there must be something happening at the earliest stage that's giving rise to toxicity."

Stanley says the team hopes to continue its research to obtain higher-resolution structural data and refine their understanding of the huntingtin protein.

"We'd like to use this small-angle neutron scattering technique in combination with others to get a better idea for how these early structures are forming and also ask the question—are they toxic or not?" Stanley said.

The research is published as "Investigating the Structural Impact of the Glutamine Repeat in Huntingtin Assembly." Coauthors are Helen McWilliams-Koeppen, Erica Rowe, and Tatiana Perevozchikova.

HFIR is a DOE Office of Science user facility. ORNL's Center for Structural Molecular Biology is also supported by DOE's Office of Science. The research on Huntington's Disease was supported in part by the Physicians' Medical Education and Research Foundation at UT Medical Center and by the National Institutes of Health.

‘Engine of explosion’ discovered at OLCF now observed in nearby supernova remnant

Data gathered with high-energy X-ray telescope support the SASI model—a decade later

Back in 2003, researchers using the Oak Ridge Leadership Computing Facility’s first supercomputer, Phoenix, started out with a bang. Astrophysicists studying core-collapse supernovae—dying massive stars that violently explode after running out of fuel—asked themselves what mechanism triggers the explosion and fusion chain reaction that releases all the elements found in the universe, including those that make up the matter around us?

Before Phoenix, one-dimensional supernovae models simulated a shock wave that pushes stellar material outward, but ultimately, succumbed to gravity. The simulations did not predict that stellar material would push beyond the shock wave; instead, infalling matter from the fringes of the expanding star tamped the anticipated explosion. Yet, humans have recorded supernovae explosions throughout history.

“There have been a lot of supernovae observations,” said the University of Tennessee–Knoxville’s Tony Mezzacappa. “But these observations can’t really provide information on the engine of explosion because you need to observe what is emitted from deep within the supernova, such as gravitational waves or neutrinos. It’s hard to do this from Earth.”

Then simulations on Phoenix offered a solution: the SASI, or standing accretion shock instability, a sloshing of stellar material that destabilizes the expanding shock and helps lead to an explosion.

The SASI provided a logical answer supported by other validated physics models, but it was still theoretical because it had only been demonstrated computationally.

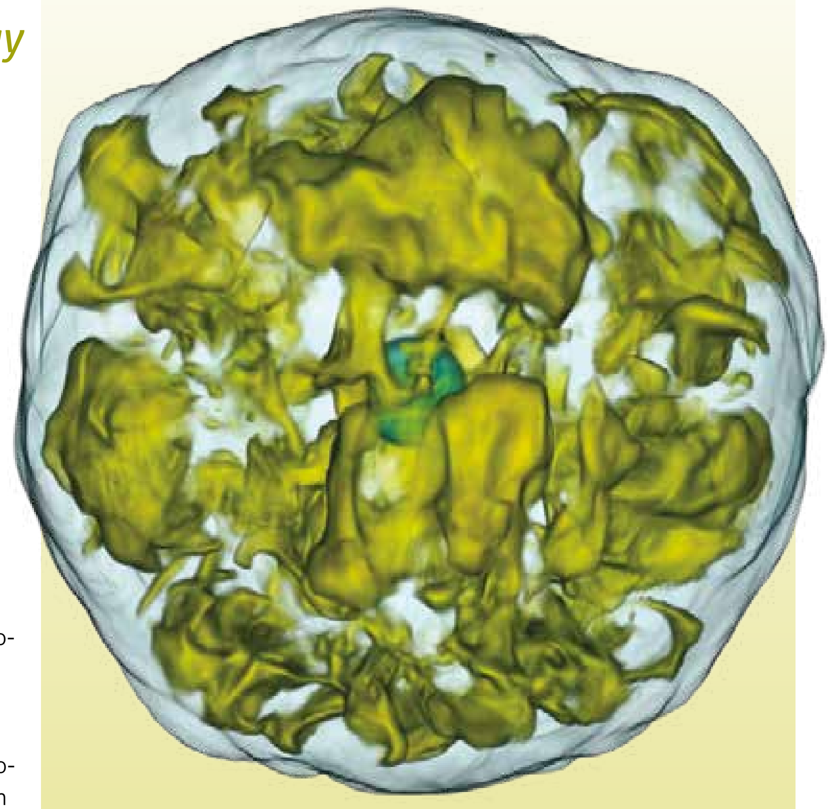
Now, more than a decade later, researchers mapping radiation signatures from the Cassiopeia A supernova with NASA’s NuSTAR high-energy X-ray telescope array have published observational evidence that supports the SASI model.

“What they’re seeing are X-rays that come from the radioactive decay of titanium-44 in Cas A,” Mezzacappa said.

Because Cassiopeia A is 11,000 light-years away (right next door, relatively speaking), NuSTAR is capable of detecting Ti-44 located deep in the supernova ejecta. Mapping the radiative signature of this titanium isotope provides information on the supernova’s engine of explosion.

“The distribution of titanium is what suggests that the supernova ‘sloshes’ before it explodes, like the SASI predicts,” Mezzacappa said.

This is a rare example of simulation predicting a physical phenomenon before it is observed experimentally.



The entropy of the inner 250 kilometers of a 15 solar-mass star during a 3D simulation of a core-collapse supernova using the CHIMERA code. Large-scale distortion of the supernova shock can be seen, along with smaller-scale convection. Visualization by Mike Matheson.

“Usually it’s the other way around. You observe something experimentally, then try to model it,” said the OLCF’s Bronson Messer. “The SASI was discovered computationally and has now been confirmed observationally.”

The authors of the Nature letter that discusses the NuSTAR results cite Mezzacappa’s 2003 paper introducing the SASI in *The Astrophysical Journal*, which was coauthored by John Blondin and Christine DeMarino, as a likely model to describe the Ti-44 distribution.

Despite observational support for the SASI, researchers are uncertain whether it is entirely responsible for triggering a supernova explosion or if it is just part of the explanation. To further explore the model, Mezzacappa’s team, including the Innovative and Novel Computational Impact on Theory and Experiment project’s principal investigator, Eric Lentz, are taking supernovae simulations to the next level on the OLCF’s 27-petaflop Titan supercomputer located at ORNL. Ⓡ—*Katie Elyce Jones* www.ornl.gov/ornlreview

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

ORNL *Review*

Editor—Leo Williams
Writers—Katie Elyce Jones, Morgan McCorkle,
Jim Pearce, Chris Samoray, Leo Williams
Designer—LeJean Hardin
Editors—Wendy Hames, Priscilla Henson
Stock images—iStockphoto™

Phone: (+1) 865.574.4160
Fax: (+1) 865.574.0595
E-mail: ornlreview@ornl.gov
Internet: www.ornl.gov/ornlreview

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

ISSN 0048-1262

OAK RIDGE
National Laboratory

U.S. DEPARTMENT OF
ENERGY