OAK RIDGE NATIONAL LABORATORY

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REVIEW

• MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY •

DELIVERING THE SCIENCE

Oak Ridge National Laboratory

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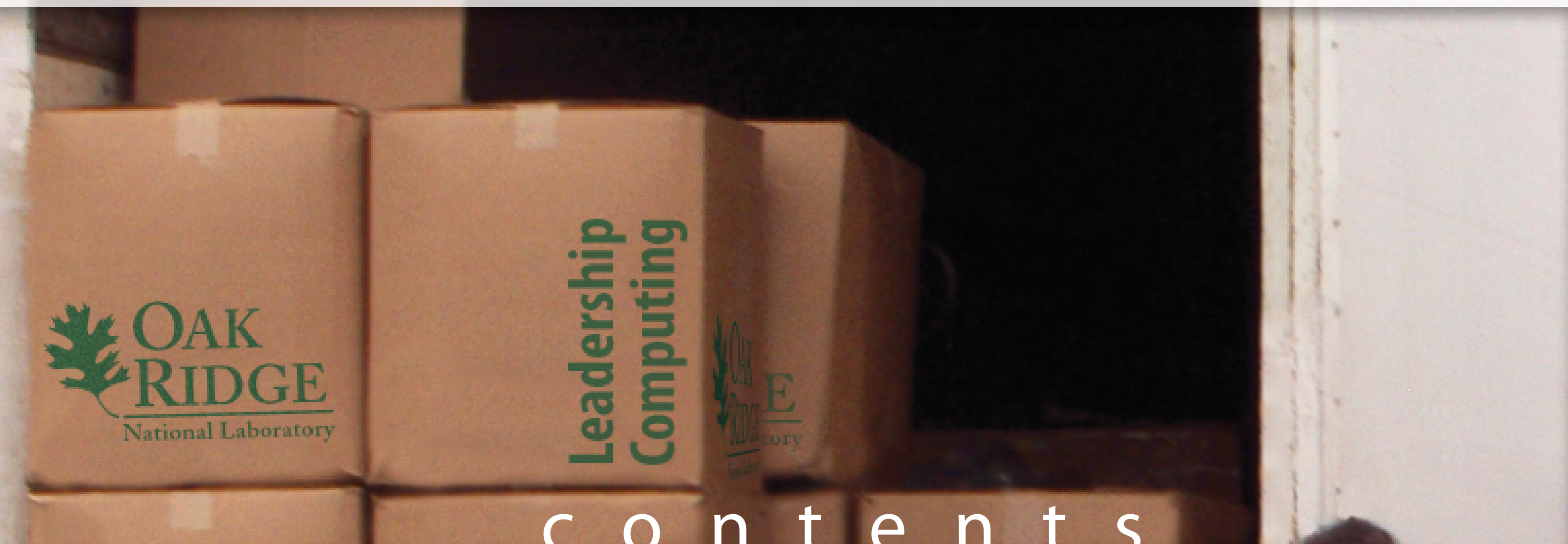

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TAKING DOWN THE FENCE

One of the most important milestones in the recent history of Oak Ridge Laboratory was the simple act of taking down a fence. Since the Laboratory's inception in 1942, the ORNL campus had been defined by miles of imposing chain link fence, interspersed at strategic points with turnstiles and guards that provided rigidly controlled access to the grounds and facilities. Not surprisingly, six decades of working in such a closed environment gradually shaped the Laboratory's culture. As the first and last thing they saw each day, the inescapable presence of the fence produced an institutional mindset among both managers and research staff that turned their focus inward, leaving many unaware and often indifferent to the opportunity for collaborations with the scientific community on the other side.

Over time, the fence had an impact—perhaps subliminal but not necessarily unintended—on a variety of ORNL operational policies that extended well beyond the security of human and scientific assets. An institution that operated behind a fence built to keep people out was not instinctively open to sharing the Laboratory's talents and technologies. Thus, while ORNL staff did a commendable job of delivering the research mission for their Department of Energy customer, the Laboratory as a whole did not fully leverage its magnificent range of research facilities by making these unique assets available to large numbers of researchers from universities, industry and other national laboratories.

Though not without controversy, UT-Battelle's decision in 2001 to take down the fence was a symbolic act designed to underscore a desire for expanded research partnerships as well as renewed access, both literally and figuratively, to ORNL's world-class capabilities. This issue of the *Review* is dedicated to the programs in a portion of the Laboratory's user facilities, where a rapidly increasing number of visiting researchers are taking advantage of what can accurately be described as a fundamental cultural change in Oak Ridge. Today, thousands of visiting researchers from around the world are spending anywhere from two days to two months at ORNL's unmatched suite of user facilities. The number is expected to increase sharply as new user facilities such as the Spallation Neutron Source complete installation of additional experimental instruments.

Indeed, for some research facilities, the growth of ORNL's user program has greatly exceeded expectations. The annual number of users at the National Center for Computational Sciences has grown from 578 to 1,030 in the span of only three years. Even more dramatic is the increase in the number of users at the High Flux Isotope Reactor, which has skyrocketed from 42 to 359 during the same period. In both instances, the number of applications for research at ORNL has expanded to the point that it now surpasses the available slots.

A change of such magnitude in ORNL's user program did not occur by chance. Guided by the Department of Energy's desire to maximize the impact of the agency's scientific investments, ORNL has undertaken a long-term commitment not only to expand the Laboratory's user program, but to do so in a way that provides visiting researchers a level and quality of support services equal to those enjoyed by resident staff.

Meanwhile, the fence, once an enduring symbol of the Laboratory, is today only a reminder of the challenge and potential that lie ahead for Oak Ridge National Laboratory.

Billy Stair

Billy Stair
Director, Communications and External Relations

News & Notes

Making ethanol in Tennessee

Dozens of federal and state officials attended the dedication of a state-of-the-art refinery that represents a new state partnership with the Department of Energy's bioenergy research program.

Funded by the state of Tennessee and located about 40 miles from Oak Ridge, the refinery is designed to demonstrate the commercial feasibility of a biofuel manufacturing process developed by DuPont Danisco Cellulosic Ethanol, a joint venture of DuPont and the Genecor division of Danisco.

Managed by the University of Tennessee, the refinery includes a process-development laboratory that will be used to scale-up production of new forms of cellulosic ethanol developed at ORNL's Bioenergy Sciences Center, operated for the Department of Energy. The unique pairing of a federal research facility with a state biorefinery will enable researchers to validate new products and processes as they develop the next generation of biofuels.

The refinery will generate up to 250,000 gallons of ethanol annually. Initially, the refinery will use corncobs and corn fiber as the raw materials for ethanol production. "DuPont Danisco has tested their technology with these materials in the laboratory and in smaller-scale units," says Brian Davison, ORNL's *Chief Scientist* for Systems Biology and Biotechnology. Davison says plans include testing switchgrass conversion technologies in the plant's process development unit. Once the corn-based demonstration project is completed, Dupont Danisco will move the switchgrass-based processes to the larger plant in 2011.

The Tennessee refinery is the first cellulosic ethanol demonstration plant that integrates all the components of research, biomass, and production. In addition to the refinery, the state's bioenergy project incorporated cellulosic research at ORNL and state subsidies for Tennessee farmers to plant switchgrass, a perennial crop that can be grown on marginal land with little fertilizer and water. State officials expect the pilot refinery will soon leverage investments of a larger, full-scale biorefinery in Tennessee.

Leveraging the assets

On January 25, Tennessee Governor Phil Bredesen signed into law legislation that will create a new graduate program in energy sciences at the University of Tennessee (UT) and Oak Ridge National Laboratory. The new program aims to add approximately 200 graduate faculty and 400 graduate students to the UT Knoxville campus. The additional faculty will comprise ORNL researchers who will be granted joint faculty status at the university. UT and ORNL currently fund about 50 joint staff who split their time between teaching at the university and research at the Laboratory.

Resembling the current partnership between Lawrence Berkeley National Laboratory and the University of California at Berkeley, Tennessee's new multidisciplinary program in energy sciences will feature a $50,000 package of stipends and tuition designed to attract some of the nation's top graduate students. The majority of the students pursuing doctoral degrees will spend two years taking classes at UT and three years conducting research at ORNL.

By seeking to increase the number of science graduates in Tennessee, the new graduate program represents the latest effort by Governor Bredesen to leverage the assets of a national laboratory and the state's land grant university for economic development. Last fall the state provided $62 million to create the Solar Institute, another joint program housed at the university and the Laboratory that will assist Tennessee's rapidly growing solar industry. On January 21, Confluence Solar announced a $200 million investment in the town of Clinton, about 10 miles from ORNL. In a press conference at the State Capitol, Confluence emphasized a desire to be located near the Laboratory's state-of-the-art research assets.

Since 2000 the state of Tennessee has provided approximately $215 million, including the construction of three joint institutes on the ORNL campus, to leverage the assets of Oak Ridge National Laboratory's research programs.

Jaguar supercomputer claws its way to the top

ORNL's Jaguar supercomputer is officially the fastest computer in the world. Capable of 2.3 petaflops, or 2,300 trillion calculations per second, Jaguar is now the research community's most powerful computational tool for exploring solutions to a variety of grand scientific challenges such as climate, alternative fuels and energy storage. The Oak Ridge machine received the designation at the SC09 international supercomputing conference in Portland, Oregon.

"Our computational center works closely with the science teams to help them use a computer system of this size and capability," said James Hack, director of the National Center for Computational Sciences, which houses Jaguar in the Oak Ridge Leadership Computing Facility.

The Oak Ridge computing complex is home to two of the world's three most powerful machines. In addition to DOE's Jaguar, a partnership between the University of Tennessee and ORNL operates another petascale Cray XT5 system for the National Science Foundation known as Kraken, which was ranked 3rd on the Top500 list with a speed of 831.7 teraflops. A third machine of comparable size will be installed this year for the National Oceanic and Atmospheric Administration.

"The purpose of these machines is to enable the scientific community to tackle problems of such complexity that they demand a well-tuned combination of the best hardware, optimized software and a community of researchers dedicated to revealing new phenomena through modeling and simulations," said ORNL Director Thom Mason. "Oak Ridge is proud to help the Department of Energy address some of the world's most daunting scientific challenges."

The early petascale results indicate that Jaguar will continue to accelerate the Department of Energy's mission of breakthrough science. With increased computational capability, the scientific research community is able to obtain results faster, understand better the complexities involved and provide critical information to policy-makers.

DELIVERING THE SCIENCE

The world's scientific community is flocking to ORNL's modern research facilities.

For nearly seven decades, Oak Ridge National Laboratory has operated some of the world's premiere scientific research facilities. During the Laboratory's early years, these facilities were shrouded in the secrecy of the Manhattan project and closed to outside researchers. Over the last half century, as the government's mission and research agenda have evolved, ORNL has opened its doors, both literally and figuratively, to the world's research community. Today, Oak Ridge enjoys a reputation for helping deliver science by making available its state-of-the-art facilities for use by guest researchers from around the world.

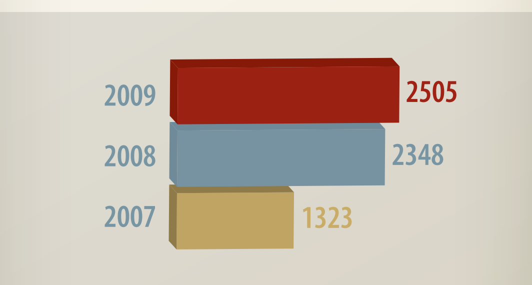
ORNL is home to a number of highly sophisticated research laboratories, known in the vernacular as "user facilities." Containing unique equipment and capabilities too large or too expensive for the academic community or the private sector, these research user facilities are designed to serve ORNL research staff, as well as leading scientists from universities, industries and other government laboratories.

In 2009 ORNL hosted some 2,500 users from approximately 550 different organizations. This record number of users reflects a decade-long expansion of the Laboratory's user program, a trend that accelerated with the addition of the Spallation Neutron Source, the Leadership Computing Facility and the Center for Nanophase Materials Sciences to ORNL's portfolio of user facilities. The opening over the last five years of these new facilities, all of which are among the world's most advanced in their respective fields, has greatly expanded opportunities for technological breakthroughs in dozens of scientific disciplines, including biomedicine, materials, climate change and alternative energy.

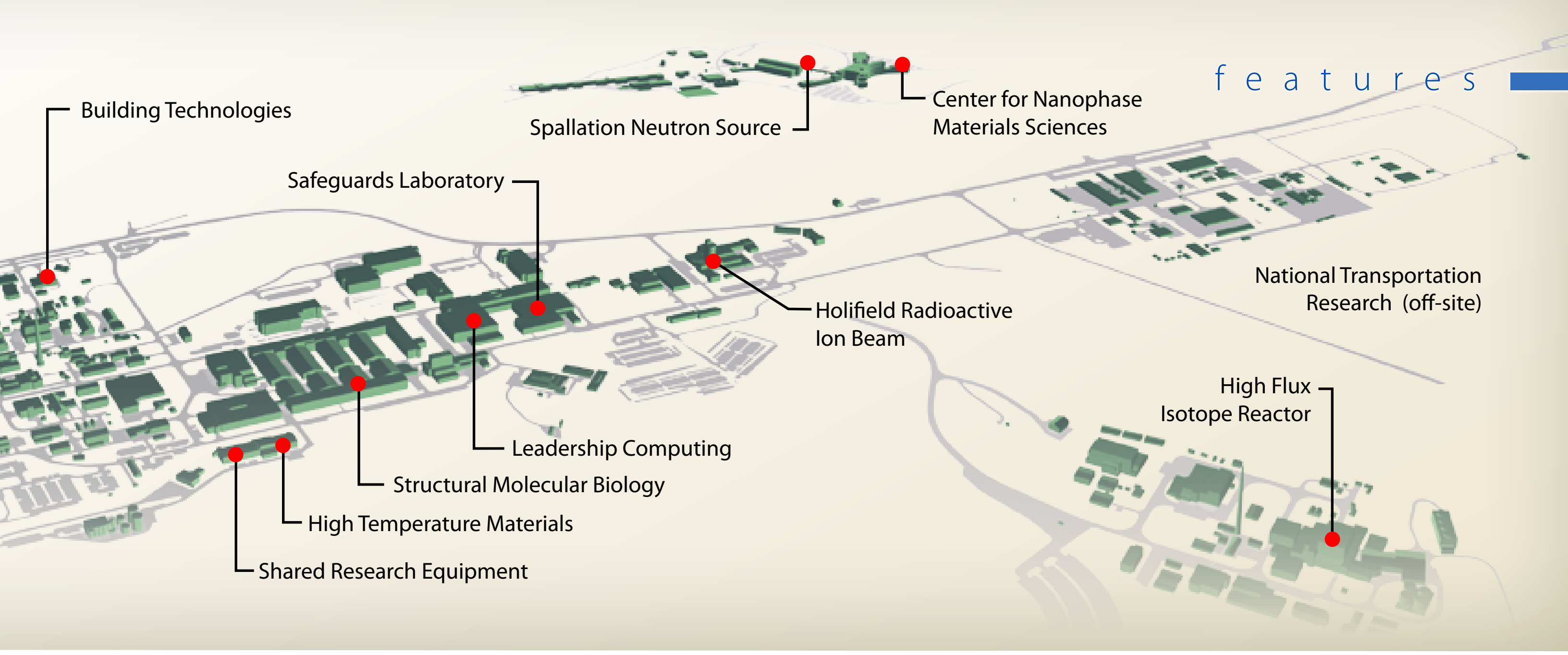
"The biggest change—and the biggest challenge in our user program over the last several years—has been the rapid addition of new facilities," said Bill Painter, Manager of ORNL's User Facilities Program Office. "For years, the number of facilities open to users was fairly static. However, with the addition of major new facilities, we are experiencing a large increase in requests by scientists wishing to conduct experiments. It's a good kind of problem, but some of ORNL's user facilities have substantially more requests than they can accommodate."

Fortunately, the capacity of some user facilities is expanding, as well. "The Spallation Neutron Source will have 17 beam lines available this year, up from 10 a year ago," Painter said. "They are accepting more research proposals and anticipating a record number of users." Similarly, the National Center for Computational Sciences, which boasts the world's most powerful supercomputer and is home to the Leadership Computing

Number of Users: ORNL



Demand for access to ORNL's user facilities is steadily rising. Some facilities now have more requests than they can accommodate.



Facility, is expanding its capacity and will soon host three petascale computers dedicated to open scientific research—the largest concentration by far of scientific computing power on earth.

A unique collection

ORNL's current emphasis on providing broad access to research facilities had its origin in 1983, when the Department of Energy adopted the official designation of "user facilities." Broadly defined, these facilities comprised unique collections of research equipment and expertise unavailable to most industrial or academic research programs. Impressed by the popularity of the user facilities, DOE gradually expanded the program by funding facilities that focused upon particular needs of the American economy or the scientific community. ORNL's High Temperature Materials Laboratory, for example, was constructed in the mid-1980s to support the competitiveness of the U.S. transportation industry. More recently, the $1.4 billion Spallation Neutron Source was designated by legislation as a user facility to provide unmatched materials research capabilities.

"By officially designating user facilities, the Department of Energy made it clear that the research capabilities of 'big science' projects would be made available to government laboratories, universities and private industry," Painter said. ORNL hosts hundreds of users in each of these categories. At facilities like the Spallation Neutron Source and the Center for Nanophase Materials Sciences, user agreements are primarily with universities and other laboratories. A larger percentage of users from industry and government agencies gravitate toward the Laboratory's "applied science" facilities, such as the High Temperature Materials Laboratory.

ORNL is careful to not permit the unparalleled technological resources of the Laboratory's user facilities to be placed in competition with private industry. Indeed, some user facilities exist precisely because there is no comparable research capability in the private sector. An example is ORNL's Building Technologies Research and Integration Center. In an era when most building material manufacturers have abandoned research and development programs, ORNL offers a state-of-the-art climate simulation laboratory that can be used to test building components under a range of weather conditions. The unique simulation capability of the center enables manufacturers to increase the efficiency of their products while decreasing the cost of production.

Similarly, ORNL's High Temperature Materials Laboratory works with the trucking industry to apply the facility's materials characterization capabilities to tasks such as making key components lighter and more durable, converting exhaust heat to electricity and removing pollutants from truck exhaust.

A competitive process

Like most programs at ORNL, access to the Laboratory's user facilities is based upon competitive proposals. An organization wishing to conduct research must submit a proposal detailing both purpose and process. Proposals are reviewed and evaluated on the basis of scientific merit, suitability for the user facility and the proposal's alignment with the Department of Energy's research objectives. Researchers whose proposals are selected are awarded use of ORNL's resources for a specified time to generate and analyze their data. If the user agrees to publish any findings in open literature, the research is free of cost.

ORNL's user program is predicated on the belief that there is a lasting benefit to both the nation and the scientific community in the sharing of research. Most user agreements contain a commitment by the researchers to publish or share the results of their work at ORNL. The philosophy of openness enables other scientists to build on the knowledge gained in these studies and to apply the findings of others to their own research projects. There are exceptions to this policy. On occasion, an industrial customer will apply to conduct proprietary research at an ORNL user facility. In such cases, the user pays the full cost of conducting the research. While some user projects involve important proprietary research, more than 90 percent of the projects conducted at ORNL user facilities contain findings that are shared with the broader scientific community.

Looking ahead, ORNL is seeking to expand even further what is already one the world's leading user programs. A unique collection of scientific facilities is bringing together an equally unique collection of talent and creativity, all inspired by the possibility of discovery. Judging by the growing number of researchers wishing to take advantage of this opportunity, ORNL's user program is just beginning to realize its potential. Ⓡ

HTML provides the user community with analytical capabilities critical to developing safe and efficient vehicles.

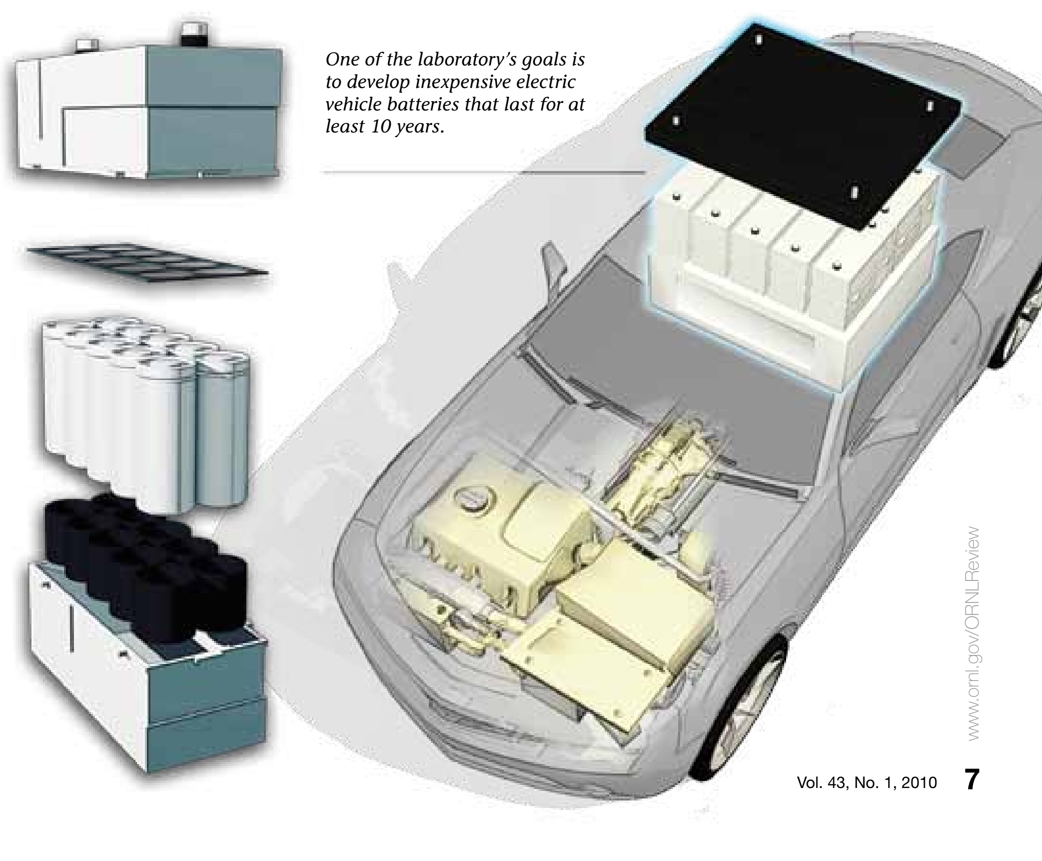
HIGH TEMPERATURE, HIGH STAKES

The High Temperature Materials Laboratory has expanded into a leading center for transportation innovation

Conceived in 1973 in the wake of the first Arab oil embargo, Oak Ridge National Laboratory's High Temperature Materials Laboratory (HTML) was originally envisioned as a place where the capabilities of high-temperature materials research programs from industry, academia and government laboratories would be brought together to develop structural ceramic materials for use in highly efficient automotive gas turbines and heavy-duty diesel engines. The facility's initial research efforts resulted in several successful collaborations with engine manufacturers, including the development of ceramic turbine components that could withstand the rigors of operating for hundreds of thousands of miles under extreme conditions.

As the price of oil moderated in the early 1980s and the urgency of the energy crisis diminished, HTML director Edgar Lara-Curzio recalls that the general level of interest in high-temperature ceramics also began to wane. "Gradually, HTML's mission evolved from simply studying high-temperature materials to analyzing a greater variety of materials for transportation technologies," he says. This broadened focus has enabled HTML scientists, as well as the users that take advantage of the facilities' unique equipment, to investigate materials-related issues across an array of transportation technologies, including advanced batteries for plug-in electric and hybrid electric vehicles; lighter, stronger vehicle components; and the recovery of waste heat using thermoelectric materials.

The expansion of HTML's research mission proved a boon to users. A large fraction of the facility's users are from industry, while the rest come from universities and other national laboratories. Lara-Curzio is quick to note that HTML continues its close relationships with engine manufacturers who have been interested in structural ceramics for gas turbines and diesel engines since the user facility was first established. "We are working with Cummins on diesel particulate filters and with Caterpillar, General Motors, Ford and others on a range of materials for transportation-related projects."



One of the laboratory's goals is to develop inexpensive electric vehicle batteries that last for at least 10 years.

HTML's user program accommodates both nonproprietary and proprietary research—the main difference being that the former is provided free of charge if users submit the results of their research for publication within six months. Proprietary users pay for the cost of conducting their research but are not required to share their results.

Lara-Curzio maintains that user programs at the national laboratories play an important role in enabling the development and implementation of new technologies by providing users with access to capabilities that are unavailable to universities or commercial research facilities. HTML staff members possess specialized skills in the area of materials characterization. In addition to their involvement in the HTML user program, most conduct research on a variety of materials used for power generation and the distribution, storage and use of energy. The ability of industrial and academic users to share these capabilities benefits both parties. "This is our goal and the role we have played from the beginning," Lara-Curzio says.

A better battery

One of HTML's top priorities in the past year was the development of tools that can be used with microscopes and X-ray and neutron diffractometers to examine the internal structure of batteries at the atomic level as they charge and discharge. Understanding these processes will enable HTML researchers to work with manufacturers to produce batteries that are longer lasting, safer and more efficient. "In one of our projects, we are working with Motorola to study the causes of 'thermal runaway' in lithium-ion batteries, a condition that causes batteries to overheat and catch fire," Lara-Curzio explains. "We are also seeking ways to enable batteries to store more energy so, for example, an electric vehicle could have a range of hundreds rather than dozens of miles between charges. The challenge is to store as much energy in as little volume with as little weight as possible."

HTML researchers currently are working on increasing the power density of batteries, a process that requires developing batteries that can provide a lot of "juice" quickly and recharge in a relatively short time. Batteries with high power density would enable an electric vehicle to accelerate and merge smoothly into highway traffic or to pass a slower vehicle comfortably. When the vehicle is parked at a charging station, the battery could be charged in a time roughly comparable to the time it takes to fill a car with gasoline.

Lara-Curzio notes that, even with all of the other technical challenges, one of the biggest hurdles on the path to a better battery is keeping the final product affordable. "A large fraction of the cost of electric cars that are available today—or that will be available in the near future—is batteries," he says. "We want inexpensive batteries to last for at least 10 years. Nobody wants to go to the car dealer every three years to replace $10,000 worth of batteries."

Lightweight materials

The greater use of lightweight materials in vehicles is one of the most straightforward ways of increasing fuel efficiency. HTML researchers are working with several industrial partners to reduce the weight of vehicles without sacrificing safety. One of the biggest success stories to come out of HTML in recent years is Metalsa, a Virginia-based truck component manufacturer that sought to reduce the weight of the truck siderails the company provides to more than 50 percent of the U.S. truck market.

Using instruments at HTML and ORNL's High Flux Isotope Reactor, Metalsa engineers and HTML scientists analyzed how weight and stress were distributed throughout the siderails. They determined the optimal locations for cutting holes in

HTML's mission has evolved from simply studying high-temperature materials to analyzing a greater variety of materials for transportation technologies.

the rails, the best methods for cutting the holes, and the types of steel that would be best suited for this new, lightweight design. As a result, Metalsa modified its manufacturing processes and was able to reduce the weight of several current production models by 10 to 20 percent. In the course of a year, the new designs could save as much as 30 million pounds of steel, resulting in an estimated fuel savings of 3.8 million gallons.

Another approach to designing lightweight vehicle components starts from the ground up, using aluminum, magnesium or fiber-reinforced composites instead of steel. Concerns about these lightweight "replacement" materials often center on their crashworthiness. HTML's specialized equipment not only can assess the amount of energy that a component will absorb in a crash but also can provide information on related issues, such as ways to strengthen welds, better choices for metal alloys and performance of lightweight components under extremes of temperature and stress.

Reflecting on HTML's 25 years as a user facility, Lara-Curzio observes that the facility's wide-ranging materials characterization capabilities have outgrown its name. "HTML continues to play a very important role in addressing one of the Department of Energy's key priorities: to reduce the nation's use of petroleum. We do that by supporting industry, universities and other national laboratories in the development of energy-saving technologies. As we pursued this goal, we expanded our capabilities in materials characterization and were aggressive in developing the infrastructure needed to support the mission of DOE's Office of Transportation Technologies." As a result, HTML today is able to provide the user community with unique analytical capabilities critical to developing safe and efficient vehicles.

Lara-Curzio is optimistic about HTML's future. "Rather than requiring a long proposal process and a long lead time, HTML responds on a timescale that meets users' needs. Our impact is both technologically and application oriented, in keeping with our mission to serve the vehicle technologies community and help solve their materials problems. We are truly a national resource for our industrial and academic users."Ⓡ

Waste to energy

One of the most exciting projects in the HTML's project portfolio is its work with General Motors on developing thermoelectric materials that can convert a vehicle's waste heat into electricity. Attaching a thermoelectric generator to the tailpipe of a car would enable some of the heat from the car's exhaust to be converted into electricity. "Internal combustion engines are only about 30 percent efficient," explains General Motors scientist Jihui Yang, "so about 70 percent of the energy from burning fossil fuel is lost as waste heat. Converting exhaust heat into electricity enables us to improve the fuel economy of automobiles and reduce the use of fossil fuel." In a hybrid vehicle, this extra power would be routed back to the electric motor to power the vehicle. In a standard vehicle, the power could be used to run electrical components, such as the electric water pump, lights, radio, GPS and air conditioning, thus reducing the generator's electrical load.

The materials involved in these studies are called "skutterudites." Skutterudites have empty places in their crystal structure filled with gas atoms. This arrangement makes them poor conductors of heat but good conductors of electricity, a requirement for efficient thermoelectric materials. Much of the research on skutterudites conducted at HTML has been aimed at gaining a more detailed understanding of how these materials are structured at the atomic level, with an eye toward developing materials that are even more efficient. The studies have also helped us understand the skutterudites' ability to conduct heat and electricity at various temperatures and their capacity to withstand thermal stress and vibrations, among other metrics.

These insights into the structure and behavior of various skutterudite-based materials have helped Yang and his colleagues identify a single material with the thermoelectric properties they seek. "In the temperature range we are working in, this is the best material in the world," Yang says. According to GM's computational models, a vehicle using a waste heat power generator based on this material should be able to increase fuel economy by up to five percent. "When we look at how much fuel is consumed by automobiles, five percent is a huge number," he says.

Yang is convinced that HTML's unique range of materials characterization equipment and expertise has helped the research project move farther and faster than would otherwise have been the case. "As far as I know, HTML is the only national user facility that can do this sort of high-temperature measurement for materials," he says. "Other places may do bits and pieces, but HTML is a dedicated facility. I only have positive things to say about HTML."

New designs and materials are reducing commercial energy costs.

ONE OF A KIND

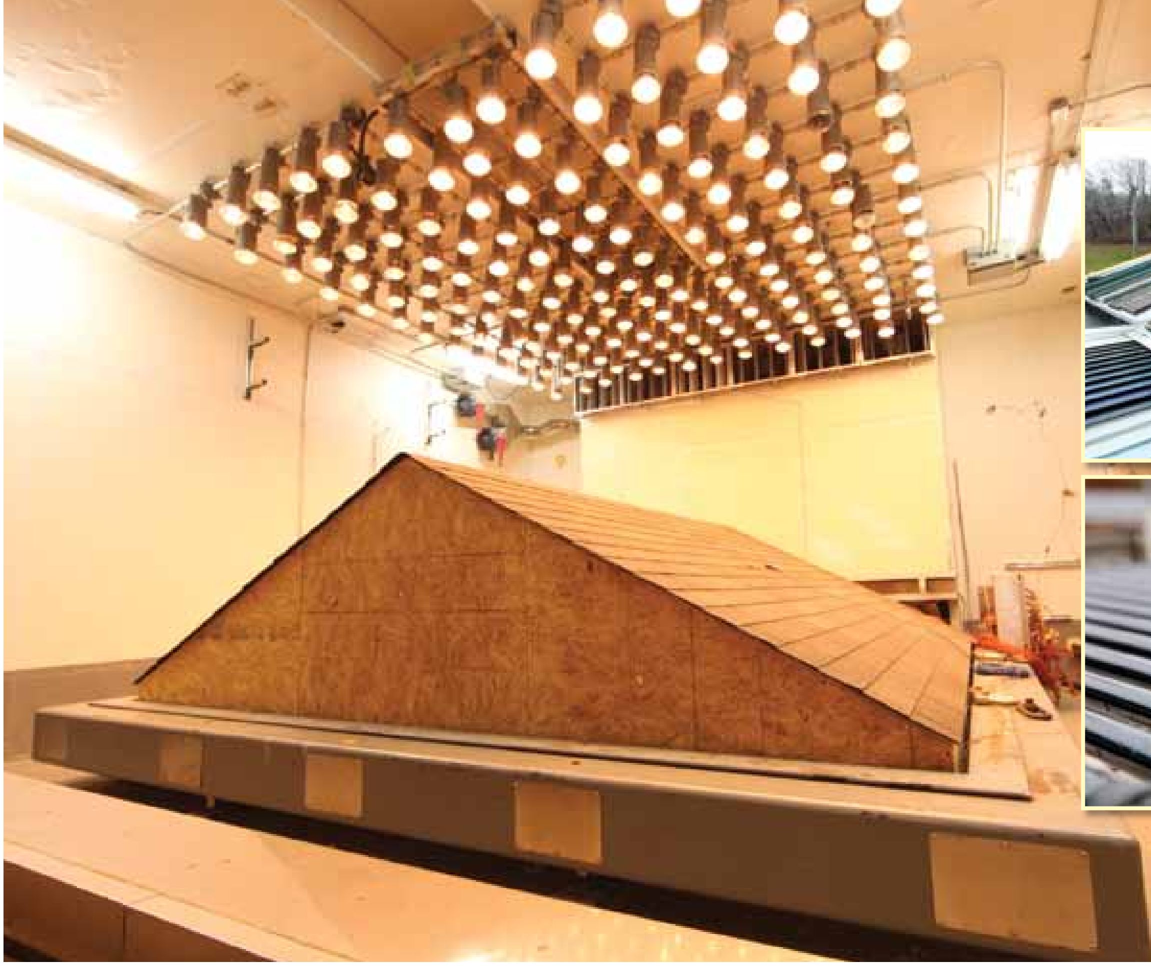
Ability and reputation. Andre Desjarlais believes these two simple words describe the primary attraction for industrial users to Oak Ridge National Laboratory's Building Technologies Research and Integration Center (BTRIC). "We have experimental capabilities that are not available anywhere else in the world," he says, "but it is the quality of our staff and their reputation for impartiality in the building materials industry that leads researchers to our door." Manufacturers know that if they need to send data to a building code agency or to a potential customer, a report with "ORNL" on the letterhead strengthens the credibility of the information.

Desjarlais recalls that, when established in 1987, the Building's Technology Center was the Department of Energy's first designated user facility at ORNL. From the beginning, DOE invested heavily in equipment for conducting state-of-the-art energy-efficiency research. With frequent upgrades, the unique equipment has remained state-of-the-art for more than two decades. The center, for example, still gathers data using the Large-Scale Climate Simulator (LSCS)—a huge apparatus that can enclose building components, such as roof or wall sections, within a highly customizable micro-climate. While most large-scale test facilities can control temperature, the LSCS offers researchers the added benefit of controlling relative humidity, sunlight, rainfall and other variables. This broader collection of data provides the user with a much more realistic testing environment and ensures a higher reliability of test results. Because of these unique capabilities, Desjarlais says ORNL is often called upon to simulate the climate of a particular city or region, noting that, "One day we'll be simulating Miami and the next day Anchorage."

Because roofs and attics represent some 25 percent of commercial heating and cooling costs, industrial users are particularly enthusiastic about using ORNL's simulator to study the efficiency of roofing systems. The LSCS has a unique advantage in these studies because, while other facilities are limited to testing flat pieces of roofs, it can accommodate three-dimensional roof and attic assemblies.

The roofing innovation that has generated the most interest in recent years is "cool roofing," a technique that involves changing the color of the roof to reflect heat away from the building. This seemingly innocuous alteration can significantly reduce air-conditioning costs for a building, particularly in America's sunbelt regions. The center at first worked with manufacturers to develop white or very light-colored roofing for flat-roofed industrial buildings because white roofing reflects the greatest amount of sunlight. However, after gathering data on sloped roofing for residential applications, scientists determined that most homeowners do not want white shingles on their roofs. "We worked with a number of paint and pigment manufacturers to come up with more traditional colors and finishes that would still reflect much of the sunlight away," Desjarlais said. This "compromise" approach kept homeowners happy and still decreased cooling costs.

Although the center was created as a test bed for increasing the energy efficiency of roofs and walls, over the years its capabilities have expanded into testing and evaluating internal building components, such as appliances and heating and cooling equipment. While perhaps less visually impressive than the LSCS, the additional test facilities provide the center with research capabilities to which 99 percent of American industry does not have access. However, despite the center's wide-ranging capabilities, the BTRIC does not compete with the private sector. "If a user wants to perform a fairly simple test that can be conducted at a commercial lab," Desjarlais said, "we direct them to those labs. We work only with clients who have exhausted commercial testing options."



The Large-Scale Climate Simulator can enclose roof or wall sections within a highly customizable micro-climate.

Despite these restrictions, over the past decade the number of users wanting access to the center's research capabilities has increased, while limited capacity has kept the number of users relatively stable. Recent funding investments by the Department of Energy, including $20.2 million to construct an Integrated Net-Zero Energy Buildings Research Laboratory, suggest that BTRIC will be able to accommodate a larger number of users in coming years.

One of the center's current users is the Metal Building Manufacturers Association (MBMA), an influential industry group that promotes the design and construction of metal buildings. Oak Ridge researchers are working with the association on a series of tests involving next-generation metal building roofing systems that have been redesigned to increase energy efficiency. During each round of testing, MBMA engineers build a section of roofing. BTRIC scientists then add instrumentation, run climate simulation experiments and share the results with MBMA. Equipped with these data, MBMA engineers redesign the prototype, and the cycle is repeated until the optimum design emerges.

MBMA engineer Dan Walker noted that the aim of these studies is to create metal building roofs that meet or exceed proposed code requirements. "Our research is designed not only to improve the performance of existing roof construction methods," he said, "but also to develop new construction methods that will result in more energy-efficient metal buildings. Our goal is to develop roofing systems that people will use, that are easy to install and that are both cost effective and energy efficient."

Walker explained that the process of developing more efficient roofing systems at the BTRIC involves a lot of give and take among MBMA and BTRIC staff. "We are providing technical expertise about our product, and Oak Ridge scientists are providing technical know-how about heat transfer fundamentals," he said. "ORNL is helping us identify areas where we can make the most effective changes to increase the energy efficiency as much as possible." The studies could have far-reaching implications if the results help the rapidly expanding metal building industry make decisions about how their designs will evolve and how these changes will affect energy efficiency. In the longer term, Walker said that MBMA is hoping to secure funding to gather whole building energy measurements on a commercial metal building to determine what changes can be made to increase the efficiency of existing buildings, as well as that of new designs.

The center's work with MBMA is emblematic of the kind of relationship BTRIC seeks to cultivate with industrial users. The research also highlights the center's primary mission: removing barriers that discourage industry from using more energy-efficient construction practices. The center does this by interacting with companies and industry groups to explore innovative ideas, accelerating promising technologies and providing sophisticated testing that is impractical to conduct in the private sector.

"We spend a lot of time interacting with the building industry," Desjarlais says. "ORNL does not have a monopoly on good ideas, so we always want to know what people in industry are working on, what interests them and what role we can play. If we discover that industry shares an interest with the Department of Energy, we put the two pieces together and try to create collaborative research projects to accelerate progress in the area of interest. When we do this, energy use goes down, costs go down and everyone gains from the interaction."Ⓡ

NUCLEAR NEEDS

ORNL is helping to replenish the skills needed to protect the world's nuclear assets.

Dating back to the origins of nuclear power in the Manhattan Project, developing and applying technologies associated with the safety and security of nuclear materials has been a core mission at Oak Ridge National Laboratory. At the close of the 1980s, the nature of that mission was in transition. Public alarm following the serious accidents at the Three Mile Island and Chernobyl reactors effectively froze expansion plans for the U.S. nuclear industry. A decade later, arms control treaties and the collapse of the Soviet Union precipitated the dismantlement of much of the nuclear weapons stockpile in the former Soviet republics. The impact of these developments on energy policy and geopolitical relationships has been well documented. Less apparent to many was the impact of these changes on the number of safeguards and nonproliferation professionals whose unique skills are critical to maintaining the safety and security of a large and diverse volume of nuclear materials around the world.

During this period when the future of nuclear power was unclear and the nuclear weapons stockpile was diminishing, a large number of engineers, health physicists and other nuclear experts gradually left the field or retired. With limited occupational options, few were trained to take their places. Jim Bogard, a scientist at ORNL's Safeguards Laboratory National User Facility, explains that one result of two decades of attrition is a cadre of safeguards and nonproliferation professionals who today are largely in their 50s and 60s. "We basically are missing an entire generation of workers in the safeguards field," he says.

To the chagrin of many in the nuclear industry, this shortfall coincides with the resurgence of nuclear energy and the emergence of nonproliferation as an issue of worldwide concern. "We see a nuclear renaissance occurring in the power industry," Bogard says. "We also see enrichment facilities being built in a number of countries, some of which are a concern from a proliferation perspective." Add to this the continuing need to dismantle nuclear weapons from the Cold War, and the challenge to develop a new generation of safeguards professionals is clear.

Addressing this challenge is the mission of ORNL's Safeguards Laboratory. The lab was established in 2000 and designated by the Department of Energy as a national user facility in 2004 to provide a range of services, including customized training for integrated safeguards methods, procedures, and instrumentation; hands-on testing of nuclear materials; and calibration of radiation measurement equipment. The lab is equipped with a world-class suite

of instruments used to measure nuclear materials in safeguard and nonproliferation settings. The facility is among only a few in America that provide a wide range of "reference samples" of nuclear materials. These sealed and closely controlled samples enable users to complete training exercises, calibrate instruments and conduct experimental activities using actual nuclear material.

Safeguards Laboratory staff members represent a diverse collection of internationally recognized nuclear engineers, certified health physicists and experts in the fields of nondestructive analysis and international safeguards. Facility users include students studying safeguards technologies and schemes. The facility also hosts users from private industry, foreign countries, and a variety of federal agencies and research laboratories.

"Physics for Feds"

Among the primary missions of the Safeguards Lab is to provide increasingly popular hands-on classroom and laboratory training in a range of areas related to the monitoring and characterization of nuclear materials. Because the lab's expertise attracts the interest of users in far-flung places, classes are sometimes taken on the road, both in and outside the United States. As ORNL's user program has broadened its capabilities, interest from the academic community has increased. In response to the growing demand for workers with expertise in safeguards technologies, a growing number of universities have created graduate programs with courses of study in nuclear safeguards and nonproliferation. Some of these universities require students to spend at least a week receiving hands-on experience at the Safeguards Lab.

Bogard believes that one of the facility's strengths is the ability to simulate difficult monitoring situations likely to be faced by inspectors in the field. The lab enables students to mock-up a number of scenarios, such as nuclear materials trapped in ductwork or in process equipment, as well as materials enclosed in various types of shipping containers. "Inspectors must know not only how to identify these materials," he explains, "but also how to estimate accurately how much of each material is present." Because the nuclear "reference samples" used in the classrooms or labs are sealed, the training can be accomplished in a laboratory setting that does not require students to be in a hazardous environment or to wear special protective gear.

In addition to providing hands-on classes for students and professionals, the Safeguards Lab also offers a specialized set of courses for federal policymakers. Nicknamed "Physics for Feds," the courses are designed to boost participants' basic understanding of the safeguards field and to provide them with greater understanding of the technical issues surrounding the handling of nuclear material.

Industry Appeal

The ORNL Safeguards Lab is of particular value to industrial users who have access to a wide selection of reference samples of enriched uranium, as well as a variety of other nuclear materials. "These materials are not available outside of DOE facilities," Bogard says. "Industrial users come to Oak Ridge, for example, to determine whether a software algorithm or a piece of detection equipment performs as expected on actual samples of nuclear material." Andrey Bosko, a researcher with the nuclear measurements company Canberra, says that working with Safeguards Lab reference samples has allowed him to acquire spectral data critical to improving Canberra's detection equipment. "We have software that uses a material's spectrum to tell us how much uranium-235 is in a particular sample. I will be able to use the data gathered here to enhance the software's algorithms, so our equipment will provide even more accurate results."

Other users, like Graham Walford, a researcher for the Fairfield Service Group, are involved in developing measurement methods and techniques used in the decontamination and demolition of obsolete nuclear materials processing equipment. Walford's company is providing technical consulting services to support the removal of Manhattan Project-era structures at the site of the former K-25 uranium enrichment facility, seven miles from ORNL.

"There's a very useful synergy here," Walford says of the Safeguards Lab. "As a measurements person, if I'm having a problem, I find it useful to be able to come here and create an equivalent measurement situation to help resolve the issue. More importantly, there are experienced staff at Oak Ridge to provide peer review on my work. This level of expertise enables users to ensure that they provide the best results possible for the equipment and time available." Walford adds that having access to the Lab's staff and reference standards is critical to producing highly accurate characterizations of radioactive contamination. "If you don't have the reference materials and the people to help use them," he emphasizes, "the result could be huge, consistent errors that could lead to over- or under-estimating the amount of nuclear material involved."

Big Impact

The Safeguards Laboratory is internationally recognized for its expertise in nuclear material measurements, arms control and virtually every aspect of nuclear safeguards and security—both domestic and international. Unlike many of ORNL's user facilities, the lab is not in the business of doing "Big Science." Instead, it pursues a more distinct mission of supporting safeguards and security research and the training of safeguards and security professionals.

With a mission that is narrow and focused, ORNL's Safeguards Lab approaches the future with a clear path forward. America is poised to expand the nuclear industry. Meanwhile, the world remains a dangerous place, made more so by the threat of nuclear proliferation. So long as these two facts define the nuclear landscape, a need will exist for skilled personnel to guide the next generation of nuclear technologies. R

FAST TIMES AT ORNL

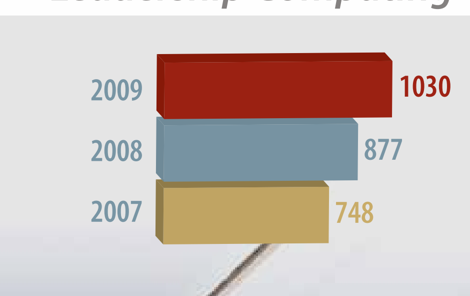
One of the world's premier computing facilities is transforming scientific research.

Many in the scientific community are surprised to learn that the world's most powerful supercomputer is not crunching numbers for classified government projects deep in the bowels of an ultra-secret agency. In fact, the computational heart of one of the Department of Energy's most successful user facilities is blazing through scientific simulations designed to help develop cleaner sources of energy and to understand the causes and impacts of climate change in Oak Ridge National Laboratory's Leadership Computing Facility (LCF).

The great majority of research conducted on this analytical juggernaut, known as Jaguar, is anything but secret. Practiced by researchers from universities, corporations and government laboratories, this "open science" philosophy is designed to provide a unique tool for addressing some of the largest and most important scientific challenges. The collection of capabilities that accompany this computing leviathan, including a breadth of scientific talent; an acclaimed support staff; and a formidable computing infrastructure of power, cooling and connectivity, has made Oak Ridge one of the world's premier computational facilities for the delivery of scientific research.

Despite the fact that in 2010 Jaguar will provide more than a *billion* processor hours of computing time, the competition by users for resources is intense. The majority of the time on Jaguar is allocated through INCITE, a program operated in conjunction with the Department of Energy's Office of Advanced Scientific Computing Research. One of the nation's most successful programs of computational research, INCITE selects from among user research proposals by evaluating both the potential and computational readiness of the research to accelerate scientific discoveries and technological innovations.

Number of Users: Leadership Computing



Research projects selected to run on Jaguar are often accelerated as a result of the massive amount of analysis conducted by the machine in a relatively brief period—in some cases, reducing from months to days the time necessary to generate data. LCF Director of Science Doug Kothe points to the Department of Education's list of the "Top 10 Scientific Achievements" over the last three years as evidence of the machine's value. "Five of those 10 achievements were the direct result of data enabled through simulations executed on Jaguar," he says.

Because of Jaguar's importance to advancing science in a number of disciplines, the supercomputer runs user experiments virtually non-stop every day of the year, relying on scheduling software to load simulations onto the system as quickly and efficiently as possible. Kothe notes that, "On any given day, the backlog of jobs waiting in the queue could be several days of simulation time. Thirty days of backlog would not be tolerated by the scientists. Likewise, a zero backlog would indicate the machine was underutilized," he says. "I am not sure what the ideal backlog would be, but there is no doubt this is a user facility achieving high availability, high utilization and high demand."

Higher resolution

Although at 2.3 petaflops, or 2,300 trillion calculations per second, Jaguar is the world's most powerful computer by a wide margin, the system's most unique attribute may not be speed, but rather its 300 terabytes of memory—about three times that of any comparable supercomputer. Jaguar's abundance of memory enables the storage of more highly detailed models and equations necessary for simulating various real-world phenomena.

The advantage of this extra memory capacity is illustrated by high-resolution climate models developed by the Computational Climate End Station Project. Headed by climate scientist Warren Washington of the National Center for Atmospheric Research, the project typically develops models that attempt to predict climatic conditions in coming decades and centuries. Washington emphasizes that while the ability to develop ever more detailed models is helpful, high-resolution models are not an end in themselves. "Resolution is important, but we must also make sure our models produce realistic simulations. This translates to improving the details of areas that we could not treat as well in the past." Washington observes that earlier models could specify only general features, such as deserts, forests or grasslands. "With additional computational power, we can now specify species of plants and examine details like how precipitation over mountainous regions migrates into river valleys and eventually flows into the ocean," he says. "With the Oak Ridge resources, we can run our models at much higher resolution than in the past."

Time will tell

From this early vantage point, it's hard to say which user communities have benefited most from Jaguar's rapidly expanding capabilities. "To some extent the answer is in the eyes of the beholder," Kothe says. "We are employing an open science system for research in a number of areas as varied as chemistry, materials science, climate, biology and astrophysics. In each of these fields, we can point to impactful work made possible by Jaguar."

In computational science, as in other scientific disciplines, time is often required for the community at large to appreciate the impact of the work being done. Koethe rarely sees a simulation in progress that can be immediately viewed as "game changing." "The point is that time—measured in years, not weeks or months—is required to know which of these impacts will be significant. We are confident, however, that the impacts will be broad and deep," he says.

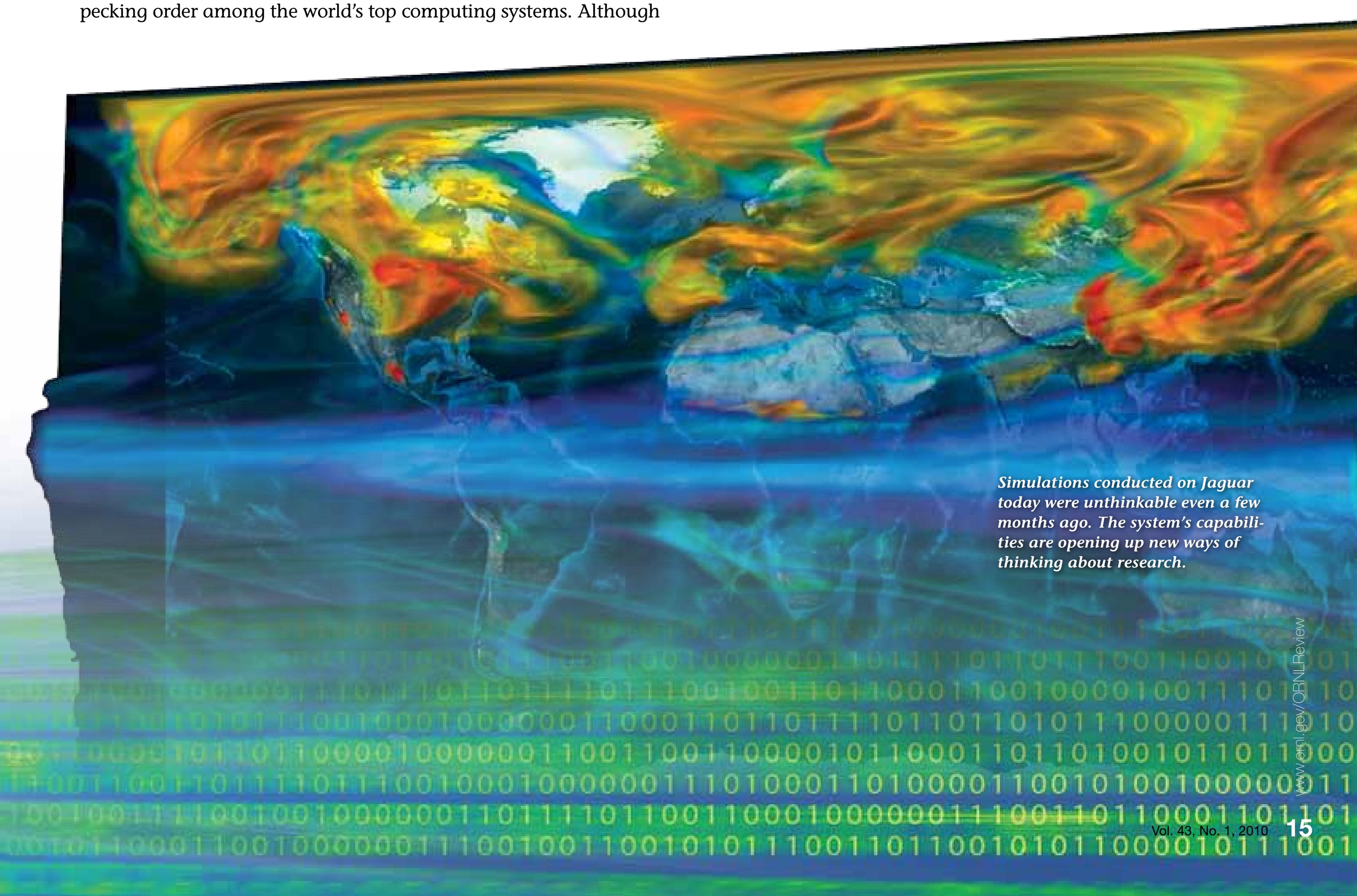
The incredible pace of change can make researchers forget that some simulations conducted on Jaguar today were unfathomable even a few months ago. For some of ORNL's users, these capabilities are opening up a new way of thinking about research. "The approach a scientist takes to designing a simulation that runs only once a week or once a year is very different than the approach he or she would take to a simulation run hundreds or thousands of times in a week," Kothe says. "The challenge is to open our minds to a more unconstrained approach to science. The sheer computing power of systems like Jaguar means that scientists are much less apt to limit the complexity of the models they construct. This ability to integrate a higher level of complexity leads to more predictive models that increase the accuracy of the simulated results."

A field of dreams

Just as computing capabilities rapidly change, so does the pecking order among the world's top computing systems. Although Jaguar is the world's top supercomputer today, the title is elusive in a field where ORNL's maximum computing capacity is 800 times greater than it was just 5 years ago. One constant over this period, however, has been the popularity of the LCF with the facility's users. When pressed about what consistently attracts users to Oak Ridge, Kothe suggests three factors. "First, Jaguar has become a field of dreams for the best scientists. To some extent one can use the cliché, 'if you build it, they will come.'" Second, he emphasizes the ability of the center's staff to meet the understandably complex and often esoteric needs of LCF users. "The ORNL support staff is continually cited by users as being second to none. We have a unique set of experts who are willing and able to help."

Finally, Kothe attributes much of the center's success to a unique support model. "When we stood up the center several years ago, we made a conscious decision to support not hundreds of projects and thousands of users, but dozens of projects and hundreds of users. This decision enabled us to assign our best staff to individual projects. As a result, we are simply not answering mundane questions like, 'Where do I get an account?' or 'How do I run a job?' Our staff members function more like collaborative members of project teams."

"One indicator that the center's model is working is the emulation from other centers," Kothe says. "Our model has been quite effective at enabling Oak Ridge to support the Department of Energy's goal of ground-breaking computational research. For our DOE customer, and for the hundreds of users who each year take advantage of this remarkable program, the impact will be nothing less than profound."



Simulations conducted on Jaguar today were unthinkable even a few months ago. The system's capabilities are opening up new ways of thinking about research.

A STATE OF FLUX

An expanding research facility provides a valuable support system for visiting scientists.

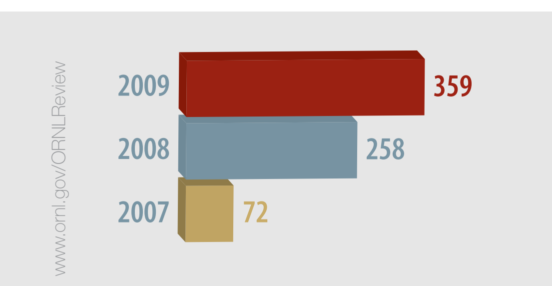
HFIR generates the most intense neutron flux of any research reactor in the world and hosts a broad selection of instrumentation used to explore the structure and dynamics of materials.

Since beginning operations in 1966, ORNL's High Flux Isotope Reactor, known among the research community as "HFIR," has provided a uniquely powerful and versatile resource tool for visiting scientists from industry, academia and other national laboratories. The research reactor, now operating at 85 megawatts, not only generates the most intense neutron flux of any research reactor in the world, but also is home to a broad selection of instrumentation used to explore the structure and dynamics of materials.

In 2009, more than 250 guest scientists conducted research at HFIR in areas ranging from physics to materials science to biology. Although the total was the largest in HFIR's history, the neutron scattering instruments in the reactor's user program consistently receive three times more user requests than can be accommodated.

Part of the reason for nearly a half-century of success is HFIR's ability to produce continuous and intense neutron beams. World-class neutron scattering research requires a high neutron flux, which HFIR provides at a quality and predictability equal to any reactor in the world. An intense source of neutrons is necessary for precise structural measurements because neutrons interact weakly with matter. As a result, a large number of neutrons must scatter to create an accurate picture of a sample's structure. "There are competing facilities in Europe," says Neutron Scattering Science Division Chief Scientist Stephen Nagler, "but Oak Ridge is as good as any of them at what we do. We can measure things at HFIR that are not measureable at any other reactor in the world."

Number of Users: HFIR



Unique capabilities

Nagler gestures at a chart detailing current and proposed neutron instruments at ORNL and notes that the Laboratory is in a unique position with regard to neutron sources. "We have the Spallation Neutron Source, which is the world's most intense accelerator-based pulsed neutron source. Researchers also have access to HFIR which, although originally built primarily to produce isotopes, has four horizontal beam tubes that are used for continuous neutron beam experiments."

Each of HFIR's beam tubes can support more than one instrument. Three of the tubes deliver "thermal" neutrons with energies comparable to the vibration of atoms at room temperature. The fourth

tube includes a "cold" source that generates lower-energy neutrons. Neutrons of different energies have a greater capability to "see" some features of materials, providing a considerable advantage for users able to conduct research at a single facility that can produce both thermal and cold neutrons. Bolstered by a recent

Focusing on the science

One of the most widely reported developments in materials science in recent years was the discovery in 2008 of a new class of iron-based, high-temperature superconducting materials. Superconductors are of general scientific interest because they may hold the key to any number of technological innovations, including super-efficient electricity generation and transmission, cheaper medical imaging scanners and high-speed levitating trains. Some of the world's earliest neutron scattering studies of these materials and related compounds were conducted at HFIR and the Spallation Neutron Source.

One researcher conducting studies at HFIR is Clarina de la Cruz, a postdoctoral researcher with a joint appointment at the University of Tennessee and ORNL. She and her colleagues are examining iron-based superconductors in pursuit of the mechanism behind high-temperature superconductivity. "For years, the only known high-temperature superconductors were copper-based," says De la Cruz. "Now, because the iron-based superconductors represent a newly discovered family of superconductors, we have a good chance of making a valuable contribution to understanding these materials."

One of the aspects of the iron-based superconductors that De la Cruz and her colleagues are studying is how the structure of the superconductors changes across temperature ranges. "Other superconductors do not indicate any structural changes in the temperature ranges in which they are superconducting," says De la Cruz. "However, these superconductors exhibit very subtle, but important, structural changes that can be detected using neutron scattering. On the basis of these studies, we are trying to determine which aspects of the structure of the iron-based superconductors might be related to their superconductivity."

De la Cruz is quick to note the importance of the HFIR user facility to her studies of superconductors and to academic users in general. "This research would be impossible to conduct in a university laboratory. Both HFIR and the Spallation Neutron Source have instruments geared specifically to study these materials. They have a much higher neutron flux that reveals more detail in less time. HFIR also has a technical staff to help set up experiments. This support makes the user experience much more efficient and allows users to focus on the science." She adds that when she started out as a user at HFIR two years ago she had no training in neutron scattering. "A lot of what I now know was learned from ORNL researchers and technical staff at the facility," she said.

Clarina de la Cruz and Jun Zhao of the University of Tennessee discuss results of measurements on an iron-based superconductor.

upgrade, HFIR has an array of instruments operating on the reactor's cold and thermal beam tubes.

SANS instruments – HFIR's cold source feeds neutrons to two small-angle neutron scattering (SANS) instruments. The instruments are normally used to look at nanoscale objects, such as proteins or polymers. One of the instruments is a general purpose SANS. The other, dubbed BioSANS, is dedicated to studying biomolecules. The instruments attract an increasingly broad cross-section of users investigating materials as diverse as biologically important proteins, polymers, metal alloys and high-temperature superconductors.

IMAGINE Single Crystal Diffractometer – The soon-to-be-installed IMAGINE Single-Crystal Diffractometer is expected to provide structural information on single crystals of a range of chemical and organic materials, yielding a hundredfold increase in performance compared with traditional diffractometers. The instrument is expected to be of particular interest to users in the pharmaceutical community.

HFIR's "cold side" also hosts a station used for neutron imaging and neutron radiography. These techniques can be used to measure phenomena involving the movement of liquids, such as the diffusion of water through soil or the motion of fluids in batteries. HFIR staff members are developing additional instruments for the "cold" beamline.

HFIR's "thermal neutron side" is home to seven instruments that measure the structure and dynamics of materials.

Powder Diffractometer – Powder diffractometry is a standard technique for examining the structure of crystalline materials, such as metals, minerals and ceramics, under a range of conditions. The advantage of neutron powder diffractometry over similar analytical techniques, such as X-ray diffractometry, is that while X-rays have trouble identifying light molecules, neutrons are sensitive to both light and heavy atoms. As a result of this advantage, HFIR's powder diffractometer is often the instrument of choice for researchers who need to analyze the structure of a newly created material.

Wide-Angle Neutron Diffractometer – Known as WAND, the instrument is also used in diffraction studies. One use is rapid data acquisition that provides an overview of several different types of structural measurements of a material in a short timeframe.

Nagler recalls one of the more interesting and unusual experiments conducted on the WAND, which involved a group of researchers wanting to study the structure of ferroelectric ice in deep space. Ferroelectric ice has been linked to various phenomena, including planetary formation.

"The researchers expected the ice to form under certain conditions at very low temperatures," Nagler says. "When they conducted the experiment, they found that some ice did indeed form. By measuring the structure of the ice, the group determined that certain astrophysical phenomena can be explained by the presence of ferroelectric ice in space. In this case, neutron scattering data that is normally used to measure very small things was used to investigate phenomena on a galactic scale."

Four-Circle Diffractometer – Unlike HFIR's other diffractometers, the Four-Circle Diffractometer is used for the studies of "single crystals," such as those in metal alloys and ceramic materials. The materials are those in which the arrangement of atoms, ions or molecules is repeated throughout their entire volume. Scientists use the wide-angle and powder diffractometers to study "polycrystals," samples that comprised a large number of single crystals that are randomly oriented throughout the sample.

Neutron Residual Stress Mapping Facility – HFIR's remaining diffraction instrument is the Neutron Residual Stress Mapping Facility. The instrument is managed by ORNL's Materials Science and Technology Division and is used to measure stress, often in large-scale materials such as jet engines, automobiles and bridges. Researchers use data from these measurements to determine the effectiveness of stress relief methods and to check failure analysis, design and life predictions provided by computer models.

Triple-axis Spectrometers – HFIR's toolbox contains three different types of triple-axis spectrometers. Generally speaking, these instruments enable scientists to study motions of atoms and their associated magnetic properties. Each of HFIR's three triple-axis spectrometers has a different emphasis. The HB3 spectrometer is a general-purpose spectrometer. The HB1 instrument is similar but can be set up to use polar-

The neutron scattering instruments in HFIR's user program consistently receive three times more user requests than can be accommodated.

Collaborations stimulated by HFIR's user program have driven the facility's research program in new directions.

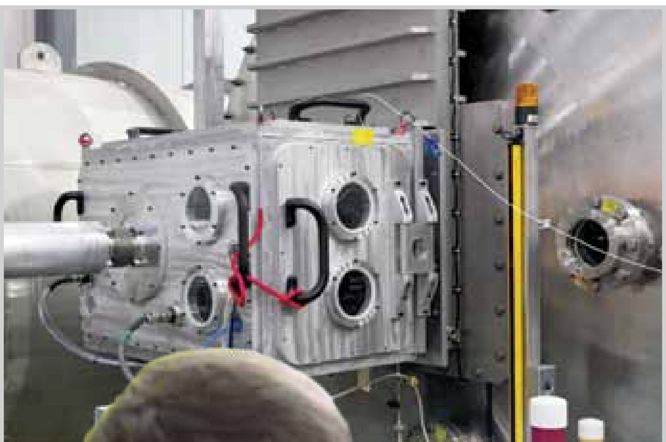
ized neutron beams that have only one magnetic state. HB1A, operated by both ORNL and Iowa's Ames Laboratory, differs from the others in that neutrons in the beam striking the sample have a fixed energy, while the other two instruments provide researchers with the ability to adjust the energy of the neutrons.

Recent experiments on the various triple-axis spectrometers have included studies of multiferroic materials that can be simultaneously magnetic and ferroelectric. Researchers anticipate that the materials could have applications in high-speed computation and communication. The spectrometers have been used to characterize some of the newly discovered class of iron-based superconductors described in the sidebar on page 17.

A unique user experience

Years of experience with the HFIR user community have convinced Stephen Nagler that one of the main advantages of running a user facility is that researchers from all over the world bring good ideas with them. "HFIR staff members certainly have their own good ideas," he says, "but we benefit by interacting with other scientists. The interaction has definitely driven our research program in new directions. Every researcher brings individual insights. This collaboration generates a tremendous amount of creative energy for our research program."

Postdoctoral researcher Clarina De la Cruz notes that the symbiotic atmosphere at HFIR also has a beneficial effect on the research process itself. "I have worked at many of the neutron scattering facilities in the U.S., but HFIR is different. At HFIR, the researchers and staff take care of you. They work with you. They don't just want you to come in and do your work. They encourage you and want you to be successful. It's a small thing perhaps, but it's something I haven't experienced at other facilities." Ⓡ



Conducting research at a facility that can produce both thermal and cold neutrons can enable users to "see" otherwise elusive features of materials.

STANDING IN LINE

One of ORNL's newest user facilities is already among the most popular.

When ORNL's Center for Structural Molecular Biology (CSMB) opened its doors in 2007, Chemical Sciences Division Director Phil Britt was a little surprised at the number of users attracted to the facility that today is helping to make ORNL a leader in neutron-based studies of bio-molecular structure. "We built the center hoping demand would be high," Britt said. "As it turns out, not only are users lining up to conduct research, but the line goes out the door and around the building."

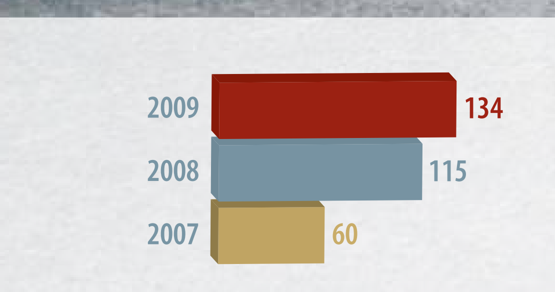
Center staff scientist Volker Urban recalls that "once the center started showing promising results, we quickly generated a backlog of users, followed by a growing number of invitations to participate in grant proposals." The center teamed with Washington University in St. Louis to win a highly competitive Energy Frontier Research Center proposal to study the biological mechanisms plants use to convert sunlight to energy, research that could lead to the development of much more efficient solar cells. In another energy initiative, researchers at the center are working with the Department of Energy's Genomes to Life Biofuels program, using unique characterization and analysis capabilities to convert biomass to bio-fuels more efficiently.

The level of enthusiasm on the part of both users and research sponsors is understandable given the center's ability to reveal the three-dimensional structures and assemblies of biological molecules, such as proteins, lipids and DNA. Understanding the molecular structure and interactions of these molecules assists researchers in determining how the molecules are formed and how they influence the function of living cells.

Specialized capabilities

"The approach we have taken provides a complete 'structure solution toolkit' for the biology community," explains center director Dean Myles. "We make available a pipeline in

Number of Users: CSMB



which users can start from a single gene and synthesize molecules at the laboratory bench, measure and characterize these molecules using neutron beams and then analyze these data using advanced computational techniques to determine 3-D models of the molecular structures. The approach represents a one-stop shop for structure solution." The center's users have access to a diverse range of research interests. To aid researchers in exploring questions related to energy, medicine and a range of other fields, the facility applies three primary research tools:

BioSANS – The cornerstone of the center's research capabilities is a small-angle neutron scattering instrument called BioSANS. Located at ORNL's High Flux Isotope Reactor, the BioSANS instrument uses a neutron beam from the reactor to probe the structure of functional biological systems at the nanoscale. This technology enables researchers to determine the structures of both individual biological molecules and molecules interacting and assembling in the functional complexes of the cell.

While similar instruments exist at other facilities, BioSANS is among only a few in the world specifically tailored to tease out the nuances of biomolecular structure. Researchers achieve this specialized capability by making several accommodations for the peculiarities of biomolecules. First, BioSANS uses less energetic, "cold," neutrons, which have wavelengths tuned to help "see" the soft material contained in most biological samples. Second, the instrument itself is designed to be extremely sensitive, minimizing sources of background noise that might interfere with measurements of small, dilute solutions of biological material. Finally, the center's biodeuteration facility (described in more detail below) enables researchers to enhance the samples further, making it possible to label individual components with deuterium and increase their "visibility" on the BioSANS.

"This combination of capabilities is unique in the United States," Britt says. "There are several similar facilities outside the U.S., but none is dedicated to biology. Moreover, at 85MW, ORNL's High Flux Isotope Reactor is the world's most powerful steady state neutron source." The intense neutron stream means that measurements taken on the BioSANS instrument can generate higher resolution data from smaller samples in less time than can be achieved at any other facility in America.

Bio-deuteration laboratory – The technique of bio-deuteration enables biological molecules to be labeled selec-

The BioSANS instrument uses a neutron beam to probe the structure of biological systems at the nano-scale.

tively by substituting deuterium, a specialized form of hydrogen, for normal hydrogen atoms. Because deuterium scatters more neutrons than hydrogen, deuterium-labeled molecules can be examined with unusual fidelity by the BioSANS. The technique is particularly effective in highlighting specific parts of target molecules, such as reaction centers, and in distinguishing the presence of labeled molecules incorporated in larger biological complexes or assemblies.

"All samples do not require this technique," Britt adds. "Individual molecules and biological complexes can often be analyzed directly on the BioSANS, but when users address more complicated questions, biodeuteration adds another dimension."

Despite obvious advantages, the technique of bio-deuteration is not without challenges. When a sample needs to be labeled with deuterium, researchers perform the work in a solution of deuterated or "heavy" water. For some biological samples, the chemistry and physics of "heavy" water can be a problem. "Most enzymes and microorganisms do not perform well in deuterated water," Britt observes. Fortunately, center staff members have a repertoire of skills and systems available to address such problems. Myles believes these techniques have advanced to the level where researchers can target and label even individual amino-acid groups in selected proteins or leave only a few hydrogen atoms in place to highlight the functional sites.

Computational modeling – To support the user program, the center has developed a suite of advanced computational tools for creating 3-D models of complex biomolecules from data collected using BioSANS. These detailed structural models are critical to providing scientists with an understanding of how biomolecules function in living systems.

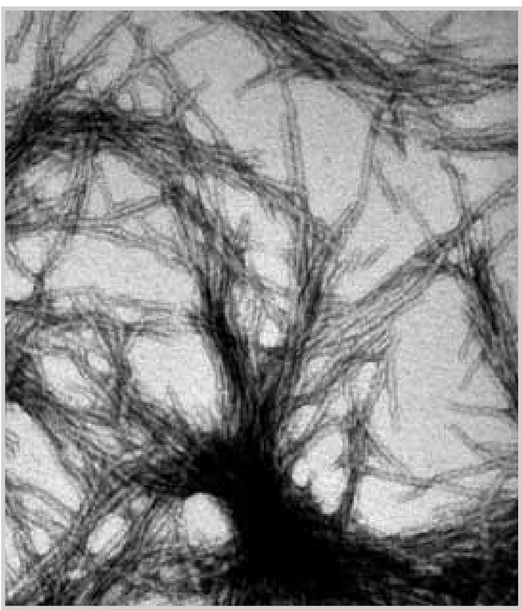
Urban cautions that, "the results we get from these studies are only as good as the software we have to analyze the data." He views computational modeling as another area in which the center's integrated approach comes into play through the development of computational tools to help interpret and understand the data. The tools enable structural information from other experimental techniques to be combined with the information gathered from the BioSANS, making it possible to develop even more complex and sophisticated 3-D models. "The process is like building a jigsaw," Myles says. "If we already know something about the individual pieces of a biological structure, these tools help us use the BioSANS data to build those pieces into more detailed models to complete the puzzle."

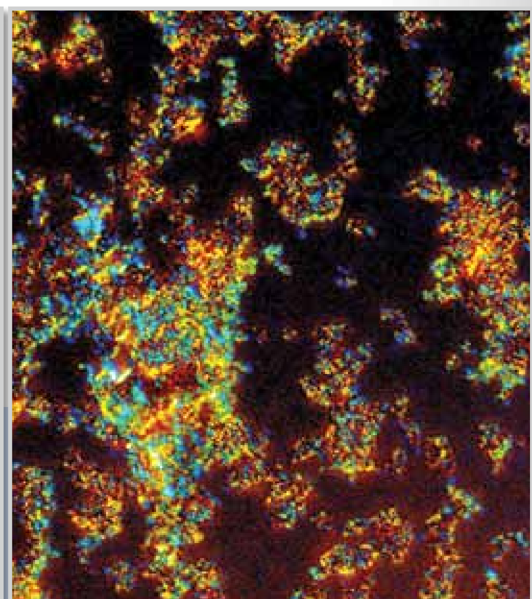
A continuing commitment

The user community's enthusiastic response over the first three years of operation make it clear that the center is not only making neutron scattering available to users in the broader biological community but is also attracting users who even five years ago would never have considered using neutron scattering as a research tool. Today, the center supports users from a range of scientific disciplines, including biophysics, chemistry, biology and computational sciences. As a result, many of the studies conducted address questions that have not, or in some instances, could not, have been answered by other techniques.

The center's success can be attributed to a unique approach and combination of analytical tools, the expertise of a world-class staff, the successful integration with other superlative research facilities such as the High Flux Isotope Reactor and the Spallation Neutron Source, and an ongoing commitment to provide users with the tools and support necessary for breakthrough research. Phil Britt sees in the collection of assets a promising future in which one of ORNL's newest user facilities continues to strengthen its reputation as one of the world's leading laboratories for neutron-based studies of biomolecular structure and function.

Below left: Electron microscopy image of Huntington's aggregates. Right: Polarized optical image of stained aggregates.





Window into a Disease

Among CSMB's most notable collaborations has been working with the University of Tennessee Medical Center, in helping to understand the molecular mechanisms behind Huntington's Disease, a genetic condition that leads to the deterioration and death of brain cells, causing problems with muscle control and certain thought processes. In its advanced stages, the disease can affect an individual's ability to walk, talk or even swallow.

Like a number of genetic diseases, Huntington's is caused by a defective protein that includes a repeated set of biochemical

The technique of bio-deuteration is particularly effective in highlighting specific parts of target molecules.

instructions. UT researcher Tatiana Perevozchikova explains that the toxic protein contains an unusually long string of 40 or more glutamine amino acids rather than the normal 15 or 20. The additional amino acids cause the protein to form thin, threadlike fibers, or aggregates, in the patients' brains that cause brain cells to deteriorate and die.

Thus far, researchers have not been able to determine at what stage of development these aggregates become toxic to brain cells. To gain a better understanding of this aspect of the disease, researchers are applying the BioSANS instrument's ability to analyze functioning biological systems to observe the aggregates at different stages of development. "The BioSANS instrument enables us to see the formation of aggregates over time," Perevozchikova said. "This kind of analysis is not possible with other techniques."

Perevozchikova notes that another advantage of the BioSANS instrument is its ability to study the protein molecules in solution. Because the molecules are large, flexible and change over time, scientists can use the BioSANS instrument to make detailed observations of the growth formation of the protein fibrils, as well as generating 3-D structural maps of both the proteins and the aggregates.

To date, researchers at ORNL have gathered a wealth of information about the differences between the toxic Huntington's protein and its normal counterpart, as well as the mechanisms that may produce the disease's toxic effects. Over the long term, scientists would like to learn how to control the process of aggregation or even eliminate it entirely. Evidence suggests that the aggregates do the bulk of their damage to brain cells in the aggregates' early stages of development. "If we can describe the toxic protein at this stage," says Perevozchikova, "the information could lead to the development of a therapeutic agent for treating Huntington's disease."

Further research planned at the Center for Structural Molecular Biology and on other instruments at ORNL's Spallation Neutron Source is expected to shed light on this and other questions related to finding a treatment for Huntington's Disease.

HERB Debban

We asked Debban about his role in providing support for the Laboratory in general, and for ORNL's user facilities in particular.

When UT-Battelle assumed responsibility for managing Oak Ridge National Laboratory almost 10 years ago, one of its highest priorities was finding a veteran facilities manager to address the challenge of aging facilities, inadequate infrastructure and an ambitious new plan for Lab modernization. A decade later, Herb Debban's accomplishments have been a key to ORNL's resurgence. His day-to-day responsibilities include planning a billion dollar renovation for the Lab, implementing a landlord-tenant model for operating facilities, helping sustain a marked increase in safety and providing the infrastructure for a growing portfolio of world-class user facilities. And that's before lunch.

What in your background brought you to Oak Ridge?

Prior to 1999, I had worked with DOE contractors for years before I was asked to help write the proposal for UT-Battelle to operate ORNL for the Department of Energy. Most recently, I was at Pacific Northwest National Laboratory and was responsible for facility operations. At PNNL we implemented customer-oriented processes that reduced cycle time and significantly improved research customer satisfaction. That's probably the main reason I'm at ORNL today.

You have more than 30 years' experience in facilities operation, engineering and management. How has the proliferation of user facilities affected the way science is done in the national laboratory system?

User facilities have really encouraged collaboration among researchers. These facilities provide users with resources that they wouldn't have access to otherwise. They also enhance the quality of the science done at the national laboratories because the research conducted at user facilities is proposal-driven. The proposals are evaluated to determine which are most worthy to pursue. Only the best proposals are accepted.

You have experience at a lot of other labs. Without naming names, how would you compare ORNL's management philosophy with that of some of those other labs?

UT-Battelle operates under a policy of simultaneous excellence. That includes excellence in science and technology, operations (environment, safety and health) and community relations. UT-Battelle genuinely believes that if an organization is excellent in science but not in operations or community relations, then the company will not be viewed by the community as a valuable asset. When laboratories have problems, it's usually a result of what they are doing—or not doing—in the areas of operations and community relations rather than the quality of their science. UT-Battelle probably emphasizes these aspects of laboratory management more than other lab operators.

What areas of research do you think have benefitted the most from ORNL's user facilities?

The areas that require the "big science" tools or highly specialized capabilities have benefitted the most. For example, in neutron science, Oak Ridge has the really big tools—the world's most powerful neutron source and a nuclear reactor with a range of unique capabilities. In the area of supercomputing, Oak Ridge now has the world's foremost facility for high-performance computing. In materials science we have the High Temperature Materials Laboratory. For nanoscale studies, we have the Center for Nanophase Materials Sciences. In the biological sciences, we have world-class facilities for both structural biology research and bioenergy studies. We also have exceptional facilities for energy, physics and transportation. Few places, if any, have such a collection of world-class research facilities.

ORNL has several extremely popular user facilities. How do you deal with the competing demands of keeping facilities available for research and maintaining them at a high standard?

We are of course concerned with availability, but we are also dedicated to keeping all of our facilities in top-notch operating condition. This has become more of a challenge recently as a result of ORNL's dramatic growth. Since 2002, we have added large new user facilities, such as the Spallation Neutron Source and the Center for Nanophase Materials Sciences. At the same time, we provided new offices for more than half the 4,700 staff at the Laboratory. The only way to manage such change is with facility managers and facility engineers who are highly customer-oriented.

We are also adding a "surge" team that can be applied to any area that has an urgent need, particularly to those facilities like the High Flux Isotope Reactor that have time-critical peak needs. When needs arise at several facilities simultaneously, there is a natural competition for resources. Our response has been the creation of a capability that we can apply in addition to the resources we would normally make available.

How do you balance competing demands such as space, power and parking for a lab that is experiencing such rapid growth?

We do a lot of planning. Normally, we have a master facilities plan that outlines several years in advance how various demands will be accommodated. However, the American Recovery and Reinvestment Act funding we recently received made it necessary to accelerate parts of our master plan. Competing demands for resources are addressed through our mission readiness process, where we collaborate with the Lab's research organizations to consider current research needs, as well as those 5 and 10 years in the future. We identify the gaps in our current capabilities and develop a plan to address those research needs with new facilities or whatever else is needed. In other words, we try to anticipate what our researchers' needs will be several years out and plan accordingly.

What is the biggest challenge of managing such a diverse set of facilities?

Our biggest challenge is to understand the evolving needs of the users—what they need to perform cutting-edge science. Once we understand their needs, it's really just a matter of setting priorities, planning and implementation. I'm simplifying this somewhat, but if we don't understand what users need, then everything else is likely to be worthless. That's why we ensure that our people are very capable and customer-oriented. This is reflected in the results of our annual customer satisfaction survey, which have gone from 70 percent satisfaction in 2002 to 94 percent last year.

What improvements have you been able to make in the operation of ORNL's user facilities?

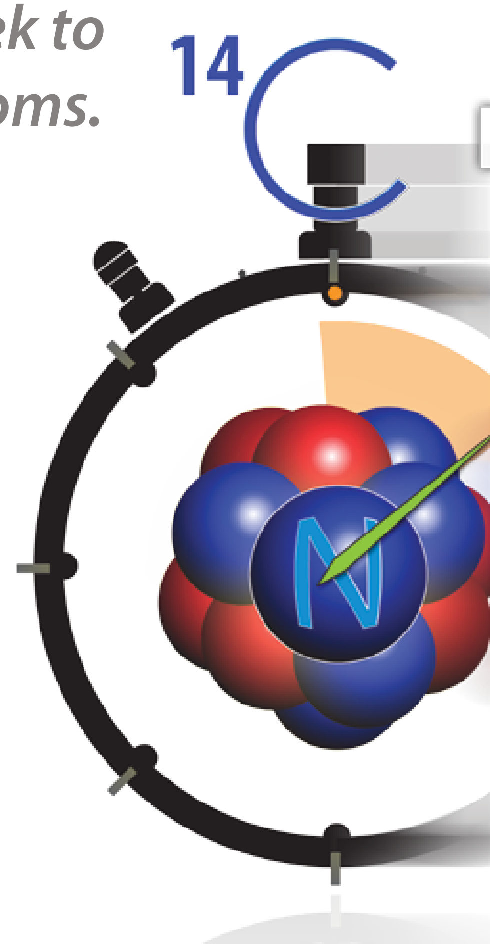
Last year we conducted a study of the efficiency and consistency of our entire user facility program. The study considered the complete user experience—from the time they write their proposals to their arrival at the Lab to the day they leave. Every research program was involved in this effort.

A number of efficiency improvements resulted from the study. However, the one all users will experience by early 2010 is the ability to create a "boarding pass" for their visits to ORNL. From the comfort of their homes or offices, users will be able to go online to fill out the necessary paperwork, take their training and print out the boarding pass. When they arrive at the Laboratory, all they will have to do is show the pass to the guard at the gate and scan it into the system at the Visitor Center. They will then be ready to get to work, instead of spending hours or even days taking training and collecting administrative approvals.

We recognize the importance of our user facilities to the research community and to the mission of the Laboratory. In many cases, the users that visit the Laboratory make or break our reputation, so we want them to leave happy. We want them to achieve their objectives, and we will do anything we can to ensure their objectives are met. R

UP TO DATE RESEARCH

By exploring carbon-14, researchers seek to understand what binds the nuclei of atoms.



For much of the public, the term "carbon-14" is among the most frequently mentioned scientific phrases heard in the popular media. The predictable decay of carbon-14 nuclei has long been used as a scientific tool for dating carbon-based materials in fields as diverse as history and archeology, yet the actual science involved with describing the physical properties of carbon-14 itself is less well understood.

When, in 1994, researchers discovered the Chauvet Cave in southern France filled with Stone Age artwork, carbon-14 indicated the charcoal drawings on the cave walls were approximately 31,000 years old. Six years earlier, when scientists examined the Shroud of Turin, results of carbon-14 analysis indicated the relic, a linen cloth believed by many to have been placed over the body of Jesus at the time of his burial, was more likely woven in the Middle Ages, more than a millennium later.

For the past half-century, carbon-14 has enabled scientists to dramatically improve the dating of both the living and inanimate elements of human history, including skeletons, ruins or anything that was once part of a plant or animal. By existing in all living things and decaying at a steady rate, carbon-14 gives researchers the ability to determine with reasonable accuracy the age of a long-abandoned community, tool or other artifact. And because, for reasons not yet understood, carbon-14 decays far more slowly than most isotopes in its weight class, the process provides researchers with the confidence to date items as far back as 60,000 years.

At ORNL a team led by David Dean is using the unprecedented computing power of the laboratory's petascale supercomputer to examine the carbon-14 nucleus. The team, which includes Hai Ah Nam of ORNL, James Vary and Pieter Maris of Iowa State University and Petr Navratil and Erich Ormand of Lawrence Livermore National Laboratory, hopes to explain carbon-14's long half-life and advance understanding of what holds all nuclei together.

"Carbon-14 is interesting to us because the physics says it should decay quickly, yet the measured half-life is much longer than expected," explained Nam, a physicist with ORNL's National Center for Computational Sciences. "The existing theoretical models used to describe light nuclei such as lithium, with six particles, or boron, with ten, have produced good results. But carbon-14, also a light nucleus, has been elusive. The models do not yield a value that matches what we measure experimentally, which means we are not capturing all of the physics."

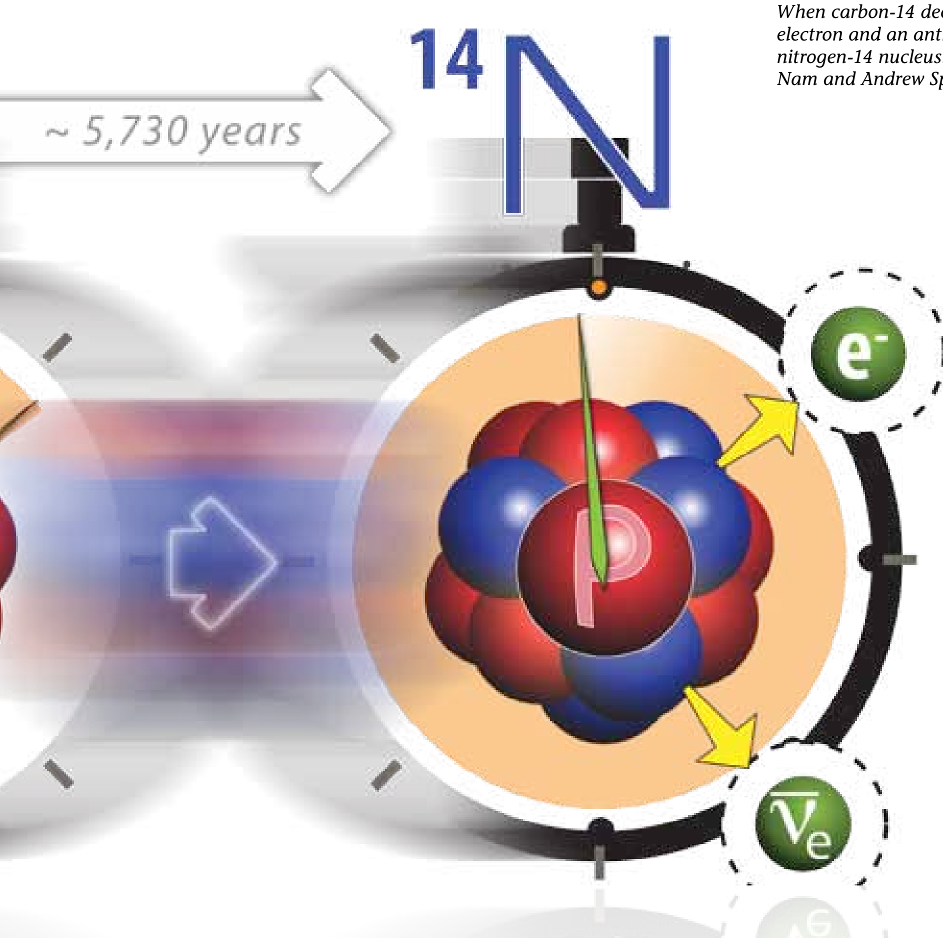
Parsing the nuclear attraction

An isotope's half-life is the time required for one-half the atoms in a sample to decay. For most light isotopes the half-life is typically minutes or even seconds. Carbon-14, with a half-life of nearly 6,000 years, is an anomaly. A simulation that reveals why the half-life of this unique isotope is so long also has the potential to illuminate the half-lives of all isotopes, both long and short, thus providing a better understanding of how the observable matter in the universe is bound together.

The task is especially challenging because some of the precise properties that bind an atom's nucleus are not fully understood. Scientists have long known that the nucleus is made up of protons and neutrons, known generically as nucleons. More recently, they have determined that the nucleons are made up of even smaller particles, known as quarks and gluons, held together by the "strong force." To nuclear scientists, the holy grail of nuclear physics would be represented by a theoretical description of the properties of all nuclei, including the stable and unstable, mundane and exotic, large and small.

Dean and his colleagues have been awarded an allocation of 30 million processor hours on ORNL's supercomputer to dissect the secrets of carbon-14 with an application known as Many Fermion Dynamics—nuclear, created by Vary at Iowa State. Dean's team will be using nearly 150,000 of the supercomputer's more than 180,000 computing cores on the project. The application is ready to scale to even more cores as they become available.

The team is using an approach known as the no-core shell model to describe the



When carbon-14 decays, the nucleus emits an electron and an anti-neutrino and becomes a nitrogen-14 nucleus. (Visualization by Hai Ah Nam and Andrew Sproles)

nucleus. Analogous to the atomic shell model that predicts how many electrons can be found at any given orbit, the nuclear shell model defines the number of nucleons that can be found at a given energy level. Generally speaking, the nucleons gather at the lowest available energy level until the addition of more would violate the Pauli exclusion principle, which states that no two particles can be in the same quantum state. At that point nucleons occupy the next higher energy level. The force between nucleons complicates this picture and creates a computational problem of enormous complexity for researchers.

Using the power of the petascale

The unprecedented computational power available at Oak Ridge enables the team to depart from other nuclear structure studies in a variety of respects. The project is taking a microscopic look at the nucleus, working with its smallest known constituents. Nuclear models have been moving in this direction for seven decades, from the liquid drop model of Niels Bohr, which treated the nucleus as a single drop of nuclear fluid, to later models that examined the protons and neutrons separately. The ORNL team is able to probe even deeper. Utilizing an ab initio, or first principles, approach, they are working from the strong-force interactions of the quarks and gluons within each nucleon. In addition, Dean's team has adopted a "no-core" strategy that incorporates all 14 nucleons and includes more energy levels in the model. The simulations also extend beyond two-body forces, which include the interaction of every nucleon with every other nucleon two at a time, to incorporate three-body forces.

"Previously we could only consider two-nucleon interactions because the number of combinations needed to describe all the different interactions is vast, even for only two particles at a time," Nam explained. "And while two-particle interactions are the dominant way that these particles interact, there are some nuclear phenomena, like the half-life of carbon-14, that cannot be described using only a two-nucleon interaction, meaning three-particle interactions or higher are also significant.

"Our project is probing whether these two approaches, using the ab initio methods and the higher number of interactions, will describe more accurately why carbon-14 has such a long half-life and help explain how all nuclei are put together."

Calculations at this scale are now possible at Oak Ridge using a supercomputer capable of 2.3 thousand trillion calculations a second—making it the world's fastest scientific supercomputer. Also critical are the machine's 362 terabytes of memory, three times more memory than other system. Prior to the system's installation in 2008, such a simulation of the carbon-14 nucleus working from its smallest known constituents would have been unthinkable.

"These types of calculations for carbon-14 were previously not possible because the research required a memory-intensive calculation," explained Nam. "Accounting for the three-nucleon force amounts to storing tens of trillions of elements, or hundreds of terabytes of information."

By making use of such extraordinary computing power, the ORNL team hopes to move a little closer to an understanding of the atom's nucleus. If they are successful, carbon-14 will become an even bigger star in the scientific galaxy.

...and the WINNERS are...

Accomplishments of Distinction at Oak Ridge National Laboratory

Ramakrishnan, Venkatraman, formerly of ORNL's Solid State Division, has received the **2009 Nobel Prize in Chemistry** from the **Royal Swedish Academy of Sciences,** for studies of the structure and function of the ribosome. Ramakrishnan was a researcher at ORNL's High Flux Isotope Reactor in the early 1980s and is currently working at the MRC Laboratory of Molecular Biology, Cambridge, England. He received his Nobel Prize for work in decoding the genetic makeup of human cells.

Markus Eisenbach and **colleagues from ORNL, Florida State University and the Institute for Theoretical Physics and Swiss National Supercomputing Center** has been awarded the **2009 Gordon Bell Prize** from the **Association for Computing Machinery.** Eisenbach and his colleagues achieved 1.84 thousand trillion calculations per second, or 1.84 petaflops, using a program that analyzes the effect of temperature on magnetic systems. **Edoardo Aprà** and **colleagues from ORNL, Australian National University, Pacific Northwest National Laboratory and Cray, Inc.,** were finalists for the award. Aprà's team achieved 1.39 petaflops on Jaguar in a first-principles, quantum mechanical exploration of the energy contained in clusters of water molecules.

Markus Eisenbach

David Singh and **Jon Kreykes** have been named UT-Battelle **Corporate Fellows.** Singh is a condensed matter theorist who is internationally recognized for his contributions to the methodology for electronic structure calculations and in applications to diverse classes of materials. Kreykes was recognized for his far-reaching accomplishments on national security issues, including nuclear weapons and nuclear materials proliferation.

Johney Green was recognized by the **Council of Engineering Deans of Historically Black Colleges and Universities**, ***U.S. Black Engineer*** and ***Information Technology*** magazines and **Lockheed Martin Corporation** as the **2010 Black Engineer of the Year**.

Julie Ezold has received the **Patricia Bryant Leadership Award** from **U.S. Women in Nuclear. Leon Tolbert, Fang Peng** and **Miaosen Shen** have received the **2009 Transaction Prize Paper Award** from the **IEEE Power Electronics Society. Hua-Tay Lin** has been selected for the **2010 James I. Mueller Memorial Award** from the **American Ceramic Society**. **Johney Green, Jamison Daniel** and **David Erickson** received the **OASCR** Award from the **Department of Energy Office of Advanced Scientific Computing Research,** for their computer visualization of seasonal CO_2 buildup and reduction in North America.

Raphael Pooser, Ivan Vlassiouk and **Zac Ward** have been selected to receive ORNL's 2009 **Eugene P. Wigner Fellowships. Cory Hauck** has received the **Alston S. Householder Postdoctoral Fellowship in Scientific Computing. Xianglin Ke** has been awarded the **Clifford G. Shull Fellowship.**

Witold Nazarewicz has been elected to the **Executive Committee** of the **American Physical Society, Division of Nuclear Physics. Amit Goyal** has been elected a **Fellow of the World Innovation Foundation** and received the **Distinguished Alumnus Award** from the **Indian Institute of Technology. Chris Pickett** has been elected a **Fellow of the Institute of Nuclear Materials Management. Roger E. Stoller** has been elected a **Fellow of the American Nuclear Society.**

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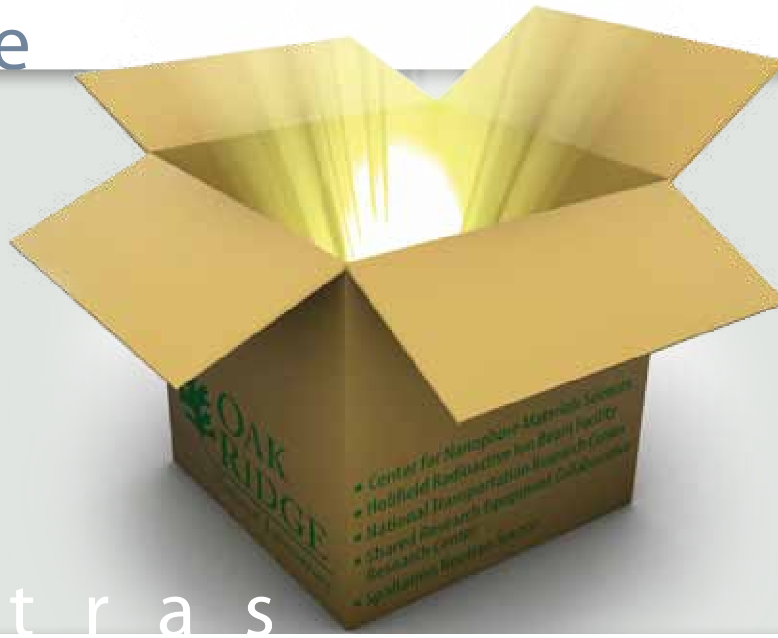
Part 2



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