Oak Ridge National Laboratory

REVIEW

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

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Boosting business, creating jobs

Power from the sea

Industrial-strength scholars

Igniting Industry

Oak Ridge National Laboratory
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Simulation of a fuel jet flame created on ORNL's Jaguar supercomputer by Jacqueline Chen and Chun Sang Yoo of Sandia National Laboratories and Ramanan Sankaran of ORNL

Delivering the Science...*and Putting It to Work*

The vital mission of the X-10 facility that would evolve into Oak Ridge National Laboratory—the pilot-scale production and separation of plutonium for the Manhattan Project—was successfully executed by a partnership that brought government, universities and industry together in an entirely new way. On a military reservation administered by the U.S. Army Corps of Engineers, DuPont engineers worked with scientists from the University of Chicago to design and construct a "chain-reacting pile," later known as the Oak Ridge Graphite Reactor, and a chemical separations plant.

This partnership achieved its goal of gram-scale production of plutonium in less than 18months, conclusively demonstrating the value of combining basic science with engineering and industrial knowledge to accelerate innovation. It also set the stage for one of the earliest examples of technology transfer from national laboratories to industry.

Once the Graphite Reactor completed its plutonium production mission, its capabilities were refocused on research and isotope production. In June 1946, an article in *Science* announced the availability of radioisotopes to the scientific public. Within 5years, Abbott Laboratories had constructed a plant in Oak Ridge so that it could use radionuclides from the Graphite Reactor to prepare radiolabeled compounds for diagnostic and therapeutic purposes. Today the production of radioisotopes for scientific, medical and industrial applications is a multibillion-dollar industry.

As ORNL evolved into a multidisciplinary institution, it continued to partner with industry, both to achieve its mission assignments and to deliver practical solutions that improve the quality of everyday life. Long before technology transfer was formally established as a U.S. Department of Energy mission, ORNL developments such as pocket radiation alarms, the zonal centrifuge and advanced alloys found their way to the marketplace, and startup companies based on ORNL technology were launched by entrepreneurially minded researchers.

In the 1980s, growing concerns about U.S. competitiveness led to legislation that provided ORNL with new tools for technology transfer. Licenses, collaborative research agreements, and cooperative research and development agreements were added to agreements that provided industry researchers with access to ORNL's expanding suite of scientific user facilities. Collaborations at the Roof Research Center, the High Temperature Materials Laboratory, the High Flux Isotope Reactor, and other user facilities led to the transfer of developments in ceramics, semiconductors, insulation and other commercially promising technologies.

When UT-Battelle assumed responsibility for managing ORNL in April 2000, the new contractor made a commitment to build on the laboratory's record of success in technology transfer, with an emphasis on engaging in regional economic development and fostering an entrepreneurial culture. The results have been impressive: nearly 100 new companies or product lines based on ORNL innovations have been launched. More than 400 jobs were created at a single plant in Louisville, Kentucky, where General Electric is manufacturing a hybrid electric heat pump water heater developed through a CRADA with ORNL. Today, ORNL has 106 technology licenses in place, and a Science and Technology Park on the ORNL campus is facilitating new and expanded partnerships.

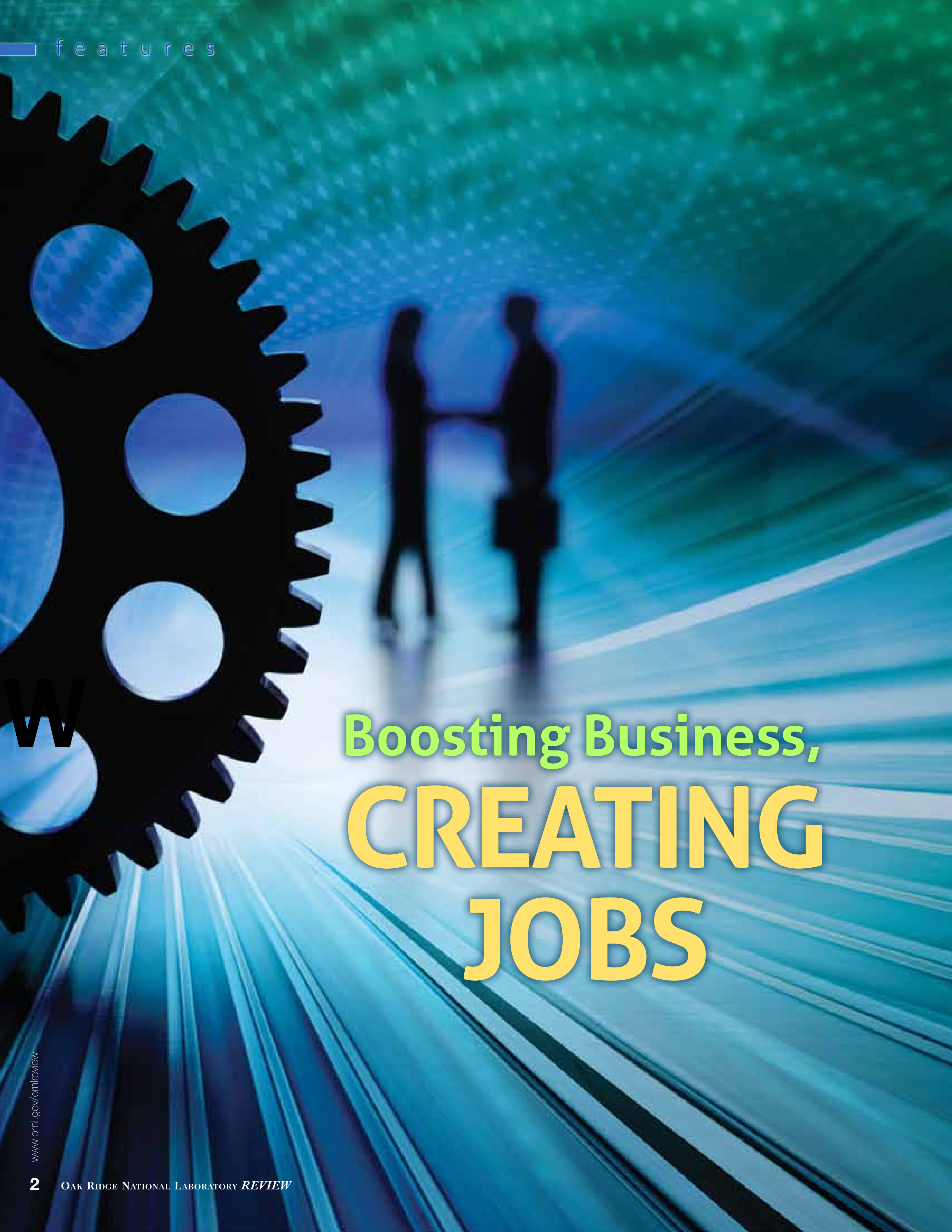
The growing recognition that innovation is the key to economic growth and global competitiveness creates new opportunities for ORNL to extend its record of excellence in partnering with industry. The need for transformative science and technology to solve problems in energy, environment and security provides a further impetus for ORNL to form partnerships that take advantage of the lab's exceptional capabilities and expertise.

We receive public funding based on the promise of a return to society in the form of jobs, improved standards of living, a more secure future, and clean and affordable energy. This promise is realized only when the science and technology that we develop makes its way into the commercial world, highlighting the importance of technology transfer to our mission.

This issue of the *ORNL Review* illustrates how we are leveraging public and private resources to strengthen our research portfolio and accelerate the translation of innovation to the marketplace. The work of the Manhattan Project partnership, which achieved its original mission and delivered unlooked-for benefits that continue to touch our lives today, is an inspiration to these efforts.

Thom Mason

Director, Oak Ridge National Laboratory



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Boosting Business, CREATING JOBS

Partnerships deliver technology to the marketplace

People don't usually think about the government's science labs as engines of economic development, but that's a role these scientific powerhouses are increasingly called on to play. In an era when private companies are cutting back their research and development divisions or sending R&D work overseas, ORNL is working with U.S. industrial partners to drive scientific and technological developments that support the economy and employ American workers. Every year ORNL's Partnerships organization hosts representatives from more than 100 companies, introducing them to the lab's capabilities and expertise and making them aware of the wide range of opportunities for scientific collaboration.

The laboratory's involvement with the business community has spiked over the last several years as the Partnerships organization has sharpened its focus on matching the laboratory's capabilities and research agenda with the needs of potential collaborators. Tom Ballard, who heads the Partnerships directorate, explains that his organization redoubled its efforts to make business and industry aware of the research capabilities of the laboratory, while at the same time helping individual scientists build or expand their relationships with business and industrial partners. "This is an enhancement of our traditional mission to license technologies and process research agreements," Ballard says. "I think this proactive approach to engaging both researchers and business partners has already benefitted the laboratory and will continue to pay dividends in the future."

Focusing on collaboration

The Partnerships organization's focused approach to collaboration with industry is characterized by developing closer relationships with researchers, actively engaging private companies and adopting more robust business practices.

Many experienced laboratory researchers, particularly those doing more applied work, already have a diverse mix of business relationships. Ballard's staff helps them build on existing relationships with funding sources at the Department of Energy, other federal agencies and the private sector, in addition to developing new ones. For younger researchers, Partnerships provides support in developing new connections with businesses. "We take the time to understand their research and its applications, so we can give them a hand in developing initial relationships that benefit their careers as well as the interests of our business partners," Ballard says.

Just as Partnerships is playing a more active role with ORNL scientists, it is also reaching out more aggressively to potential business and research partners nationally and even globally. Ballard's team is finding that companies are increasingly receptive to working with the laboratory to address specific research needs and gain access to world-class scientific facilities that will enable them to advance their research programs.

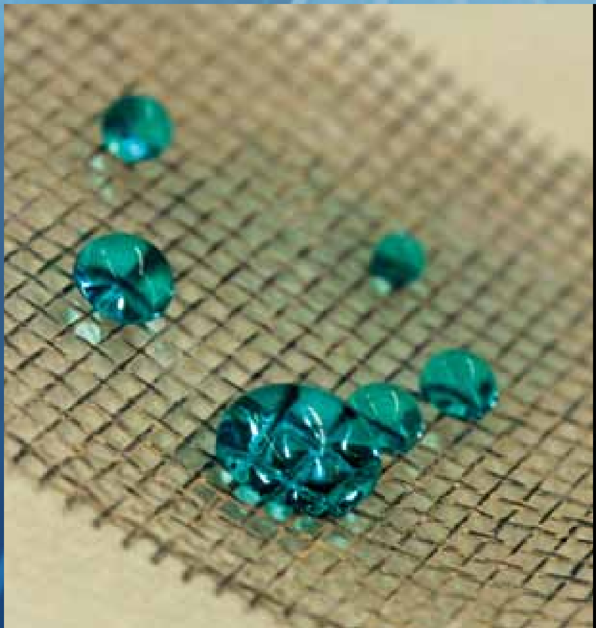
Ballard says his organization owes part of its recent success to what he calls "robust" business practices. That means taking a very proactive approach to implementing research agreements with the business community. "When we find opportunities to collaborate, we expedite all of the agreements that need to be in place for the research to begin as quickly as possible," he says. "It's like buying a car—you may shop around for a long while, but when you make a decision, you're ready to get the deal done. When the laboratory decides it's going to have a research relationship with industry, we work aggressively to get things started."

Companies work with the laboratory through either CRADAs (Cooperative Research and Development Agreements) or nonfederal WFO (Work for Others) agreements. Ballard explains that, in general, WFO agreements are made when ORNL will be doing most or all of the R&D needed to solve a problem. In a WFO partnership, the company usually has an R&D problem it wants to investigate, and ORNL has expertise or facilities that can't easily be found in the private sector. "Basically, the company is hiring us to do the research needed to solve their problem," Ballard says. CRADAs, on the other hand, happen when both the company and the laboratory have R&D resources. In these partnerships, scientists from both parties work together to solve the problem.

Building on success

The laboratory has always placed a premium on partnering with industry. However, Ballard recalls that the experience of competing for, and winning, the right to host a prestigious DOE collaborative research facility in 2004 raised the level of intensity of his entire organization and showed them what was needed to compete on a higher level. "Our transformation began with the competition that brought the Bioenergy Science Center to the laboratory," he says. "We had never pursued a research opportunity of that magnitude before. We had to develop a number of complex agreements among national laboratories, universities and industrial partners. This experience required close and dynamic interaction with a range of research partners. The intensity and pace of interaction that we developed on that project have become a part of our standard operating procedure."

Ballard recalls that before the BESC competition, Partnerships staff primarily waited for scientists to come to them with technological advances and then matched those advances with potential business



partners. Their experience with BESC showed them the necessity of being more proactive and knowledgeable about the research being done at ORNL and more closely engaged with potential research partners. "Now we are much more in tune with the laboratory's R&D portfolio, as well as with the needs of business," he says. "In the longer term, this can only lead to more success in commercializing ORNL-developed technologies."

Pursuing economic development

Not long after winning the BESC competition, the laboratory began to establish itself as an important economic development resource for the region. In 2007, several years into this effort, Partnerships received what turned out to be a fortuitous request from representatives of the city of Chattanooga and Hamilton County, Tennessee, asking for help in convincing Volkswagen to locate its new automobile factory in Chattanooga. "We're a 'national' laboratory," Ballard explains, "so if the people in Michigan or Alabama had asked us, we would have tried to help them, too; but it just so happened that the people just down the road in Chattanooga asked. Of course it made perfect sense for them to come to us. The laboratory has the largest transportation program in DOE, and we have many longstanding relationships with automotive industry through DOE's National Transportation Research Center."

After meetings with representatives of ORNL and a number of other organizations around the region, Volkswagen decided to locate its new factory in Chattanooga and has since hired 2000 workers. Ballard says he likes to think that the laboratory played a role in sealing the deal with the automaker. "It was obvious that the laboratory's research portfolio—particularly our materials expertise—was of great interest to Volkswagen," he recalls. "Since that time, we have set up collaborative research agreements with them to investigate lightweight carbon fiber components and battery storage. The big story here is that, by working with economic development organizations, we also opened up a pipeline of opportunities with a business that might not have otherwise explored a relationship with ORNL."

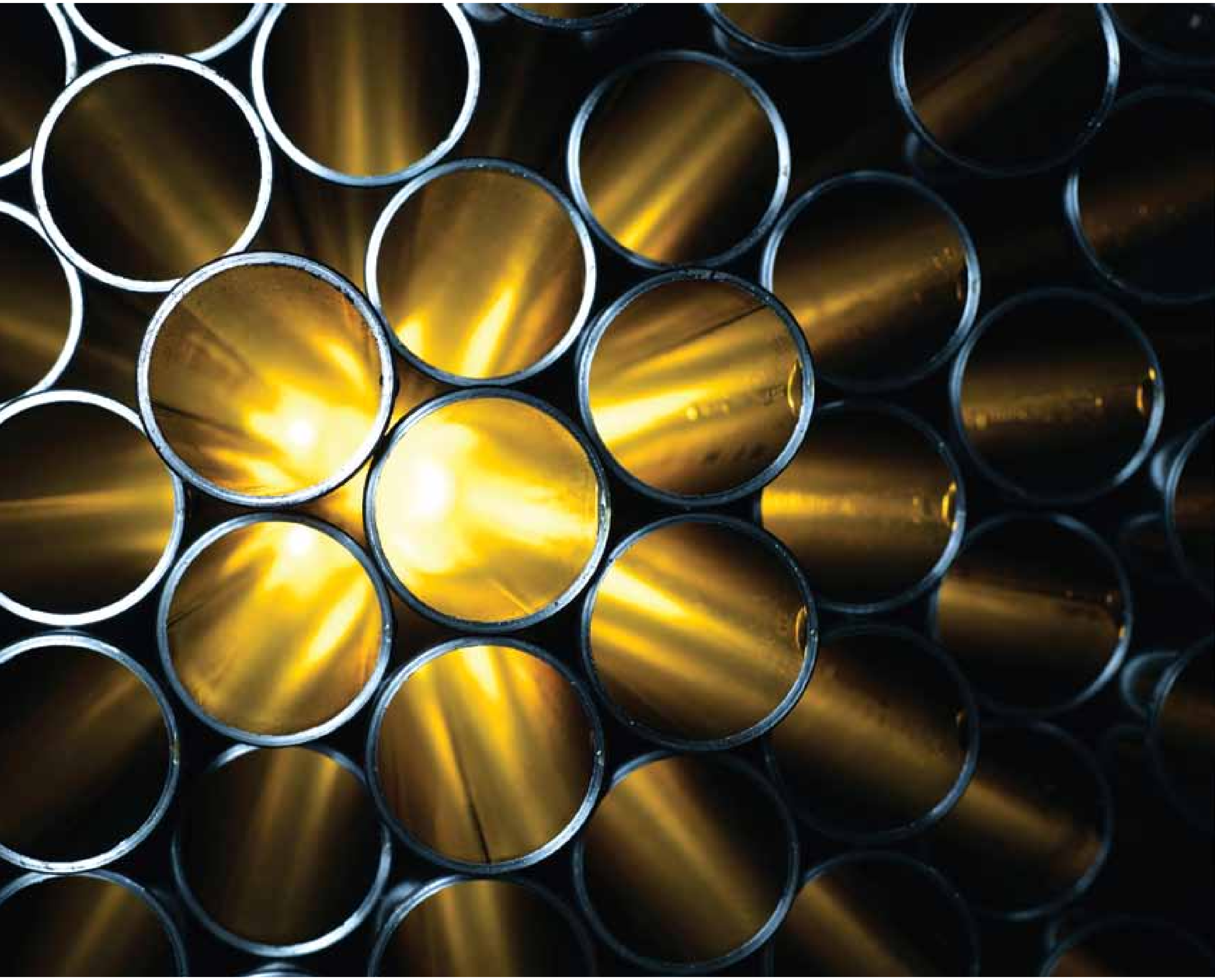
Ballard reasons that the biggest contribution the laboratory can make to economic development is to provide an incentive for companies to locate research divisions in the region. "Those facilities would provide good jobs," he says, "and there's some evidence that having a regional research and development base helps keep the associated manufacturing jobs in the region as well."

Ongoing opportunities

Partnerships has enjoyed continued success, playing a key role in bringing the Consortium for Advanced Simulation of Light Water Reactors to the laboratory. CASL is a collaborative effort among several national laboratories, the nuclear industry and the nonprofit Electric Power Research Institute to accelerate the development of the nation's next generation of light water reactors using ORNL's supercomputing and simulation capabilities. Ballard notes that his organization was part of the proposal team and continues to work as an intermediary among the various players. Ballard expects Partnerships to play a similar role in the competition to host DOE's Batteries and Energy Storage Hub sometime in 2012.

"We are always working to identify the next big opportunity for the laboratory to collaborate with industry, based on market needs, the players in the market and our research expertise," Ballard says. "ORNL will only be successful in fulfilling its mission and expanding its research portfolio by engaging in mutually beneficial collaborations with industry. At the end of the day, our goal is to deliver ORNL-developed technology to the marketplace where it can grow U.S. business, create jobs and enhance our global competitiveness." ®—*Jim Pearce*

ORNL is working with U.S. industry to drive scientific and technological developments that support the economy and employ American workers.



Getting an edge on the competition

Collaboration produces an award-winning, new technology

The R&D 100 Awards presented by *R&D Magazine* to scientists and engineers for their technological prowess are sometimes referred to as the "Academy Awards of Science." This year ORNL won seven, and four of them went to researchers in the laboratory's Industrial Technologies Program. ITP Manager Craig Blue says the program provides a way for ORNL to collaborate with industry to develop energy-related technologies that improve the ability of U.S. industries to succeed in an increasingly competitive global marketplace.

One of this year's award-winning technologies is CermaClad, a process for creating wear- and corrosion-resistant coatings on a wide range of metal surfaces. Developed jointly by ORNL and MesoCoat of Euclid, Ohio, and in collaboration with the Edison Materials Technology Center of Dayton, Ohio, CermaClad is expected to be used initially as a protective coating on the inner surfaces of pipelines used in oil and gas transportation—both above and below ground.

Laboratory roots

Blue notes that the CermaClad process makes extensive use of technologies that were originally developed at ORNL. In fact, Greg Engleman, MesoCoat's chief technology officer, worked at the laboratory from 1998 until 2007. Engleman says he and Blue helped install the lab's first plasma arc lamp facility. "At the time, I heard there was a company called Powdermet looking at this technology for processing coatings," Engleman recalls. "So I decided to venture out and go to work for them. MesoCoat was spun off from Powdermet in 2008 with the intention of promoting both plasma arc lamp technology and a drop-in powder feedstock for thermal spray technologies."

"The laboratory's main contribution to the CermaClad collaboration was providing the plasma arc lamp technology," explains Blue. This technology uses an infrared plasma arc lamp for "liquid phase fusing" of ceramic/metallic coatings. The process involves spraying a metallic or composite material onto a surface. Then to ensure a good bond between the surface and the coating, the coating is heated until it turns liquid. The result is a wear-resistant coating on a metal surface. Researchers use plasma arc lamps that can fuse an area up to 30 centimeters wide, whereas traditional fusing uses a centimeter-wide laser beam. This approach is more energy-efficient and provides a more homogeneous coating than other fusing technologies.

Engleman says that when MesoCoat licensed the plasma arc lamp technology from ORNL, the lab also provided a great deal of information about potential trouble spots in applying the technology and how to get past those problems. "That information was very helpful in our effort to get this technology to market. All of the basic research done at the laboratory gave us an advantage over the competition when we started to look for capital to move this technology forward."

Faster, cheaper, better

CermaClad coatings encompass a range of applications, but they are primarily focused on improving corrosion and wear resistance. The most popular application is currently CRA materials—corrosion resistant alloys—for use in the oil and gas market. MesoCoat is using CRA materials to coat the inside surfaces of 12-meter-long oil pipes. The coating reduces corrosion and increases both the lifetime of the pipe and the efficiency of the pumping process. "We can use this technology in any pipe from 20 centimeters in diameter up," Engleman says. The process that MesoCoat is using is 25 to 180 times faster than traditional weld or laser cladding, and speeding up the process results in considerable cost savings. "We are still establishing a price point, but our intention is to be below the price point of weld overlay claddings," he adds.

MesoCoat is also working with a major oil company to explore the use of CermaClad pipe for undersea use as well. This potential customer wants to use CermaClad coating to improve the efficiency of oil pumping. Engleman explains that current methods of pipe cladding create small ridges inside the pipe. Those little ridges create turbulence, which slows down the flow of oil and requires higher pumping pressures. The CermaClad process puts down a smoother coating that reduces ridges and allows smoother flow of oil through the pipe.

While the oil industry is the first market MesoCoat is exploring, the company is also looking into a number of other applications. Engleman sees potential applications in the transportation industry for a product called CermaClad-LT, which would be used to treat cargo tanks for corrosive materials or chemicals and prevent corrosion and wear in containers used to store spent nuclear fuel.

Maintaining an edge

ORNL's relationship with MesoCoat has been an unqualified success and shows no sign of ending any time soon. Engleman says that in addition to their ongoing research, the two organizations have signed an agreement to conduct further studies on wear- and corrosion-resistant materials and are discussing collaborative research in other areas as well. "These joint projects will allow us to develop materials to improve the CermaClad process, maintain our edge in the market, and introduce more products more quickly. The opportunity to partner with ORNL on this research has been invaluable; there is no place else we could have performed this work."

"Our relationship with MesoCoat is a good example of what a national laboratory can do to support U.S. industry," Blue observes. "Our job is to develop a technology to the point where private companies like MesoCoat can apply this know-how to create successful commercial products." Ⓡ—*Jim Pearce*

The CermaClad process will to be used to apply a protective coating on the inner surfaces of pipelines used in oil and gas transportation.

Neutrons probe inner workings of batteries

Designing long-lasting, reliable batteries is the key to wider acceptance of electric vehicles

Listen for any length of time to Ke An, lead scientist for the VULCAN engineering diffractometer at the Spallation Neutron Source, and you're sure to hear "Nobody has done this before" and "couldn't be done anywhere else." And he's right. VULCAN has capabilities available nowhere else, and the instrument has become a popular tool for researchers in industry, even though it has been available to users for only a little over a year.

As its name suggests—Vulcan was the Roman god of fire and metalworking—the instrument was built with industrial applications in mind, says Xun-Li Wang, lead scientist for materials science and engineering in ORNL's Neutron Sciences Directorate. In addition to excellent neutron optics, the instrument features an open sample area that accommodates specimens ranging from a few grams of material to jet engines and vehicle bodies. The open space also enables in situ studies of materials behavior under realistic, simulated operating conditions.

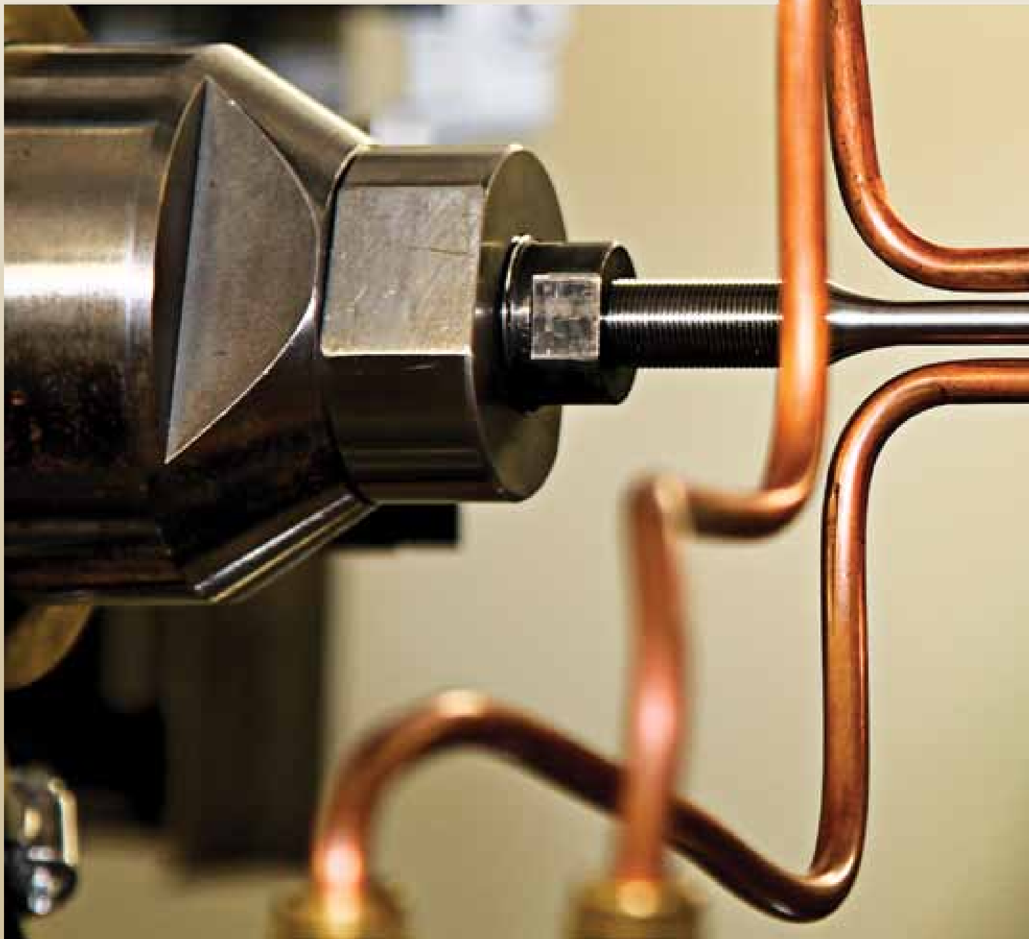
The massively capable instrument is a big draw for scientists and engineers working to advance battery technology. Before VULCAN officially opened to users, a research team led by Zhili Feng of ORNL's Materials Science and Technology Division, Wang, and An used it to conduct pioneering experiments on lithium-ion batteries as part of an ongoing collaboration with industry. Since then, the ORNL team has been working with General Motors, Dow Kokam and other battery manufacturers. Besides these direct collaborations, academic researchers are using VULCAN to explore the inner lives of batteries to improve their performance.

Better batteries are essential to transitioning vehicle drive systems from internal combustion engines to electrical motors. To succeed as power sources, batteries must be quick and convenient to charge, long-lasting, reliable and able to power a vehicle for a reasonable distance without recharging. Li-ion batteries are popular for the automotive market because they store a lot of energy and are relatively lightweight. But performance degradation as batteries are depleted and recharged hundreds of times is a persistent issue and a barrier to widespread adoption of electric vehicles.

To slow battery degradation, scientists and engineers need to understand atomic-level mechanics of the process under working conditions. That requires looking into the battery's molecular structure and observing chemical phenomena occurring in a battery's anode and cathode as it works. "VULCAN lets us observe the structural evolution in both electrodes in real time. Its unique capabilities and the unique power of the pulsed SNS neutron beam allow us to take 'snaphots' of the process at closer time intervals and and collect more comprehensive data faster than ever before," An says.

"Seeing" internal changes

The initial GM experiments examined battery cells for electric vehicles after hundreds of charge/discharge cycles. (An EV battery consists of hundreds of such cells.) Neutrons were used to map several points inside the molecular framework of the cells to see how internal stresses and irregularities were distributed. The cells were then charged and mapped again on VULCAN to show structural differences between the charged and discharged state for a degraded battery. They were



also probed with neutrons during a series of charge/discharge cycles, allowing the GM team to "see" structural changes inside the batteries as they occurred.

The GM team was very surprised by the power of VULCAN and satisfied with the results it obtained, says An, and soon returned to VULCAN for a second set of experiments on a new EV battery. This time, they were able to observe, in real time, lithium ions being absorbed into the carbide structure of a battery as it charged and discharged. "This was the first time data have been collected in real time at such close intervals using neutron scattering," An notes.

"We used high-intensity neutron beams to observe the real-time charge and discharge of a battery—not a slow discharge over several hours, but a real-time discharge, in real-world conditions, in less than an hour," An explained. The neutrons showed the actual chemical reactions as lithium moved from one side of the battery electrode to the other. "We now can use neutrons to see this; once we understand this process, we can tune it," he says.

Inconsistent conditions, such as charge levels, current densities, and temperatures across battery cells are suspected of accelerating degradation, but there is little quantitative information about how they do so, says Stephen Harris of the GM Technical Center, an expert in Li-ion battery research. VULCAN's ability to measure transient phenomena like these at microsecond time steps allowed the experimenters to precisely track environmental conditions in different areas of the battery cells as charging/discharging progressed.

An added advantage is that the high power of the SNS neutron beam—the most intense pulsed beam in the world—enabled the team to complete its studies in less than a week.

The team completed a third set of measurements on the GM batteries at VULCAN during early 2011 and has an experiment on a degraded battery scheduled for later in the year, says Feng. "For the coming experiment, the battery we studied before will be charged and discharged by several hundreds of cycles or more to be degraded," he says. "We'll cycle the battery to 50 to 70 percent of its original capacity and repeat the experiment we did before, looking at the structural and chemistry evolution to understand the degradation mechanism."

The Vulcan instrument can analyze samples ranging in size from a few grams of material to jet engines and vehicle bodies. (Photo: Jason Richards)

Reaching out to industry

With a set of 25 instruments in the user program at SNS and the High Flux Isotope Reactor, ORNL is broadening its outreach to potential industrial users. VULCAN is one of several instruments at SNS and HFIR with a user base in industry. The Neutron Residual Stress Mapping Facility and General Purpose Small-Angle Neutron Scattering Diffractometer at HFIR regularly conduct experiments driven by industrial needs, notes Wang. HFIR staff members are working with a number of American manufacturers to improve product lines such as diesel engines, heating and cooling systems and batteries. The research at SNS and HFIR is also closely watched by research and development departments across a swath of other industries, including pharmaceuticals, electronics, solar cells, fuel cells, nuclear power, plastics, transportation, mining and petroleum, says Thomas Proffen, leader of Neutron Sciences's powder diffraction group.

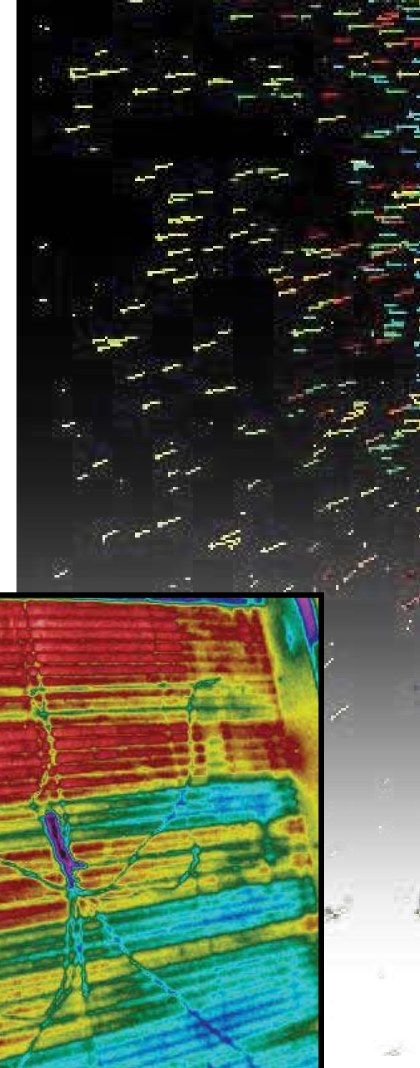
ORNL is eager to show industrial users that neutron scattering can provide them with the information they need, Proffen says. Researchers from industry tend to have a different agenda than academic scientists, who explore problems at great length and value even inconclusive results, he says. Industry researchers "want to know enough to answer a question. The pressure is on them to obtain reliable results they can report back quickly."

Neutron Science's strategies for growing its industrial user base include holding workshops to show potential users what neutron research can do, making access to the facilities easier, and providing tools to help users analyze their data.

"It's a matter of finding out what problems industry is trying to address," Proffen says."Once we know that, we connect the people who know the research techniques with the people who have the problems and move on from there." R—*Deborah Counce*

Air-conditioning the desert

Boosting heat pump efficiency reduces power demand and consumer cost



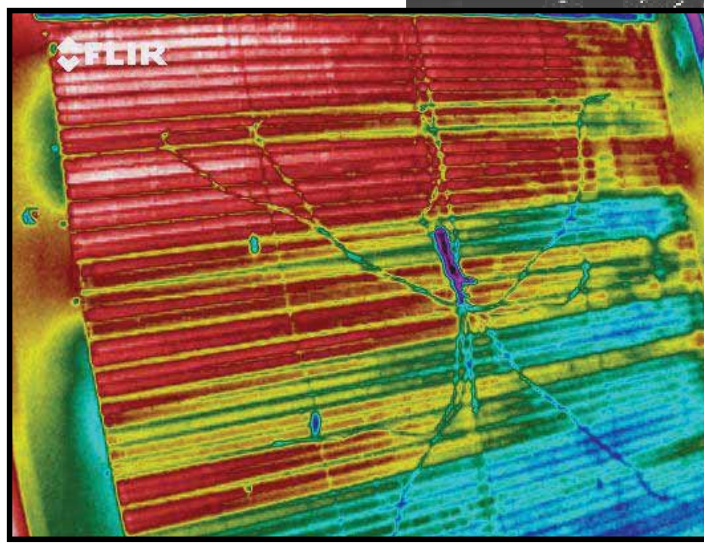
Over the last decade the population of Las Vegas, Nevada, ballooned by nearly a third. At the peak of the surge, 5000 families were moving to town every month. As it turns out, the population boom has been a bust for local electric power plants that rely on scarce water resources for their cooling towers in this arid part of the country. To help reduce the demand for electricity, several local utility companies encouraged customers to supplement their electricity usage with natural gas appliances. One of these companies, Southwest Gas, went so far as to design its own natural gas-powered heat pump. Gas heat pumps are a particularly attractive option in the Las Vegas area because they not only use 85 percent less electricity than electric units, but they also enable customers to avoid premium charges for electricity use during peak-demand hours.

When Ed Vineyard's group in ORNL's Energy and Transportation Science Division heard about Southwest Gas's plan to lighten the load on the Las Vegas electric grid, the unusual nature of the project captured their attention. "Utilities aren't normally in the business of designing heat pumps," Vineyard says, "but Southwest Gas had a prototype for small commercial buildings they wanted to have evaluated, so we asked if they wanted us to do some testing."

An efficient solution

In Las Vegas in the summer, a heat pump's primary job is the same as that of an air conditioner: to pull warm air out of a building and through a heat exchanger, cool it down and pump it back inside. The more efficiently this happens, the less it costs to do it. That's where ORNL's test facilities come in. ORNL is nationally respected for its expertise in testing and evaluating heat pumps and other HVAC equipment, and laboratory researchers have worked with several of the major manufacturers to evaluate and improve the efficiency of their units. The laboratory tests heat pumps in two large environmental chambers. The units are evaluated at industry standard temperature and humidity levels for both heating and cooling. By measuring the temperature of the room while a heat pump is running, researchers can calculate the heating and cooling capacity and efficiency of the unit.

When Southwest Gas sent its initial prototype to Oak Ridge, Vineyard's group ran a battery of efficiency tests on it and found that its performance has plenty of room for improvement. "As it turns out," Vineyard recalls, "the heat exchangers weren't functioning efficiently." To do a thorough study of the problem, ORNL and Southwest Gas sought and received funding from the Department of Energy to develop a more efficient prototype of a gas heat pump.



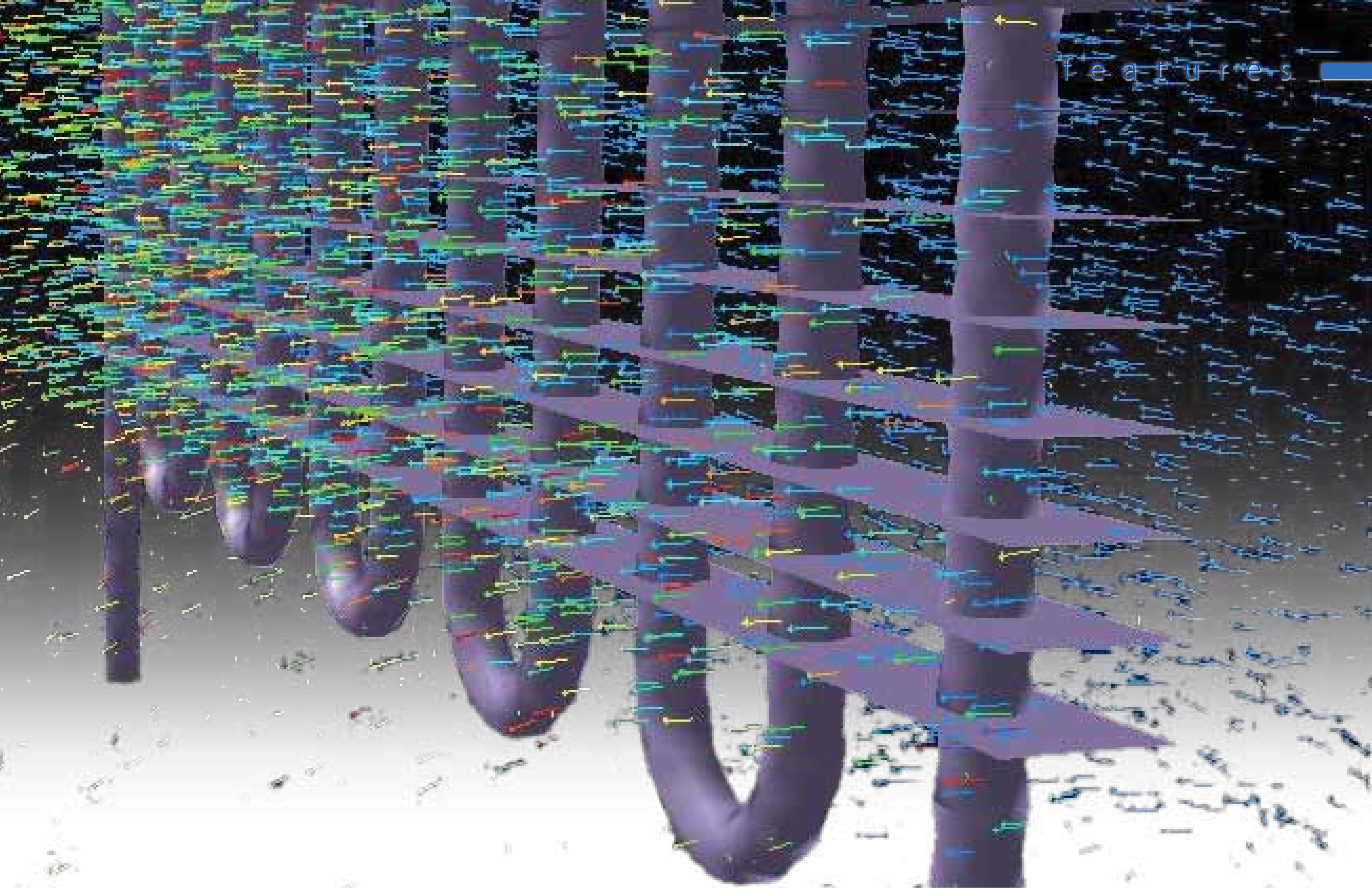
Using sensitive thermal cameras and computer modeling, ORNL and Southwest Gas developed a heat pump that is about 25 percent more efficient.

During the course of the collaboration, the laboratory and Southwest Gas shared design responsibilities. Southwest Gas built the prototypes, and ORNL created the computer models and did the testing and analysis of the unit.

Through several rounds of testing and analysis, Vineyard's group paid particular attention to the efficiency of the unit's heat exchanger, making a series of measurements using sensitive thermal cameras. These studies found that uneven airflow across the heat exchanger caused a 10- to 15-degree temperature difference between the warmest and coolest parts of the device.

Building a better heat pump

Normally heat pump airflow problems can be addressed by rearranging components inside the unit, allowing more room for the air to circulate. However, because this heat pump was a rooftop unit, both size and weight were concerns. "We wanted to have an efficient



airflow path and the most compact system possible," Vineyard recalls. "Generally, those parameters are at odds with one another." Eventually, using fluid dynamics modeling to build computer simulations of the air flow paths within the unit, the research team developed a configuration that greatly increased the efficiency of the heat exchanger within the available space. "When we do fluid dynamics modeling," he explains, "we build the model in pieces. For example, we model the air flow through the heat exchangers, through the radiator for the gas engine and through the exhaust fans separately. Then we put them together to build a model of airflow through the entire unit." Several computer models and prototypes later, the result of this process was a unit in which the temperature variations across the heat exchanger were reduced to 1 or 2 degrees Fahrenheit.

Vineyard says that the improved prototype developed by Southwest Gas and ORNL is about 25% more efficient than the original unit. The cost savings provided by this increase in efficiency suggest the unit could pay for itself in about 3 years, depending on the price of natural gas and electricity.

Not long after this highly efficient unit was completed, the technology behind it was licensed and brought to market by Intellichoice Energy under the name NextAire. The design and performance of the NextAire Packaged Gas Heat Pump was impressive enough to earn ORNL, Southwest Gas and Intellichoice Energy a 2011 R&D 100 Award from *R&D Magazine*. R&D 100 Awards honor the 100 most outstanding advances in technology for the year and are chosen by an expert panel of independent judges and the magazine's editors.

Encore performance

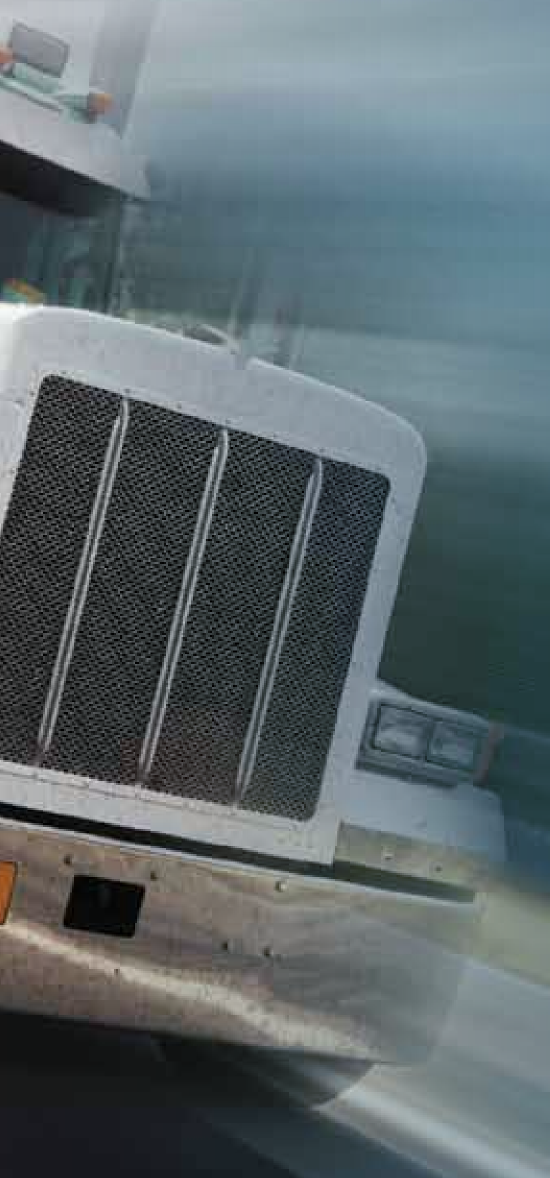
The successful conclusion of the laboratory's original collaboration with Southwest Gas won't be the end of the partnership between the organizations. The research team is currently working on improving the overall efficiency of a smaller, residential gas heat pump by incorporating water heating and using engine heat to improve overall system efficiency. In addition to heating and cooling, plans for the residential prototype include adding an alternator and storage batteries to enable the system to generate and store electricity during off-peak hours.

Vineyard notes that while working with a gas heat pump enables designers to build in a lot of extra functionality, the primary goal of the collaboration is still to design a system that offers a significant improvement over the state of the art and is competitive in the commercial heat pump market. "That's a big challenge," he says. "Once that's taken care of, we'll think about adding features to it." Ⓡ
—*Jim Pearce*

Designing a SMART TRUCK with the power of Jaguar

One of these days as you're traveling down the interstate, don't be surprised if you see a an 18-wheeler that looks more like a low-flying airplane than the familiar big rig. A perfect storm of factors is providing the impetus to revolutionize truck design, including high fuel costs, heightened environmental awareness, and mandates from state and federal agencies to boost fuel efficiency and reduce carbon emissions. Today's trucks average only 6 mpg or less and add a whopping 423 million pounds of CO_2 to the atmosphere every year. However, new California Air Resources Board regulations mandate a minimum mileage improvement of 5 percent for long-haul trucks operating within the state's borders.

For truck owners, CARB is a headache. For SmartTruck Systems in Greenville, South Carolina, the new rules present a golden opportunity. Says Mike Henderson, CEO of SmartTruck, "CARB and the other regulatory rules impacting the trucking industry are opening up an entirely new market for us." Before founding SmartTruck Systems, Henderson was a 30-year veteran of the Boeing Company. He and his team of engineers are specialists in the design of aerodynamically advanced aircraft as well as racing and motorsports vehicles. That experience includes the use of advanced modeling and simulation techniques made possible by computational fluid dynamics (CFD) software running on high-performance computers—a set of skills that they now apply to the problem of making Class 8 trucks more fuel-efficient and less polluting.



Retrofitting what's already on the road

SmartTruck took a both short- and long-term approach to complying with present and future mandates. First, given the impending CARB regulations, completely redesigning the long-haul trucks from the tires up was not an option. Instead, they needed an economical, efficient solution that could be applied to trucks already on the road. Then they could turn their attention to a "clean sheet" design for the truck of the future. SmartTruck's answer to its immediate need was to launch the Smart Truck program.

"Our first goal is to design add-on parts for existing trucks to make them more aerodynamic," Henderson says. "By reducing drag we boost fuel efficiency and cut the amount of carbon that's being dumped into the environment. Once we have the existing fleets retrofitted, we can turn to creating a brand new, highly aerodynamic vehicle with optimum fuel efficiency."

A Class 8 truck consists of two parts—the tractor, a motorized vehicle that is used to tow a trailer, a large container unit without an engine, front wheels, or front axle. Combined, the two units are called an 18-wheeler, referring to the truck's total number of tires.

Initially, the SmartTruck team used a high-performance computing cluster to model drag-reducing parts for the trailer by simulating the action of complex airflows over and around a typical unit. The team used a conventional HPC cluster with a limited number of computing cores—and they were not happy with the results. "On the conventional cluster we had to simplify the problem," Henderson explains. "We couldn't handle the really complex models—the solutions lacked accuracy. We could explore possibilities, but we couldn't run the detailed simulations needed to verify that the designs were meeting our fuel-efficiency goals."

SmartTruck Systems was, as they say in computer industry jargon, computebound. Its engineers needed orders of magnitude additional computing capability, both to run highly detailed, accurate models of the trailer retrofit components and to get the results in time to meet the looming CARB deadlines.

Hunting a Jaguar

At the recommendation of some aerospace colleagues, SmartTruck approached the Oak Ridge Leadership Computing Facility at ORNL. Through the laboratory's Industrial HPC Partnerships Program, SmartTruck applied for and received access to the extraordinary computational capabilities of the Jaguar high-performance computer.

Access to Jaguar allowed SmartTruck Systems to design the UnderTray System, a unique group of aerodynamic add-on parts that minimizes drag associated with the trailer's underside components. The UnderTray System compresses and accelerates incoming airflow as well as injecting high-energy incoming air and attached airflow from the top of the trailer down into the trailer's wake.

On the smaller HPC clusters that SmartTruck was using before moving to Jaguar, running a model of a typical UnderTray component might take 4 days and use every resource the cluster had to offer. Jaguar allows the SmartTruck engineers to break the truck into hundreds of pieces in order to calculate drag with a high degree of accuracy. Says John Anastos, SmartTruck project engineer, "Breaking the model down into that many pieces and resolving the flow on each one is something you can't do with a small cluster—it would take weeks to get a solution. But with Jaguar we can do whatever we want in terms of complexity and still get reasonable results that allow us to turn the design around in hours instead of days. All we leave out are the nuts and bolts—every other detail is represented in the computer."

Impact at a glance

Jaguar is DOE's flagship supercomputer. With almost a quarter of a million processing cores and a theoretical peak computational capability of 2.3 petaflops, the world's largest Cray XT was more than able to provide SmartTruck Systems with all the computational power it needed. (A petaflop is a measure of a computer's processing speed and refers to a thousand trillion [one quadrillion] floating point operations per second.) In addition, SmartTruck opted to run the FUN3D application, the National Aeronautics and Space Administration's CFD software that is used widely in the aerospace industry.

Challenge

- Design retrofit parts for Class 8 long-haul trucks (18-wheelers) to improve fuel efficiency in time to meet looming California regulations

Solution

- Tap into the power of Jaguar, the Department of Energy's flagship high-performance computer at ORNL, to run detailed simulations in record time

High-performance computing impact

- Run simulations based on the most complex tractor and trailer model ever devised instead of simplified models, and run them faster
- Dramatically shorten design turnaround from days to a few hours
- Eliminate the need for costly and time-consuming physical prototypes

Business benefits

- Significantly reduce time-to-market for new products from more than 3 years to 18 months
- Pass EPA tests with new parts on first attempt, an unprecedented result in this industry
- Increase revenue and market share opportunity
- Assume leadership position in an emerging industry with great potential
- Strengthen the manufacturers engaged in production

Design digitally, confirm physically

Access to Jaguar led SmartTruck to the holy grail that many manufacturers seek: the ability to substantially reduce or completely bypass the costly and time-consuming process of creating multiple physical prototypes in the design phase of new product development.

Comments Henderson, "Developing these parts through physical experimentation is a real exercise in frustration, which is one reason it hasn't been done. It's extremely expensive, and you don't learn with a CFD solution. So we develop our designs computationally, and then confirm them physically through testing to be sure we haven't

Trailers equipped with SmartTruck Systems components can achieve seven to twelve percent better fuel mileage. (Images: SmartTruck Systems)

overlooked a problem. With the speed and power of Jaguar, we were able to create and evaluate the most complex model of a trailer to date and dramatically accelerate that design process."

The approach worked. When it came to correlating the computer-generated simulations with physical tests in the field, the SmartTruck team scored an A+. The team's test truck, loaded with prototype components and telemetry, was put through its paces on the world's longest, smoothest concrete landing strip—the 18,000-foot runway at the Kennedy Space Center. These tests confirmed the accuracy of the CFD simulations and the operational efficiency of the new add-on component designs based on those simulations.

From calculation to compliance

"We were pleased to see how close our CFD simulations matched the physical test results," says Henderson. "The process works—physical test results were within 1 percent of our CFD calculations, and we were able to pass Environmental Protection Agency fuel tests on the first try—something almost unheard of in our industry. Without Oak Ridge and Jaguar it would be impossible to be where we are today."

The EPA SmartWays program has certified the UnderTray system components with a 6.8 percent fuel savings, designating them as CARB-compliant for use in California. This goal was reached with a minimum package; a full set of UnderTray components provides nearly a 12 percent savings. If all of the 1.3 million Class 8 trucks in the country were configured with just the minimum package of new components, the United States could annually save almost 1.5 billion gallons of diesel fuel; reduce CO_2 by 32.7 billion pounds (16.4 million tons); and save $4.42 billion in fuel costs.

Launching an industry

In the highly competitive industrial world, cool designs matter only if they generate hard cash. By bringing products to market faster, SmartTruck Systems will realize revenue earlier and move into a leadership position in a new industry. With this early-to-market advantage, the companies should capture even greater market share, increasing their revenue opportunity.

However, the positive economic impact extends beyond SmartTruck. The parts for the Smart Truck retrofits are being manufactured in Georgia by Cellofoam, and the various metal hardware components, such as screws and brackets, are being manufactured by a variety of metal companies in South Carolina. In today's stressed economic environment, the addition of any type of domestic manufacturing is beneficial to both the region and the country as a whole, providing economic stimulus at the local and national levels.

Next steps

Market receptivity has been positive and quick. *Heavy Duty Trucking* magazine, a leading industry publication, named the new UnderTray system one of the top 20 products of the year. The first production UnderTray products are being installed on fleets owned by SmartTruck Systems customers Frito-Lay, Swift Transportation, and Conway Truckload, permitting the fleets to move products into and throughout California. The company has embarked on the next phase of its truck-retrofitting program with the design of a new aerodynamic trailer configuration and fuel-efficient modifications to existing tractors.

At the same time, SmartTruck is taking the first steps toward its long-term goal: the design of a highly aerodynamic truck from the ground up—an ambitious "clean sheet" project. In the not too distant future, this work will culminate in the creation of "Super Truck," a futuristic vehicle with astonishing fuel efficiency that may bear little resemblance to the classic big rigs currently on the road. R

—John Kirkley

a BIOENERGY ecosystem

BESC partnerships translate R&D into biofuels

Paul Gilna, director of the BioEnergy Science Center at ORNL, is a man on a mission. In fact his entire organization is working under a Department of Energy mandate to focus the world's leading scientific minds and resources on revolutionizing bioenergy production. When the center was created in 2007, this innovative partnership of national laboratories, a private research foundation, universities and industries set out to break down the barriers to developing viable and affordable biofuel alternatives to petroleum-based fuels from plants that do not compete with food crops, such as switchgrass or poplar trees. Four years into a five-year mission, they have already provided considerable evidence that that they can achieve what they set out to do.

Breaking down barriers

Gilna cites three main areas where the BESC collaboration has made significant progress. First, the center achieved its primary goal by demonstrating that scientists can genetically modify a biofuel crop, or feedstock, to increase the amount of biofuel it produces. This breakthrough is critical to the future of biofuels because it promises to significantly reduce the cost of the entire biofuel production process.

The center has also made huge strides toward its goal of developing consolidated bioprocessing microbes—genetically altered microbes, such as yeast, that can digest plant material, extract its sugar content and turn it into ethanol or more advanced biofuels. This research has advanced to the point where one of BESC's industrial partners plans to build a commercial-scale biofuel production facility that employs microbes developed in collaboration with BESC partners.

Finally, the center has collaborated on a regional level with industrial partners to develop what Gilna describes as the beginnings of "a tightly woven bioenergy ecosystem." "We are working with the biotech firm Ceres to develop more efficient feedstocks based on our science. Once regulatory hurdles are satisfied, we can see a day where Ceres will in turn work with Genera, a University of Tennessee bioenergy spinoff company, to grow those feedstocks with the cooperation of a consortium of Tennessee farmers. The crops the farmers produce will be delivered to DuPont Danisco's Vonore, Tennessee, ethanol production facilities to be processed into biofuel." All of this is happening at a demonstration level, but Gilna expects biofuel production in the southeastern U.S. to become a self-sustaining industry. As evidence of this, Gilna notes that DuPont, Inc., has openly discussed plans to construct a cellulosic ethanol plant in the Southeast, possibly in Tennessee.

Although centered in Tennessee, BESC works with scientists at institutions throughout country. However, the regional flavor of the center's efforts to form a "bioenergy ecosystem" is intentional. In fact, there are three regional DOE bioenergy research centers across the U.S. The other two are the DOE Great Lakes Bioenergy Research Center, led by the University of Wisconsin in collaboration with Michigan State University, and the DOE Joint BioEnergy Institute, led by DOE's Lawrence Berkeley National Laboratory. Gilna says he is sometimes asked why the DOE needs three different bioenergy centers. "The strength of our complementary approaches lies in their very diversity," he says. "The biofuels industry in the U.S. will be likely be highly regionalized, so what works in the Northwest may be different than what works in the Southeast." As a result, having a geographically diverse set of centers, and therefore a diverse set of approaches to making bioenergy a viable option, increases the likelihood that the U.S. will meet the goal of increasing biofuels production nationwide.

Evolving relationships

BESC's closest relationships are with its partners, which include fifteen federal or academic research institutions, the Samuel Roberts Noble Foundation and three private companies. "Our industrial partners are part of the fabric of the project," Gilna says. "Ceres focuses on the development of biomass feedstocks, ArborGen develops wood-based biomass, and Mascoma is a multifaceted bioenergy company. Their personnel are an integral part of our research and development activities."

The center also has a second tier of commercial collaborators, called "affiliates." These companies have a business interest in the center's activities, but they are not directly involved in BESC's research and development program. Affiliates are provided with "additional, though not exclusive" access to information and activities. For example, they are notified of the center's invention disclosures—also available to the public—and they can attend BESC's annual retreat, where the normally widely distributed project staff come together to present and discuss their research.

Gilna notes that BESC's relationships with its research partners have evolved over the last four years. "As our research has progressed, we have often had to adjust how we work with our partners," Gilna says. "For example, we never envisioned we would be ready for field trials of genetically modified feedstocks as quickly as we were. However, we were able to adjust course and accelerate an effort with one of our partners to capitalize on this advance and get the field

Clyde Thurman of Monroe County, Tennessee, and his 76 acres of switchgrass. Thurman was among the first farmers to grow switchgrass as part of the University of Tennessee Biofuels Initiative. (Photo: Ken Goddard, UT Extension)

BESC scientist Jonathan Mielenz works with biomass-degrading microbes that thrive in an oxygen-free environment. (Photo: Jason Richards)

trials started early." Having a close scientific relationship with bioenergy companies has occasionally led to cooperation between BESC partners and ORNL in areas outside the bioenergy center. Gilna observes that BESC's research partners now have greater awareness of the range of ORNL technologies that could be useful to them.

Publications in scientific journals produced by BESC researchers have also been a catalyst in moving technological advancements from the laboratory to the private sector. Gilna cites several examples of research partners' applying published BESC research directly to their commercial enterprises. "For example," he says, "we made genetic changes to switchgrass that resulted in a 25 percent higher yield of ethanol. Shortly after we published the results of the work in a scientific journal, one of our partners applied the modification to other commercially available strains of switchgrass. They are still in the process of determining whether they will see a similar improvement in ethanol yield, but the main message here is that they had enough confidence in our work to make an investment in this technology based on their association with us."

Future focus

DOE's mandate for the first five years of BESC's life was to understand the chemistry and genetics behind the unwillingness, or recalcitrance, of plants to release their sugars and then to develop ways of modifying plants and microbes to overcome that recalcitrance. Having accomplished the lion's share of what they set out to do, BESC is hoping to receive a five-year extension of its mandate to build on its progress and completely eliminate recalcitrance as a barrier to the economical production of biofuels.

"It's all about reducing the cost of biofuel production to the point that it is competitive with other fuels," Gilna says. "Developing affordable, sustainable biofuels and reducing our dependence on foreign oil will boost our economy and have huge implications for the nation's transportation sector. This is an exciting and noble goal that will truly make a difference, and we believe we know how to get there." Ⓡ—*Jim Pearce*

POWER from the sea

Innovation at the crossroads of global security and green energy

Technological developments are generally incremental changes that slip mostly unnoticed into business practices, industrial processes and daily routines. Those aren't the kind of scientific advancements Lockheed Martin Corporation's Open Innovation Program seeks to address. Johnnie Cannon, who heads up ORNL's Global Security Directorate's collaboration with the program, says its goal is to develop "disruptive" technologies that leapfrog the competition, rather than making gradual, predictable progress. Currently Cannon's collaboration portfolio consists of active projects in a range of disciplines, including advanced materials, quantum computing and ocean thermal energy conversion.

"One of our highest profile collaborations with the Open Innovation Program is Ocean Thermal Energy Conversion," Cannon says. "It represents a substantial investment by LMC over several years." OTEC can be used to address the U.S. military's energy needs in parts of the world where long supply lines or distant power-generation facilities make generating power problematic.

Power from the sea

OTEC uses temperature differences in the world's oceans to create energy. In the tropics, the surface water temperature is about 25 degrees C; and at 3000 feet down it's about 5 degrees C. "That's a difference of about 20 degrees C, and can be used to generate power," says James Klett of ORNL's Materials Science and Technology Division. The OTEC power generation system works by using this temperature difference to drive a closed-loop Rankine cycle power plant. The Rankine cycle begins by pumping the 25 degree C surface water through a heat exchanger to boil ammonia. The ammonia becomes a gas, which is used to spin a turbine-generator to produce power. Then, the 5 degree C water is used to cool the ammonia, which condenses to its liquid state within a heat exchanger called a condenser, and the cycle starts over again.

Given the state of current OTEC technology, a commercial-scale OTEC power plant would require at least 20 very large heat exchangers. That's where the graphite-foam-based heat exchangers developed by Klett and his research team come in. Graphite foam combines a tremendous amount of surface area with a high capacity for conducting heat, enabling these heat exchangers to improve the performance of standard thermally conducting units while reducing their size and cost. Making heat exchangers twice as effective means an OTEC power plant could cut the size of its heat exchangers in half, shrinking the capital expenditure for the plant and making OTEC a much more practical green energy alternative. Alternatively, the same size heat exchangers could produce twice the power for the same cost.

Studies have estimated that the heat exchangers for a 100 MW OTEC power plant would account for roughly 25% of the total capital costs, and the graphite-foam-based heat exchangers have the potential to reduce that figure by 50%. Because heat exchangers are a large part of an OTEC plant's footprint, and OTEC plants are located on offshore platforms like those used for oil and gas drilling, reducing the footprint by half will also enable a plant to fit on a standard size platform, rather than requiring a costly custom-built alternative.

Plentiful, reliable energy

"There are several compelling advantages to the system," says Klett. "First, it produces totally green energy; there are no by-products. It's also very much like geothermal, solar or wind power in that it does not take any fossil fuel to drive it, so costs are limited to construction and maintenance." In addition, Klett is particularly emphatic about the availability of OTEC power. He notes that consumers don't always understand that the only kind of "green" energy that is currently available as "base power"—power that is available 24 hours a day, 7 days a week—is geothermal. "With other renewables," he says, "when the wind stops, you don't have power. If it's a cloudy day, you don't have power. Even hydroelectric power is at the mercy of fluctuating water levels. OTEC can actually be used for base power." Estimates suggest that, in tropical latitudes, OTEC has the potential to generate 3 to 5 terawatts of power without affecting the temperature of the ocean or the world's environment. "That's more than the electric generating capacity of this country," he says. "If we can supply a large fraction of our base power needs with green energy, we can revolutionize power generation."

Klett and his colleagues at Lockheed Martin are building a laboratory-scale heat exchanger that is 3 feet in diameter and 20 feet long and are shipping out to Hawaii to test at the National Energy Laboratory of Hawaii Authority (NELHA). Hawaii, which is also rich in geothermal resources, has made a commitment to eliminate its dependence on foreign energy sources by 40% in the year 2030. OTEC is viewed as a very attractive alternative to accomplish this goal.

Unique capabilities

Klett notes that the technology used to build heat exchangers for OTEC could be used to increase the efficiency of other types of power plants. "Potentially, any technology that uses heat exchangers, from heat pumps, desalination, LNG re-gasification to power plants, could benefit from this development," Cannon adds. ORNL's experience collaborating with Lockheed Martin through the Open Innovation Program has opened the door to working with them outside of the program on other research and development projects, Klett says. "The more they learn about us and the unique capabilities that we have, the more they come to us for help in areas outside of the Open Innovation Program.

As for the future of OTEC technology, Klett says, "I think this is a case where if we build it they will come. If we can build a power source that doesn't require fuel and only requires maintenance, then we won't have to worry about the price of fuel going up and down. The price of energy generated by an OTEC plant will be tied to the cost of maintenance—and if we come up with cheaper ways of maintaining the plant, the price of the OTEC energy could actually go down, and hopefully be competitive with conventional power plants."

"The demonstration of the project is scheduled for this winter in Hawaii," Cannon says. "If everything works as expected, it could be a game-changer in terms of generating green energy." R—*Jim Pearce*

Graphite foam's tremendous surface area and high capacity for conducting heat boost the performance of heat exchangers while reducing their size and cost.

INDUSTRIAL-SCHOLARS

CIRE student, Kemper Talley (Photo Jason Richards)

A new degree program in energy sciences and engineering, led jointly by ORNL and the University of Tennessee, is preparing graduate students to meet the nation's increasing energy challenges with a transformational approach to interdisciplinary and innovative research.

The program, administered by the ORNL-UT Center for Interdisciplinary Research and Graduate Education, continues a longstanding relationship between the two research institutions and offers students a chance to experience the best of both worlds.

The opportunity to gain research experience in a national lab attracted students like Kemper Talley, one of 19 students in CIRE's inaugural class. Talley, who recently graduated from Clemson University with a bachelor's in physics, says the history and vision of national labs piqued his interest in CIRE.

"I see the national lab as a center for innovation and a center for fundamental research," said Talley, who is a recipient of a 2011 National Science Foundation Graduate Research Fellowship. "This program fit the bill for me because I wanted to do fundamental science, and I also enjoy interdisciplinary research."

The mission-oriented nature of national labs is also attractive to industries that hire new PhDs, says Jim Roberto, ORNL's Associate Director for Graduate Education and University Partnerships. As co-leader of a task force to develop CIRE, Roberto helped conduct interviews with senior-level representatives from industries including Siemens, DuPont, Chevron, GE, and Exxon Mobil to understand what companies require from new hires.

"Industries appreciate that national labs are problem-oriented, so the students develop an expectation that there is an outcome beyond their research," Roberto said. "They value the fact that the students work in multidisciplinary teams, so they learn communication skills and how to work across disciplines."

Breaking the mold

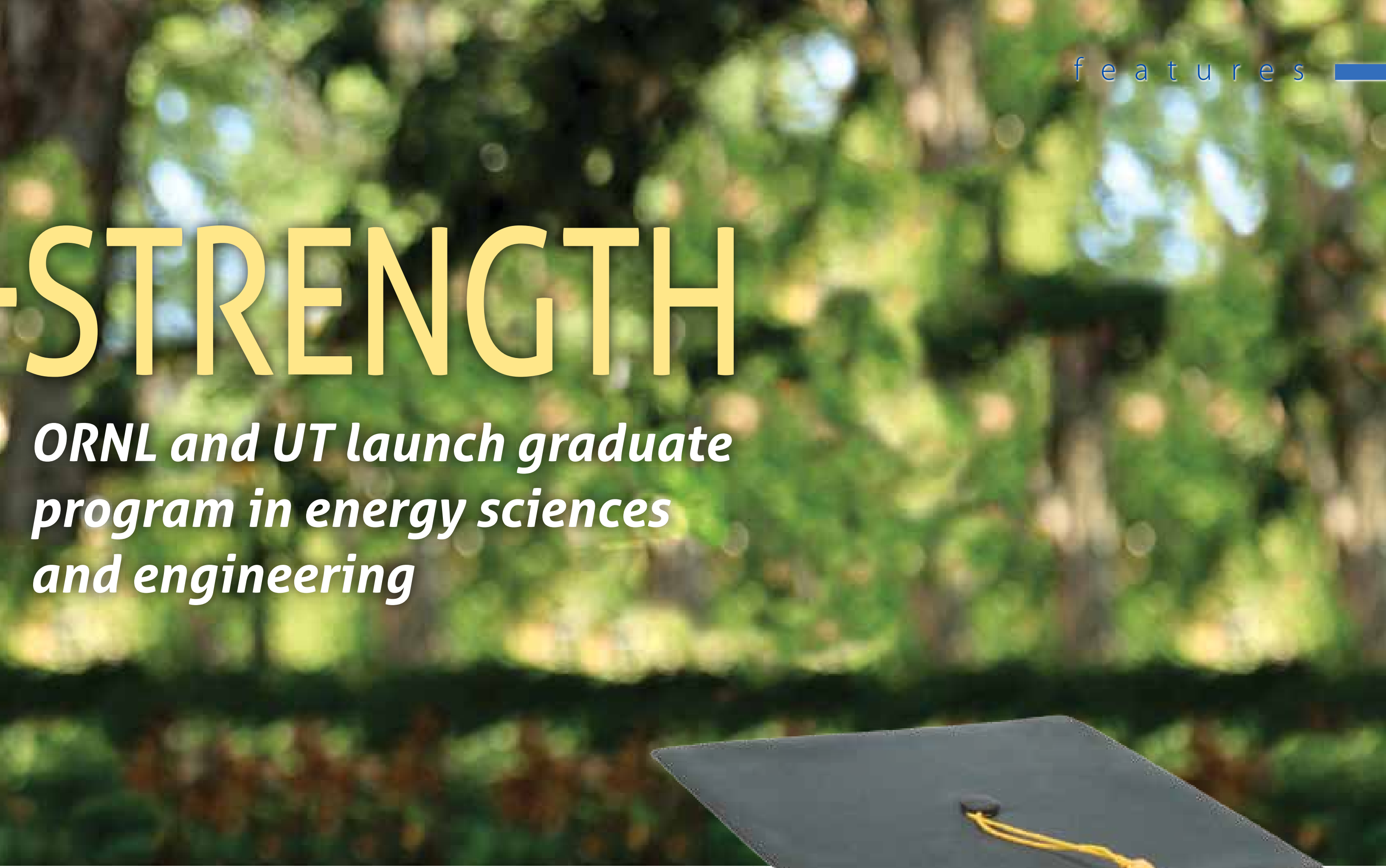
CIRE student Talley knows first-hand about the necessity of communicating across disciplines. Before beginning classes in August, Talley kicked off his research experience by spending his summer working in ORNL's Reactor and Nuclear Systems Division. His research focuses on using and improving theoretical models for nuclear data.

"I'm working with a nuclear physicist and a nuclear engineer who had never met before, even though their offices are 10 minutes away from each other," Talley said. "The ultimate goal of my doctorate is to bridge the gap between theorists and engineers and help them talk to each other."

CIRE's curriculum includes breadth courses such as policy, law or management classes to help students understand the larger context of energy issues. Talley says these broadly scoped courses will create opportunities to engage not only the scientific and industrial community but a more general audience as well.

"Too often, we get in our own corner and just deal with our science," Talley said. "We're not actively taking part in educating politicians and the community. CIRE is trying to break that mold. I think CIRE is going to give us training in the science and engineering, and then say, you need to be able to communicate this to everyone. We don't want to be isolated; that's the idea of the interdisciplinary research."

Even as the CIRE program exposes students to interdisciplinary research, it still requires a "deep dive" in an energy-related focus area. Roberto emphasizes that the program's depth and breadth create a "T"



STRENGTH

ORNL and UT launch graduate program in energy sciences and engineering

shaped curriculum, which ensures students have a solid grounding in fundamentals while understanding broader contextual issues.

Specialization areas include nuclear energy, bioenergy and biofuels, renewable energy, energy conversion and storage, distributed energy and grid management, and environmental and climate sciences related to energy. The initial group of 38 CIRE faculty members includes 18 ORNL scientists and engineers who work within these specialization areas.

"Typically, when we think about interdisciplinary research, we're thinking about one person working in several different fields—that's not the right view. What industry does and what the lab does, is to pick experts—in nuclear engineering, materials science or chemistry—and bring them together, so they span the disciplines," Roberto said. "No single person has survey knowledge of everything. It's people who are experts in their particular areas working as a group. When you put them together, you get a team that can solve a problem that crosses disciplinary boundaries."

Engaging with industry

As part of the breadth curriculum in the CIRE program, students have the option to pursue an entrepreneurial track. Roberto says this option encourages interested students to develop skills that could lead to forming a technology-based company. Students who want to pursue the entrepreneurial track can partner with UT's College of Business Administration to develop and implement a business plan.

"We want to encourage students to think about entrepreneurship and think about deploying their technologies," Roberto said. "Many graduate students go through school with the understanding that the outcome is a research paper, which is great. They're contributing to the growth of knowledge, which is an important component, but that's not the end. How is that going to get applied? Where are the innovations, and how are they deployed? This allows graduate students the choice to take that additional step."

Roberto notes that the inspiration for the CIRE's business-oriented track stems from the fact that many successful companies in recent history were started by students, including such economic powerhouses as Google, Facebook and Microsoft.

"We want to create an environment where students who have an interest in that dimension can find support in developing themselves and their ideas," Roberto said.

CIRE's relationship with industry may grow further as the program evolves. Program administrators are talking to industry about sponsoring fellowships for students and providing summer research experiences to create a unique workforce development program. Ⓡ
—*Morgan McCorkle*

ORNL's Technology Transfer Division Director,

Mike Paulus

is responsible for ensuring that the lab's technological developments are accessible to U.S. business and industry so they can make the fullest use of the nation's investment in research and development. Paulus' team fulfills this mission by licensing ORNL technologies to industrial partners and negotiating agreements to make the laboratory's scientific expertise and research facilities available to external partners.

Before joining ORNL's Partnerships Directorate, Paulus served as vice president of product management with Siemens Molecular Imaging. He also served as co-founder (along with ORNL scientist Shaun Gleason) and CEO of ImTek, Inc., an ORNL spinoff company and market leader in computed tomography imaging. Paulus has nineteen years of experience as a research and development engineer; has co-authored more than 100 peer-reviewed publications, book chapters, and conference proceedings; and holds 14 patents.

We asked Paulus how his organization benefits both ORNL and its research partners.

How do partnerships between national labs and industry benefit the nation?

The U.S. government and taxpayers have made a significant investment in creating unique research facilities at the national laboratories. They expect that, as a result of that investment, the nation will be better off economically and its citizens will have a better quality of life. At ORNL, we try to create these benefits in part by licensing technological developments to companies that will convert them into products or services that will help them grow their business or start a new business. We also provide companies with access to our research staff through research collaborations, as well as through work-for-hire agreements that enable our scientists to help companies address specific technical challenges.

Our goal is to make the lab's capabilities, research and resources available to support U.S. businesses, create jobs and strengthen our economy.

What areas of R&D currently provide the greatest opportunity for partnerships?

Opportunities for partnership exist in every corner of the laboratory. However, energy-related research is always of particular interest because it is at the core of the DOE mission and because the U.S. usually deploys its energy solutions through commercial entities. If we're going to help move the nation away from petroleum-based fuels, reduce our dependence on foreign oil, and reduce our greenhouse emissions, that's going to happen in partnership with the private sector. An important part of our mission is facilitating those partnerships.

What do you see as ORNL's greatest success in partnering with industry?

There is no single example that's head and shoulders above the rest. Our best license in terms of units sold is a composite of aluminum oxide and microscopic silicon carbide whiskers we licensed to Advanced Composites Material Corporation in 1986. This material was used to manufacture cutting tools which could, among other things, machine jet engine components ten times faster than tools made of competing materials. We have also had a very successful partnership with American Superconductor for developing the process for manufacturing superconducting cable. We started working with them in 1989, and our relationship is winding up this year. Our partnership with Caliper Life Sciences to develop the "lab on a chip" technology that is used in a number of medical diagnostic tools began in 1995 and continues to this day.

Based on your years of R&D experience in the private sector, what attracts industrial partners to ORNL?

The two main reasons private sector organizations collaborate with the lab are its unique scientific capabilities and facilities and the opportunity to take advantage of government-sponsored programs that match their research and development needs. When we show businesses our user facilities and research programs, they see the huge potential for collaborating with us for the benefit of their companies.

What role do the laboratory's user facilities play in these relationships?

Three of our user facilities most engaged with private industry are the High Temperature Materials Laboratory, the Building Technologies Research and Integration Center, and the Oak Ridge Leadership Computing Facility. These facilities illustrate the role user facilities play in getting the results of federally funded R&D into the hands of industry. HTML collaborates with all of the major automotive companies and a large fraction of the companies that develop materials for use in high-temperature, high-stress environments. BTRIC works with many of the top building materials companies to create new products and to improve their existing product lines. Earlier this year, OLCF and SmartTruck Systems used the laboratory's Jaguar supercomputer to develop aerodynamic design changes for tractor-trailer rigs that resulted in fuel savings of 7 to 12 percent.

Because many businesses no longer maintain corporate research centers, the national laboratories are fast becoming the last bastions of fundamental research for these companies and are critically important for them.

How do you expect the laboratory's partnerships portfolio to evolve over the next several years?

The laboratory's research agenda is set by the Department of Energy, so as the goals and mission of DOE change, so will our mission. That means our research portfolio will evolve as well. From my perspective, it's clear that eliminating the country's dependence on foreign oil and reducing our greenhouse emissions are multidecade goals at least. I'm sure those focus areas will remain with us for a very long time and that ORNL will play a key role in meeting these challenges. R

Computing for the next generation

ORNL scientists provide the building blocks for quantum information science

Researchers are recreating the capabilities of a half-million-dollar laser table on a silicon chip the size of a fingernail. The silicon wafer above will be cut into 20 to 25 individual chips. (Photo: Jason Richards)

Just the name of ORNL's Cyberspace Science and Information Intelligence Research (CSIIR) group conjures images of enigmatic, cutting-edge science. As it turns out, this impression is pretty accurate—at least for the computing research being done by quantum information scientist Phil Evans and his colleagues.

Evans' efforts are concentrated on applying principles of quantum physics and optics to developing the building blocks needed to realize the goal of quantum information processing. He notes that, because QIP is so new, there are a variety of approaches to the problem. "Programs at other laboratories and universities work with trapped ions or groups of electrons traveling in superconducting loops," he says. "However, at ORNL our research is focused on doing QIP with photons."

The advantage of QIP over traditional data processing can be roughly illustrated by looking at the basic units of information used by the two approaches. "Classical" digital information is based on the binary digit, or "bit." A bit can have a value of 0 or 1. The basic unit of information in QIP is the quantum bit, or "qubit." Its value can be 0, 1 or a superimposition of the two, meaning both 0 and 1—as well as all the values in between. While the concept is a little hard to get one's head around, the ability of a qubit to simultaneously represent a theoretically unlimited number of values points to the potential of devices utilizing QIP to become orders of magnitude more powerful than today's technology.

The path forward

Evans sees the ongoing evolution of quantum information science as a four-step progression that he expects will lead to the development of quantum-enhanced devices and applications.

The first generation, he says, was focused on an information security technique called "quantum key distribution." Technology companies have already begun to apply quantum principles to the problem of encoding and decoding communications such as email. QKD is an attractive option because it not only enables users to swap secret "keys" used to encrypt and decrypt messages, but it also tells them when someone is eavesdropping on the exchange.

Evans notes that the security of these exchanges is guaranteed by quantum physics—to a point. A well-publicized weak point in existing QKD implementations is the single-photon detector used in every QKD system. QKD systems manufacturers are constantly looking for ways to reduce the detectors' tolerance for noise—errors introduced by irregularities in the system's physical or network environment. Error tolerance is necessary to ensure that exchanges can take place under less-than-ideal conditions. However, tolerance for mistakes in transmission also provides an opening that can be exploited by hackers, so, while the physics behind QKD is unassailable, the technology used to implement it needs to be airtight to ensure its security.

The second generation of quantum apps includes a range of projects such as those spearheaded by Evans' colleague, quantum scientist Raphael Pooser. Pooser's research into quantum noise reduction and quantum sensors reboots traditional optical technologies by applying quantum principles to make them smaller, more sensitive and more precise. Evans cites Pooser's work with atomic force microscopes as an example of this quantum refinement. Traditionally, AFMs have gathered data by shining a laser onto a cantilever and measuring its movement as it is pulled across the surface of a material. "There is always a certain amount of quantum noise, or uncertainty, associated with laser-based measurements," Evans says. "However, replacing the laser beam with a beam of light that has been engineered to have less quantum noise improves the resolution and sensitivity of the microscope."

Quantum chips and Q-STILLs

One of the roadblocks to faster development of QIP technologies is the cost of the highly specialized optical equipment required to conduct quantum information research. "We tell our sponsors about the gains that can be made using this technology," Evans says, "but we can't expect them to pay for the half million dollars' worth of equipment it takes to support each laser table." It's also not practical to develop a quantum sensor package that requires a table-sized collection of equipment with substantial power if its ultimate application is going to be on a submarine or aircraft or anywhere else space and power may be limited.

Fortunately, Evans has an alternative in mind. He and his colleagues are working on a process that places the capabilities of a half-million-dollar laser table on a silicon chip the size of a fingernail. A downsizing challenge of this magnitude might seem a bit daunting, but Evans reasons that this is no different than the trend toward smaller, more powerful microprocessors that drove the personal computing revolution. "I guess you could say that we're trying to do the same thing with quantum technologies," he says. "One of the big challenges is to make the current technology scalable."

Evans leads the Quantum Lightwave Circuit project, which is supported by the Laboratory Directed Research and Development fund. The fund supports cutting-edge research across ORNL. The QLC project aims to develop a scalable framework for designing, simulating and fabricating any photon-based quantum device to perform any task. One of these circuits is called the Q-STILL (quantum states integrated with lightwave logic). Q-STILL also means "quantum still," a tongue-in-cheek reference to East Tennessee's moonshining heritage. "It's the same principle," he says. "We feed in the raw material—in this case "unentangled" photons—and interesting stuff—"entangled" photons, come out the other end."

To make a silicon chip do the work of a table full of equipment, Evans uses a process called electron-beam lithography, as well as other tools located at the laboratory's Center for Nanophase Materials Sciences, to create nano-scale waveguides—raceways for photons to follow—on a silicon wafer. The wafer is then cut into individual chips. Once a chip has been processed, researchers shine a laser through a specially designed crystal to produce pairs of entangled photons. When the photon pairs are injected into the chip, they can be split, rotated, combined, or manipulated in various other ways. "Pretty much any effect we can create on a laser table, we can duplicate on a chip—more quickly, far more cheaply and in a much smaller space," Evans says.

Because entangled photons are intimately related at a quantum level, their physical properties are precisely correlated. As a result, manipulating the photon pairs as they move through the circuits on the chip enables researchers to use these quantum correlations as the basis for calculations. Photon-based QIP may eventually use optical chips in the same way that traditional computing uses semiconductor chips—to perform various logical functions and calculations. Increasing the number and complexity of calculations that can be handled on a chip is another step toward the goal of realizing QIP. Evans suggests that classical computers, such as ORNL's Jaguar supercomputer, could eventually be used to study the production and application of these very-large-scale optical circuits.

Step by step

In the next 5 years, Evans estimates, researchers will begin to create third-generation applications, including the ability to produce optical chips that can simulate quantum objects, such as individual atoms, molecules and complex quantum processes such as photosynthesis. Because quantum chips control and manipulate photons—which are themselves quantum objects—researchers expect this type of simulation to be more accurate and in some cases faster than simulations conducted on traditional computers. "Quantum simulators are where you'll see the early stages of the marriage between classical computing and quantum computing," he says. "This is where we will be able to supplement the function of machines like ORNL's Jaguar with quantum co-processors."

Evans expects that the fourth generation of quantum applications, or true quantum computing, will require meshing several quantum technologies. He notes that, while photon-based technologies are good for transporting information, they're not likely to be useful for creating the computational core of a quantum computer. "This is more likely to be achieved using trapped ions or a gas vapor," he says. "A separate technology may be used to serve as a memory device, and all of these elements might be linked using photons. By the time we achieve quantum simulation and quantum computing, we'll start to see the number of technologies narrowed down and implemented and integrated together."

Next stop: metamaterials

To reach the third and fourth generations of quantum information science with optical chips, Evans reckons that progress will have to be made in the area of optical "metamaterials," materials engineered from the ground up to provide certain optical characteristics. "For example, Evans says, "some optical metamaterials have a negative index of refraction, providing a way to "cloak" materials hidden inside them. We're not interested in cloaking, but we would like to be able to develop optical materials that enable us to steer photons one way or the other or make them interact in one direction but not the other. It would also be useful to find a way to store photons for a short time before throwing a switch and releasing them. This is all part of the drive toward quantum simulation and quantum computing." Evans notes that quantum technology could play a key role in the development of new optical metamaterials by using QIP to leverage the laboratory's expertise in the areas of materials science, neutron science and nanotechnology.

"ORNL and CSIIR have great resources for this sort of research and a group of people with a keen interest in quantum information science," Evans says. "As a result, we have been able to build on developments made both at the lab and at other institutions and push them toward applications. Our next step will be finding out if we can build a quantum sensor that uses meta-materials for great resolution or great sensitivity. If we can do that, then we can build toward quantum simulation and quantum computing." —*Jim Pearce*

Moving materials to market

Large and small companies can benefit from targeted collaborations

When taxpayers invest in the national laboratories, they have a right to expect results in the form of technologies that help private businesses increase their productivity, introduce new products, and create jobs for American workers. ORNL's Partnerships organization delivers on that obligation by accelerating the movement of technology from the laboratory to the marketplace. In the R&D world, sometimes the most direct route to commercializing a technology is working with a startup company. Other times, an established business partner is a better bet. Either way, when ORNL works with business, Tom Rogers' Industrial Partnerships and Economic Development group is closely involved from start to finish.

Rogers says that the laboratory's approach to getting technologies to market is more about market pull than technology push. "Often large research institutions devote a lot of their time to telling people what they've got," Rogers says. "We take the opposite approach by inviting companies to come and talk to us about their research needs and priorities to see if they match our capabilities." Each year Rogers' group hosts about 75 of these targeted company visits. "If it looks like we have a good match in terms of research interests and available resources," Rogers says, "we'll have follow-up discussions on what we can do to help the company and how we can work together."

Two of the laboratory's recent partnerships have been with Ampulse, a solar energy startup company, and industry giant Dow Chemical.

Teaming up on solar cells

Ampulse is part of a three-way research and development project with ORNL and the National Renewable Energy Laboratory to develop a groundbreaking method of manufacturing solar cells. The basis of this effort is a technology called "rolling-assisted biaxial textured substrates," or RABiTS™, which was first discovered and refined at ORNL. The RABiTS part of the new manufacturing process involves creating a specially textured metal base, or substrate, that causes materials deposited on top of it to have a high degree of grain alignment in all directions. "It makes a really effective base on which to grow silicon for low-cost silicon solar cells," says Ampulse President and CEO Steve Hane.

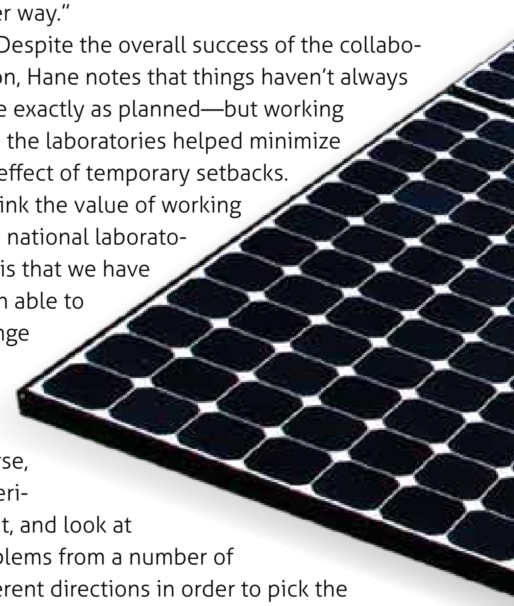
The technology behind depositing and growing the silicon on top of the substrate and the solar architecture techniques needed to create finished solar cells is provided by NREL. Hane explains that Ampulse is working with the two laboratories to combine these technologies and then plans to accelerate them toward a commercial product, with the help of the Ampulse development staff.

"While crystalline silicon itself is a great material for building solar cells, it's expensive to manufacture in wafer form," Hanes says. "The advantage of this new technology is that it allows researchers to deposit silicon onto the textured RABiTS substrate and basically have a finished product. This eliminates a number of intermediate steps and reduces the cost of the entire process. "Normally, when you make a silicon wafer," Hane says, "you have to melt polysilicon, grow crystals from it and saw it into wafers. This involves a lot of waste, processing time and energy intensity. Our new method is more like spraying a gas onto a metal surface to create a finished silicon wafer." The process is expected to reduce the cost of manufacturing silicon wafers for use in solar cells by 60 to 70 percent.

The company that provided the seed money for Ampulse is Battelle Ventures, the venture capital arm of the Battelle Memorial Institute. "Battelle knew about the specialized silicon deposition techniques the NREL researchers were using, and they also knew NREL was looking for a specialized surface that cut time and labor out of the manufacturing process," Hane says. "Because of Battelle's involvement in managing ORNL, they also knew about RABiTS. So they signed agreements with both laboratories and Ampulse to start the collaborative effort.

"Historically," Hane says, "solar energy has been a fairly expensive technology and has required government subsidies to make it affordable. Our goal is to create a technology that can stand on its own two feet without any subsidies and be on a par with or beneath the cost of electricity generated any other way."

Despite the overall success of the collaboration, Hane notes that things haven't always gone exactly as planned—but working with the laboratories helped minimize the effect of temporary setbacks. "I think the value of working with national laboratories is that we have been able to change course, experiment, and look at problems from a number of different directions in order to pick the best, most cost-efficient path forward," he says. "When you're starting out and you don't have a lot of capital to work with, you need to be able to draw on a variety of resources as you need them. Working with ORNL and NREL allowed us to do that."



Closing in on carbon fiber

Dow is working with ORNL to produce carbon fiber using polyolefin, a relatively low-cost plastic.

Before Doug Parks, Global Business Director of Government Markets and Lightweight Materials, came to work for Dow Chemical, he headed up business development for the state of Michigan, where he dealt with ORNL on a number of automotive-related projects. Parks notes that in Michigan, some of the biggest research and development opportunities are in the areas of wind power and transportation. Recently, a state-funded project to boost research into applications of low-cost carbon fiber in these areas brought Dow and the laboratory together.

Dow's specific interest is in developing a process to use polyolefin, a relatively low-cost plastic, as the raw material, or precursor, for carbon fiber production. At the right price, strong, lightweight carbon fiber could be used to produce a range of products, including the blades for giant wind turbines and lightweight body and chassis components in the transportation industry. Currently the precursor of choice for producing carbon fiber is polyacrylonitrile, or PAN. Polyolefin is much cheaper than PAN and has the potential to make carbon fiber production faster and more efficient. "In order to develop broader industrial acceptance of carbon fiber," Parks says, "the aim of the program is to develop a precursor with a low, stable cost. Over 50% of the cost of producing carbon fiber is the precursor material."

Park notes that the supply of carbon fiber is dominated by the fortunes of the aerospace industry. "When aircraft manufacturers are building lots of planes, supplies are down and prices are up," he says. "When they're not, supplies are up and prices are down." Proponents of expanding the use of carbon fiber in the manufacturing sector contend that identifying a low-cost carbon fiber precursor would result in broader adoption of carbon fiber across several industries, which would, in turn, help maintain a stable, lower price for the material.

In the area of wind power, carbon fiber is used primarily in the blades of wind turbines, which can span close to 100 meters. Because carbon fiber is stiffer than fiberglass, carbon fiber blades can operate closer to the housing of the turbine's drivetrain, eliminating wear and shortening the shaft that drives the blades. Carbon fiber blades can also be up to 50 percent lighter than fiberglass, providing similar durability benefits for turbine components.

Low-cost carbon fiber is also being considered for use in several other areas, including automobile manufacturing. Using lightweight carbon fiber components would increase fuel efficiency and reduce vehicle cost. In the oil and gas industry, where cables are used to tether drilling platforms to the seabed, carbon fiber would have significant advantages over steel or carbon-fiberglass composite cables.

"We are about a third of the way through the project with ORNL," Parks says. "Research teams are working both at Dow headquarters in Midland, Michigan, and in Oak Ridge, with some researchers dividing their time between sites. Most of the work on creating the carbon fiber precursor is being done at Dow, while the work on carbonizing the material and producing carbon fiber is being done in Oak Ridge."

Recently, Dow became a member of the Oak Ridge Carbon Fiber Composites Consortium and hopes to be an active player in the carbon fiber pilot facility the laboratory is building. "Dow's satisfaction with Oak Ridge has been very high," says Parks. This project has helped us realize the significant positive impact a national laboratory can make in a research project, and we hope to do a lot more work with ORNL."

Transformative technologies

"When we have the opportunity to translate our research and development accomplishments into transformative technologies for American business," Rogers says, "it is truly important and a cause for celebration. People look to the national laboratories to provide solutions in areas like materials science, alternative energy, high-performance computing and many others. That's exactly the kind of return on investment that national labs provide. Our interactions with private companies run the gamut of technology available at ORNL, and these relationships are crucial to the economic well-being of both the region and the nation."—*Jim Pearce*

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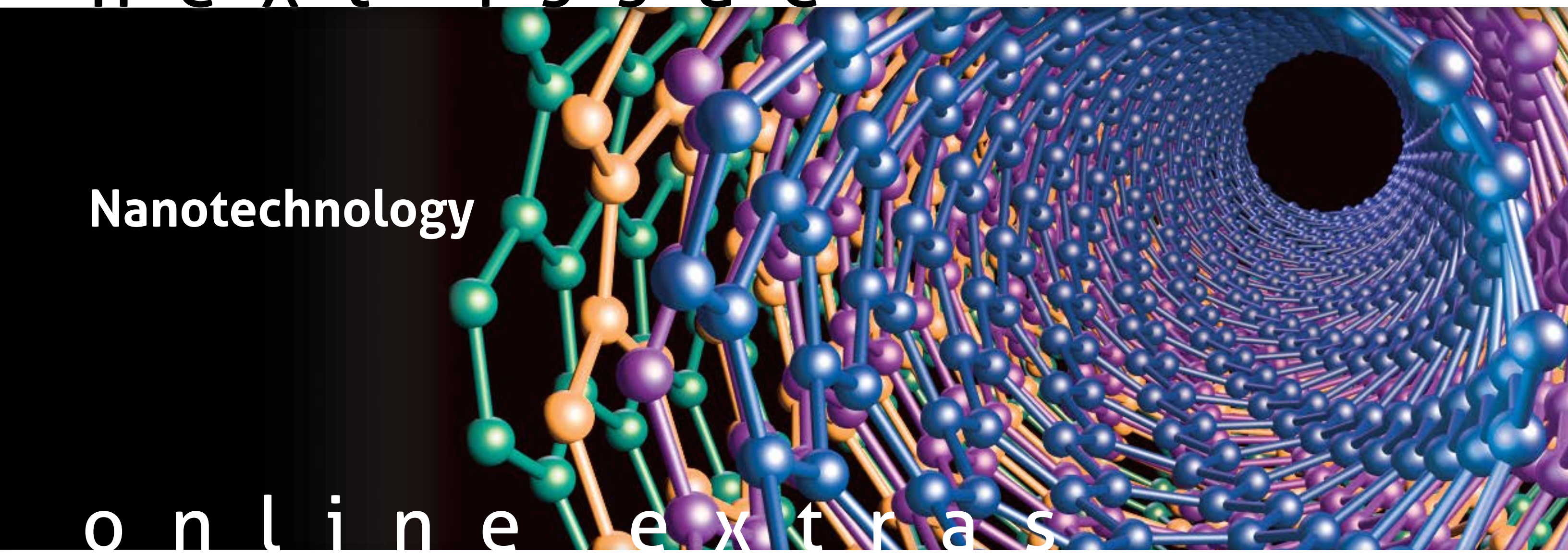

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