Oak Ridge National Laboratory

REVIEW

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

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Innovation Nation

Synergistic R&D

Printing the future

Strategic science

OAK RIDGE NATIONAL LABORATORY

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Vol. 45, No. 2, 2012

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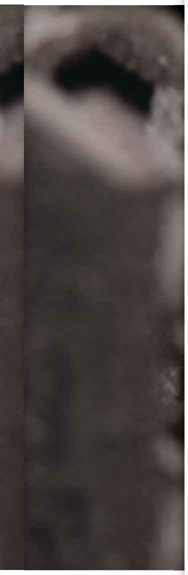
Optical fibers sprout from photomultiplier tubes in a cross-fiber neutron detector that is built for ORNL by PartTec, an Indiana-based scientific equipment manufacturer. Read more about the teamwork behind this instrument on page 18.

Photo: Jason Richards

Generating Innovation



Energy Secretary Steven Chu is fond of saying that America has the world's greatest innovation machine. At Oak Ridge National Laboratory, our mission includes not only delivering the scientific discoveries and technical breakthroughs that are the feedstock for the nation's innovation machine, but also carrying out the translational research and development needed to accelerate the deployment of solutions to the marketplace.

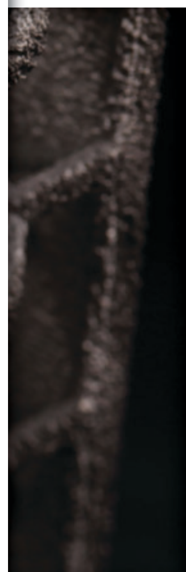
This issue of the *ORNL Review* offers a closer look at how we are executing that mission, with an emphasis on advanced manufacturing processes and materials technologies. The importance of a dynamic domestic advanced manufacturing sector to our national security and economic prosperity was highlighted by President Obama's announcement in June 2011 of the Advanced Manufacturing Partnership, which is focused on helping US manufacturers reduce costs, improve quality, and accelerate product development. The US Department of Energy is supporting the AMP by investing in the development of transformational manufacturing technologies and innovative materials that could enable industrial facilities to dramatically increase their energy efficiency.

ORNL has a long history of collaborating with industry partners who have made use of our distinctive capabilities. We are building on that history and exploiting new facilities and mechanisms to accelerate innovation in this key sector of the nation's economy.

For example, we are participating in the Department's pilot project for a new partnering mechanism, the Agreement for Commercializing Technology, which is intended to give private-sector companies a new means of working with the national laboratories. ORNL helped to develop ACT, which provides more flexible terms than existing technology transfer mechanisms.

We are also working to accelerate the implementation of ORNL innovations by encouraging entrepreneurial activity within the laboratory. We have established a new Research Conflict of Interest Committee to expedite the consideration of outside professional activity requests by ORNL staff. In addition, we are investing discretionary resources in innovative new projects with the promise of near-term societal or economic impact. Entrepreneurially minded staff members are given the opportunity to compete for R&D funding and access to external mentors, to develop new ideas, and to transform these ideas into commercial applications.

Innovation begins with an idea, and we have plenty of those. But turning ideas into reality requires perseverance, creativity, flexibility, and a willingness to take considered risks. At ORNL, we are committed to doing all we can to keep the innovation machine running smoothly.

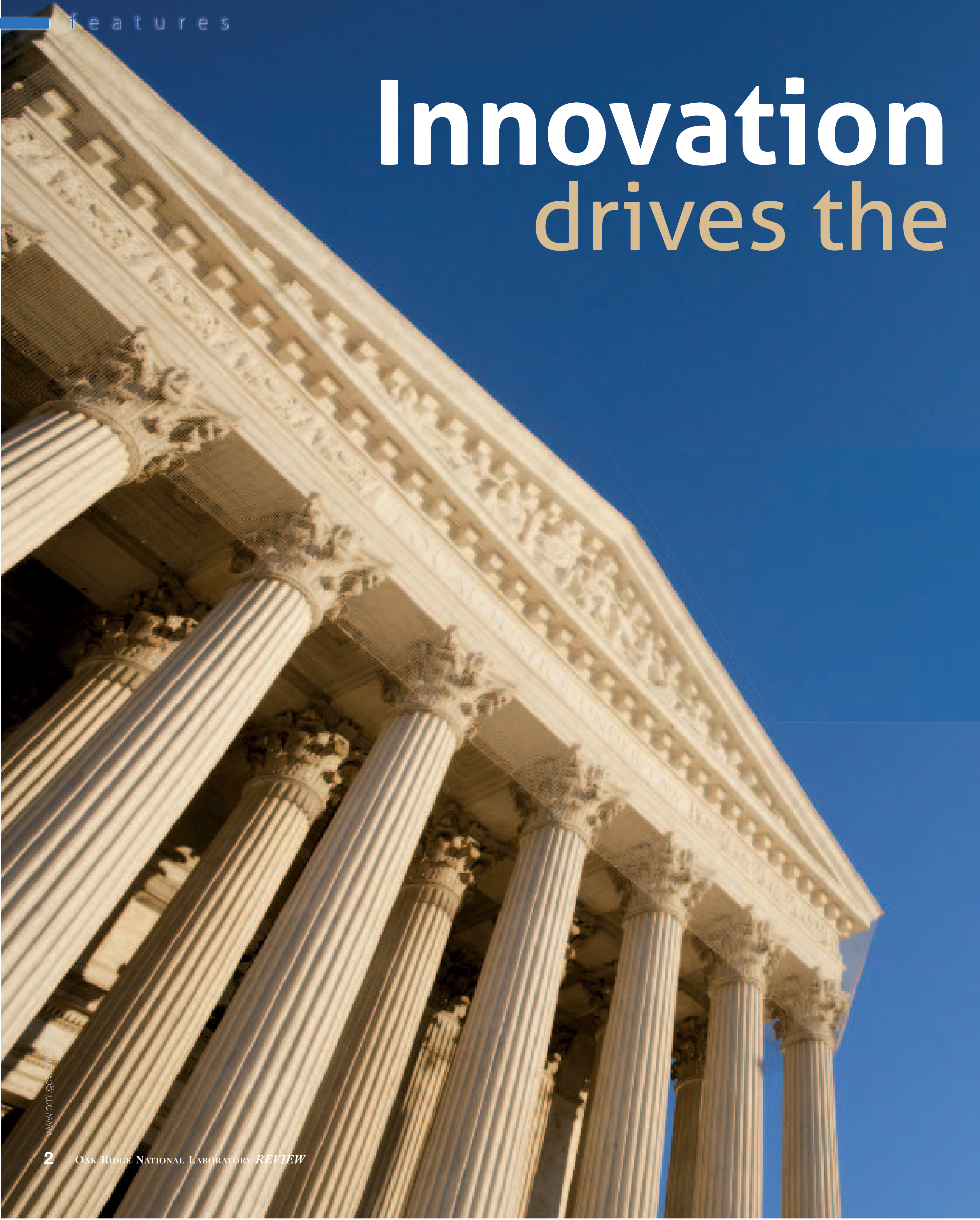


Thomas Zacharia

Deputy Director for Science and Technology

Oak Ridge National Laboratory

Innovation drives the



nation

For businesses competing in the global marketplace, innovation increasingly requires complex interdisciplinary research and sophisticated science. Companies need skilled researchers and unique facilities in a variety of disciplines, and ORNL is well positioned to meet this demand.

"It's like a Greek temple. We have a foundation supporting many pillars, which in turn support the roof."

Always handy with a metaphor, Laboratory Energy and Environmental Sciences head Martin Keller turns to classical architecture to describe ORNL's capacity for supporting advances in manufacturing. "Our program is like a Greek temple," he says. "The fundamental research disciplines—neutron physics, biology, materials science and supercomputing—are the foundation blocks." Fundamental researchers analyze, simulate and create materials with the goal of understanding their structure, how that structure can be modified, and how the materials interact with the world around them. For example, laboratory biologists studying the genetics of certain plants have found that a handful of genetic changes make the plants much easier to process into biofuel, which could have important implications for the economic viability of biofuel production.

That knowledge, in turn, is used to develop technologies to improve products or manufacturing processes, especially in the areas of transportation, energy generation and storage, and additive manufacturing. "These technologies are the pillars of the temple," Keller says.

Research and development projects provide the roof, putting these transformational technologies to work in a manufacturing environment. The Carbon Fiber Technology Facility, nearing completion a few miles from ORNL, is a textbook example of such a relationship. ORNL scientists and their industrial partners are applying decades of carbon fiber research to accelerate the development and commercial adoption of carbon fiber in manufacturing lighter, stronger components for cars and trucks, aircraft and wind turbines, among other uses.

Because the laboratory's expertise in a number of key R&D areas is similarly broad, ORNL is in a position to be a major player in the effort to develop a range of technologies needed to strengthen American industry and expand the nation's economy.

Fundamental tools

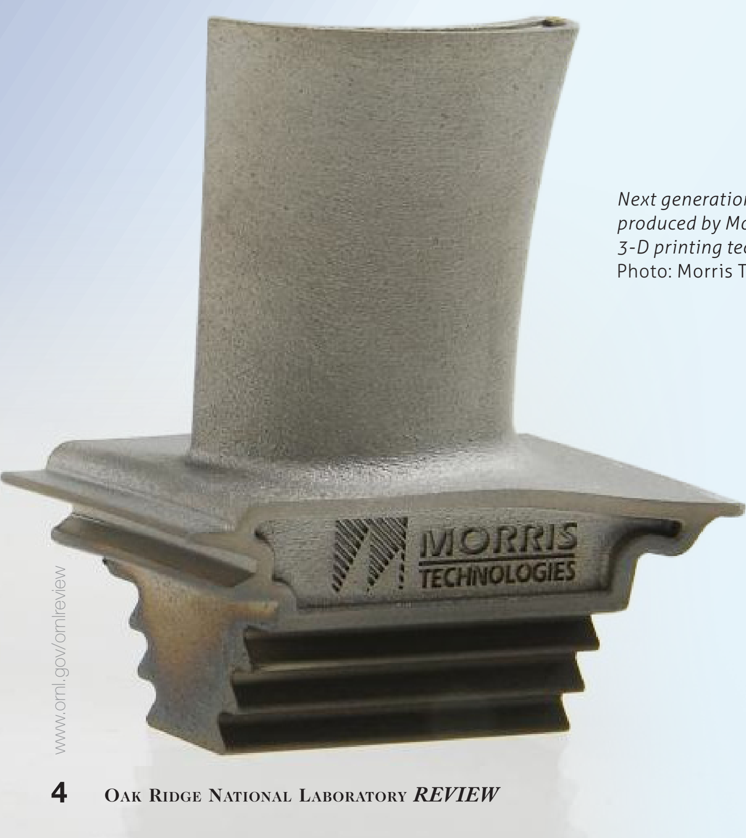
To help illustrate ORNL's multidisciplinary expertise, Keller holds up a durable, lightweight turbine blade produced by Morris Technologies using a process called additive manufacturing—a technology that enables manufacturers to design parts on a computer and then "print" them out in 3-D.

"These blades are used in jet engines," he explains. "When the engine is stopped, they are curved, but when it is running and the turbine is spinning at high speed, they straighten out." In order to perform in the unforgiving environment of a jet engine, these rugged components have been designed to exacting standards—a process that required the expertise of several ORNL research groups. "What alloys should we use?" Keller asks rhetorically. "We consulted materials experts. What is the most efficient design? We developed simulations on our supercomputer. What stresses are being placed on various points in the structure? We determined this using neutron analysis at the Spallation Neutron Source." This collaborative approach is increasingly necessary to address complex research challenges, particularly those that involve working with manufacturers to translate basic research into marketable products.

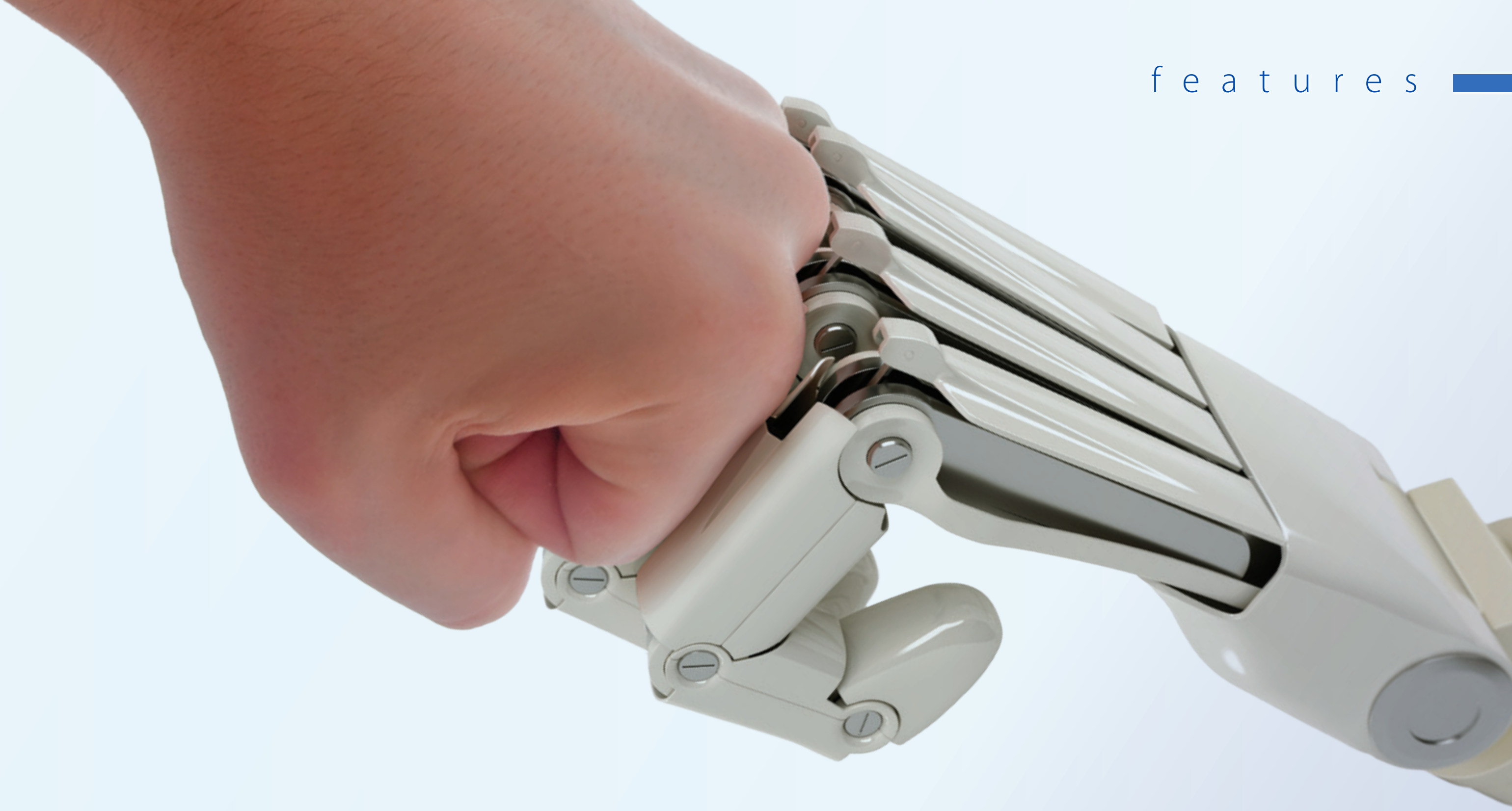
The extent to which technology permeates modern life is also a factor that pushes "applied" research projects in the direction of multidisciplinary collaborations. For example, one of Keller's keen interests is the prospect of creating transportation systems that are both economically and environmentally sustainable. He notes that it's no longer enough to focus narrowly on optimizing the energy efficiency of engines. "That only addresses a small part of the question of sustainability. What about making vehicles lighter using carbon fiber composite materials? What about avoiding congestion by incorporating 'smart' sensors into our cars and roadways? What about electric vehicles and their implications for the nation's electrical grid? Fifty years ago you could work on one specific problem and make a big impact," Keller says. "That's no longer the case. These days, problems are more complicated and cross traditional boundaries. As a national lab, we are poised to address this kind of problem."

ORNL has a long record of success in working with industrial partners to apply its unusually broad spectrum of capabilities. For example, 1,300 jobs were created when General Electric moved a manufacturing facility from China to the United States to manufacture superefficient water heaters based on technology developed in a GE-ORNL collaboration. The laboratory's supercomputing expertise also enabled BMI Corp. to develop add-on parts for 18-wheel, long-haul trucks that could save up to 1.5 billion gallons of diesel fuel and $5 billion in fuel per year. Similarly, laboratory materials experts are working with a California company, Campbell Applied Physics, to address heat exchange problems in water desalination plants. A solution promises to cut their energy needs in half.

Keller emphasizes that the advanced testing and analysis required for these projects is out of the reach of most companies. "For the most part, they can't do these things by themselves," he says, "but we have the tools and the expertise to help them. This is the role ORNL needs to play in the new generation of manufacturing. We have the ability to link fundamental research to



Next generation jet engine turbine blade produced by Morris Technologies using 3-D printing technologies.
Photo: Morris Technologies



industrial applications and to enable the production of products like reliable turbine blades, lightweight carbon fiber for cars, and robotic limbs for injured soldiers. As a laboratory, we need to be part of the manufacturing process, helping companies improve processes and products with our understanding of fundamental science and our ability to translate that understanding into applications."

Tearing down walls

Keller explains that, historically, scientists' ability to play this kind of role has been hampered by the metaphorical wall between fundamental and applied studies in many research organizations. "At ORNL, we have been tearing down that wall," he says, "and our efforts have been paying dividends." Keller cites the example of a recent biofuels project that teamed fundamental researchers—experts at developing catalysts that improve the speed and efficiency of biofuel production—with applied scientists who were tasked with testing the performance of the fuel in engines. As they worked together, the two groups developed a greater appreciation for how their contributions ultimately fit together in the larger project, enabling them to tailor their efforts to meet each other's specific needs.

This sort of successfully synergistic research has, in part, led to a tighter focus on the outcomes of research projects in both the applied and fundamental sciences. Keller notes that, as a result of this change in emphasis, applied researchers, whose contributions may have tended to be overlooked in the past, are now likely to find management paying more attention to their work. "I am finding that ORNL does much more applied research than I was aware of a couple years ago," he says. "The talent the laboratory has in this area is amazing."

Tremendous opportunities

While the ability to work across disciplines poses scientific and logistical challenges, it also presents tremendous opportunities. "A lot of people come to the laboratory because they see the potential of doing cross-disciplinary research," Keller says. "This is our strength. Our new research centers, like the Consortium for Advanced Simulation of Light Water Reactors and the BioEnergy Science Center, make it much easier for researchers from ORNL and our industrial and academic partners to cross disciplines and gain the insights they need to solve pressing problems."

Keller notes that future prospects for collaborations, both between national labs and industry and across disciplines within ORNL, are looking brighter. "When young scientists get out of school today," he says, "they're in a job market where their ability to collaborate and apply their findings is critical." He recalls that it was a different story when he reentered the job market several years ago after 10 years in the biotech industry. "The reason I came to ORNL," he says, "was that this was one of the few places I could do collaborative research with scientists from across the organization."

Innovation drives the nation

Keller, who became a US citizen in 2009, notes that one of the nation's strengths is the ability of its people to pull together in tough situations. "We are the most creative nation on earth," he says, "and we have the best chance of coming up with solutions to the difficult problems facing the world today. Historically, innovation has been the driver of our nation, and I predict that will increase in the coming years. The national laboratories are playing a key role in encouraging innovation by taking a more integrated approach to research and development and working closely with a range of industrial partners. We can't just innovate and then ship the resulting technology overseas so someone else can do the manufacturing. That's not sustainable."

Keller realizes that this surge of innovation won't happen overnight, but he is convinced that the national laboratories will be critical to meeting the challenges faced by America's manufacturers. "If you were to do a survey of ORNL scientists and ask them why they are working at the laboratory," Keller says, "they would tell you they're here to do exactly that sort of thing—to innovate, to overcome obstacles, and to solve the hard problems. We have to aim high to fulfill our mission." R *—Jim Pearce*

Printing out the future

ORNL leads a wave of collaborative research in additive manufacturing

ORNL is opening its doors to companies interested in using 3-D printing for products ranging from heavy equipment to biomedical implants. Photo: Jason Richards

It's 4 p.m. on a Friday, and robotics engineer Lonnie Love needs a new set of mechanical fingers. A few decades ago, he might have spent days or weeks tooling down a hunk of metal, like a sculptor painstakingly carving a statue. Today, all Love has to do is pull up a computer drawing and push a few buttons. In a couple of hours, a kiln-like machine spits out the parts to form a hand made out of titanium mesh.

It's called additive manufacturing, and it's not a fictitious technology from the *Terminator* movies. Also known as 3-D printing, additive manufacturing is still in its infancy compared to traditional manufacturing techniques, but it has a growing number of applications, such as biomedical equipment, aerospace parts, and military suppliers.

Love, an ORNL researcher, is part of a team funded by the Department of Energy's Advanced Manufacturing Office that is working to apply new technologies like 3-D printing on an industrial scale, with an aim of reenergizing the American manufacturing sector.

Unlike conventional methods that have been used since the Industrial Revolution, additive manufacturing entails building a product from scratch by putting down layer after layer of a raw material such as a metal powder or a plastic polymer.

"Additive manufacturing is when you grow parts rather than removing parts," Love says. "You add material only where you need it."

The process allows the team to quickly fabricate oddly shaped or complex parts—like fingers for a prosthetic hand—that would be difficult or even impossible to produce with traditional manufacturing methods.

"It redefines what it means to design to manufacture," Love says. "If you think it, you can make it."

Interest in 3-D printing has exploded in recent years as the technology has improved and printer prices have plummeted. Once prohibitively expensive, printers are now starting to move outside high-tech research labs into homes and high school classrooms. But while these desktop systems may be fun for hobbyists, the real opportunity for 3-D printing lies with industrial applications, says Craig Blue, who directs ORNL's advanced manufacturing program.

"We're focused on taking it from a prototyping or modeling technology to a manufacturing technology," Blue says. "If you look at 3-D printers found in high schools, the materials they use don't have engineering properties. In other words, you can't use the parts they produce for practical applications. You can use them for models, but you're not going to put the final product on an aircraft or a car. When we're done, you will be able to do just that."

Testing the waters

To help turn additive manufacturing into a mainstream practice, ORNL is opening its doors to companies that are interested in using 3-D printing for applications from multiton material-handling equipment to tiny biomedical implants. Hundreds of companies are already working alongside ORNL staff to take advantage of the lab's newly completed Manufacturing Demonstration Facility, or MDF, funded by DOE's Advanced Manufacturing Office.

With approximately 20,000 square feet of space that houses state-of-the-art 3-D printers and processing equipment, the MDF offers companies large and small the chance to test the waters of additive manufacturing by trying out their ideas in a reduced-risk environment. But access to equipment isn't the only draw. Blue says a distinguishing feature of the MDF is a staff with decades of expertise in materials research and development, combined with ORNL's other unique facilities.

"From a materials standpoint, we're basically unparalleled," he says. "We can bring large science tools like ORNL's Spallation Neutron Source to help rapidly qualify a material or process."

In addition to introducing companies to the potential of additive manufacturing, ORNL is working to advance 3-D printing technologies by collaborating with equipment providers like Stratasys and Arcam to improve the systems and controls on commercially available machines. ORNL researchers are also experimenting with feedstock materials, including new types of metal powders that could open up possibilities for new applications by offering increased strength and lower costs.

Shipping electrons

Beyond its transformational impact on the manufacturing industry, Blue explains that benefits of 3-D printing could spread into areas like logistics and supply chain management. Military supply lines, for instance, which are typically dangerous and costly areas of operation, might reap major benefits if 3-D printers could be used to help troops repair equipment more efficiently.

"We have military systems that are 20 or 30 years old, so you have to maintain the supply chain for that equipment for 30 years," Blue says. "It would be nice to only keep track of electrons. What if you just could carry around a CD of all the part drawings to take care of a piece of equipment? That would be unbelievable—to print a part on demand."

In the face of an increasingly global economy in which companies are moving more manufacturing facilities and jobs overseas, 3-D printing also provides companies with incentives to bring business back to the United States by offering rapid prototyping and quick turnarounds on finished products.

"If you're in a dynamic industry, you can't depend on materials shipped from China," Blue says. "If you're shipping electrons, you get it instantaneously. One of the mantras for additive manufacturing is 'design anywhere, build anywhere.' You can have these machines distributed so that you don't have to think about shipping costs. If these machines are in every town, then you can ship the electrons to wherever you need to have your product."

The increased efficiency of additive manufacturing provides additional savings to interested companies in terms of materials and energy. For example, the average component in the aerospace industry requires eight pounds of raw materials to produce one pound of aerospace-ready product. Since 3-D printing uses only just enough material to get the part done, it can reduce this "buy-to-fly" ratio from 8:1 to nearly 1:1.

The benefits of a distributed system of 3-D printing machines would not be limited to industrial customers either. Blue says the dream for additive manufacturing could extend to the average handyman who needs a customized part for a home repair.

"There's a vision in the future that you'll go to Home Depot because you want this polymer elbow for a fitting," Blue said. "You'll touch a machine and your part will come out. We'll ship electrons; we won't ship parts anymore." R —*Morgan McCorkle*

Next-gen engineers meet next-gen manufacturing

Hundreds of East Tennessee students are getting a taste of additive manufacturing through ORNL's participation in the FIRST robotics competition, an annual nationwide event that promotes science and engineering for high school students.

Over the course of 10 weeks in the spring semester, students meet with ORNL engineers and scientists after school and on weekends to design robots that can meet the challenges of the year's competition. Students learn the ins and outs of additive manufacturing as they develop prototypes and create working components and systems for robots that are required to perform tasks such as playing basketball.

ORNL robotics engineer Lonnie Love, one of the FIRST mentors, says the competition is one way that the lab is preparing the future workforce for high-quality jobs in the additive manufacturing field.

"We're exposing the next generation of engineers to the next generation of manufacturing," he says. "The younger generation isn't encumbered by what it means to design to manufacture, so they come up with some very innovative things."

ORNL became involved with the FIRST robotics competition in 2011 by mentoring a team from Knoxville's Hardin Valley Academy in its rookie season and helping the students learn how to design, fabricate and test components. Three HVA students later conducted their senior project at ORNL with a focus on additive manufacturing, and their work resulted in an invention disclosure and interest from multiple robotics companies in licensing the technology. HVA was selected as the top rookie team in regionals and was invited to nationals in St. Louis, where they were again named one of the top rookie teams.

In 2012, ORNL expanded its support to eight high schools and opened up a workspace in its new Manufacturing Demonstration Facility to those interested in learning and using additive manufacturing technologies. In addition, ORNL provided financial assistance, encouraging more ORNL research staff to volunteer as mentors and engaging additive manufacturing companies in providing financial support and hardware donations. Of the eight participating teams, two ranked in the top five in the regional competition, with Oak Ridge High School winning top rookie team honors and HVA receiving an award for engineering excellence.

Love credits Dean Kamen, the founder of FIRST, with giving students a reason to get excited about careers in science and engineering.

"Dean noticed that high school students were aspiring to be actors and athletes," Love says. "He wanted to inspire kids to become scientists and engineers by getting them to work hand in hand with engineers to see what happens when you create something."
—Morgan McCorkle

Hardin Valley Academy student Michael Goins prepares a robot for competition (left). Addie Chambers, daughter of ORNL researcher Jeff Chambers, tagged along for the day. She's holding a robotic arm made from titanium powder.
Photo: Curtis Boles

Synergistic R&D

Shrinking the product life cycle

Got the latest smartphone? The lightest mountain bike? The longest range electric car? Too bad. They're soooo 1994.

The ugly truth for technophiles and neo-Luddites alike is that it takes about 18 years for the average product to move from conception to production. That's a big problem for scientists who are trying to address the pressing problems facing the world in the areas of energy and the environment.

"Eighteen years is too long to wait," says Bobby Sumpter, a chemical physicist who works at ORNL's Center for Nanophase Materials Sciences. "That's a fact Congress recognized when it established the Materials Genome Initiative. This program is aimed at integrating experimentation, computing, simulation and fabrication in a synergistic fashion to shorten the product life cycle to perhaps five years."

More computing, less serendipity

Sumpter explains that one of the most powerful tools researchers have for accelerating the R&D process is high-performance computing and its ability to simulate and screen millions of possible materials to find those that are best for a particular application. "For example," Sumpter says, "if I wanted to make a greatly improved electronic device with particular characteristics, it may not be practical to simply keep trying different materials because testing each device can take a lot of time. I might accidentally stumble on the right material, but that's sort of like winning the lottery. Serendipity happens, but it's not a good strategy for materials development and design or for solving many of the current materials problems."

Fortunately, high-performance computing can allow this selection process to be guided by a set of calculations and computer simulations that analyzes the physical characteristics of each material and enables researchers to narrow the myriad possibilities to a handful that meet their specifications. Sumpter notes wryly that "it's a lot easier to make three and test three than it is to make a million and test a million."

Currently, computers can sort through some material properties better than others, based on the available data and computational approaches. For example, one problem that lends itself to computational analysis is the selection of materials that might be good candidates for use in battery cathodes. Scientists can consult a large database of material structures to enable the computation of electronic properties for selecting the most promising candidates for a particular battery configuration. Ensuring that battery components, such as cathodes, have the potential for improved capacity is one important step along the product development line for manufacturers of products ranging from tablet computers to electric vehicles.

Applied simulation

Simulations also allow researchers to investigate alternatives to increasingly scarce elements that are commonly used in industrial applications, such as electronics, energy conversion (solar panels, catalytic materials, magnets for wind farms), and automotive and aircraft production. In order to build useful simulations of materials, researchers need to have a thorough understanding of their structures. For example, many of the materials that Sumpter and his colleagues study are crystalline—meaning that their structures have well-defined characteristics that repeat throughout the material. This regularity, generally speaking, makes them easier to simulate. The irregular structure of noncrystalline materials or materials with structural defects, on the other hand, requires more complicated models.

As it turns out, these irregularly structured, materials have shown considerable promise as substitutes for hard-to-find elements and in other novel applications.

Synthetic polymer chemist Deanna Pickel investigates materials designed to increase the efficiency of solar cells.
Photo: Jason Richards

Computer simulation recently helped a multi-institutional research team develop a cheap, renewable nanotube sponge material that can absorb up to 100 times its weight in oil. Photo: Courtesy of Jeff Fitlow/Rice University

Sumpter notes that carbon, one of the most abundant elements on the planet, can be modified to perform in a number of unexpected ways. Applications of this versatile material range from lighter, stronger car parts to thermal insulation. Sumpter and his colleagues have made progress in adapting carbon to new purpose by developing simulation tools that allow them to better understand the properties of carbon-based materials with structural defects as well those of amorphous and composite materials.

These tools enable materials researchers to use computer simulations to "tweak" the properties of carbon to change its characteristics—a process that would be more difficult and time-consuming in a laboratory. "Imagine we have a sheet of graphene, a type of carbon." Sumpter says. "A single sheet has very interesting electronic properties. If we cut the sheet into smaller pieces, such as nanoscale ribbons, they have interesting magnetic properties. However, if one graphene ribbon comes into contact with another, the desirable properties can disappear—unless the sheets are aligned in a particular way. You might not know about any of these characteristics without first-principles simulations. This is a situation where using a computer model helps us take a nanoscale property and apply it at the mesoscale and the macroscale. Then, guided by the simulation, we can better determine how to achieve the same results in the laboratory."

A good example of what can be accomplished through the use of simulation and engineered carbon structures is a 3-D carbon nanotube sponge recently devised by a multi-institutional research team that included Sumpter. "It absorbs oil exceptionally well," Sumpter says. "It's also cheap, renewable and can be grown in large quantities." The nanotube sponge illustrates how nanoscale properties can translate into a useful macroscopic structures—in this case into a material that can absorb 10 to 100 times its weight in oil.

The discovery of the nanosponge was a result of an effort to grow clumps of carbon nanotubes by introducing boron atoms into the network of carbon atoms that make up nanotubes. Simulations of various arrangements of the new atoms indicated that they would result in "elbow" junctions in the nanotubes that would cause them to grow into a sponge-like 3-D network—which turned out to be correct.

In addition to being superabsorbent and far more efficient than other materials commonly used for oil remediation, the nanosponges are tough. The absorbed oil can be wrung out of them and recovered, or burned out—either way the sponges can be recycled and used over and over again.

Simulations have also shown how carbon-based systems can be useful for the catalytic production of synthetic fuels. Such a process typically depends on transition metal catalysts to convert a gaseous mixture of carbon monoxide and hydrogen into liquid hydrocarbons. However, recent simulations have found that carbon-based materials with specific defects can promote the catalytic process more effectively.

Collaboration and codesign

Working directly with industry is another way to compress the product development life cycle. These research relationships often involve not only laboratory work but also theory, modeling and simulation aimed at enhancing the properties of materials. Collaboration among researchers from all stages of the product life cycle can speed a product toward production just as surely as employing computer simulations.

Sumpter notes that a good example of this kind of collaborative design can be seen in the preparations researchers are making to move from the current generation of supercomputer to the next one, which will be a thousand times more powerful. "We don't just want a faster computer," he says, "we want it to be usable on critical problems as soon as the hardware is available. We can't develop a computer and spend 10 years writing software to take advantage of it. If we do that, the product life cycle hasn't been changed."

Sumpter says that to be sure they're ready on day one, the strategy is to employ a process of co-design."That means experimental scientists; computational scientists; the computer manufacturer's hardware designers; and the mathematicians, computer scientists, and engineers who apply the results of research are all working directly with one another to design viable next-generation computers. The hope is that this process will result in a system that, from day one, can be used by scientists and engineers to solve critical problems.

Sumpter suggests that a similar model could be used to improve efficiency in any area of science. It's just a matter of clearly defining what needs to be accomplished at the end of the process. "Sometimes the key to success is finding a way of expressing ideas that can be understood among all the different disciplines," he says. "It's not trivial; it's a cultural thing."

A new approach

Sumpter foresees that efforts in the areas of computation and collaboration will radically change the traditional approach to the design and deployment of materials and will shorten the time required to bring a concept to market.

"These changes will result from the integration of theory, computing, characterization and synthesis, from multiple disciplines," he says. "The way a physicist looks at a material is very different from the way a chemist or biologist looks at it, and this expanded perspective has already enabled us to overcome some tough challenges."

"We have the facilities; we have people with really good ideas and lots of energy, and we have problems that need to be solved. There's no reason we can't go forth and solve them." Ⓡ —*Jim Pearce*

Computation and collaboration will change the design and deployment of materials and will shorten the time required to bring a concept to market.
Photo: Curtis Boles

Strategic science

Leveraging R&D to benefit American manufacturers

Carbon fiber composites are super-strong, super-light materials that manufacturers would swap for high-strength materials like steel in a heartbeat—except for one problem. They're also super-expensive.

Engineers estimate that if CF could be produced for $5 to $7 a pound instead of the current $10 to $15, the typical car would include 200 pounds of the stuff—replacing twice its weight in steel and increasing fuel efficiency.

Thinking ahead

So that's what ORNL is trying to do—find a way to pare up to 50 percent of the cost from the CF production process and open up a potential market that has been estimated at 300 million pounds per year, just for automobiles—if the current price for CF can be halved. That's three times the current market, and that's what got Tom Rogers and other folks at ORNL thinking about developing a commercialization strategy for CF.

"We believe that a combination of new materials and new processing technologies can lower the cost of CF by as much as 50 percent," says Rogers, director of Industrial and Economic Development at the laboratory. "We're building a $35 million pilot plant to help commercialize new materials and processing techniques and put low-cost CF into the hands of industry. This new facility is the result of a huge team effort on the part of laboratory staff and our industrial partners."

The 400-foot-long Carbon Fiber Technology Facility is being outfitted with state-of-the-art processing equipment and is scheduled to be producing CF by early 2013.

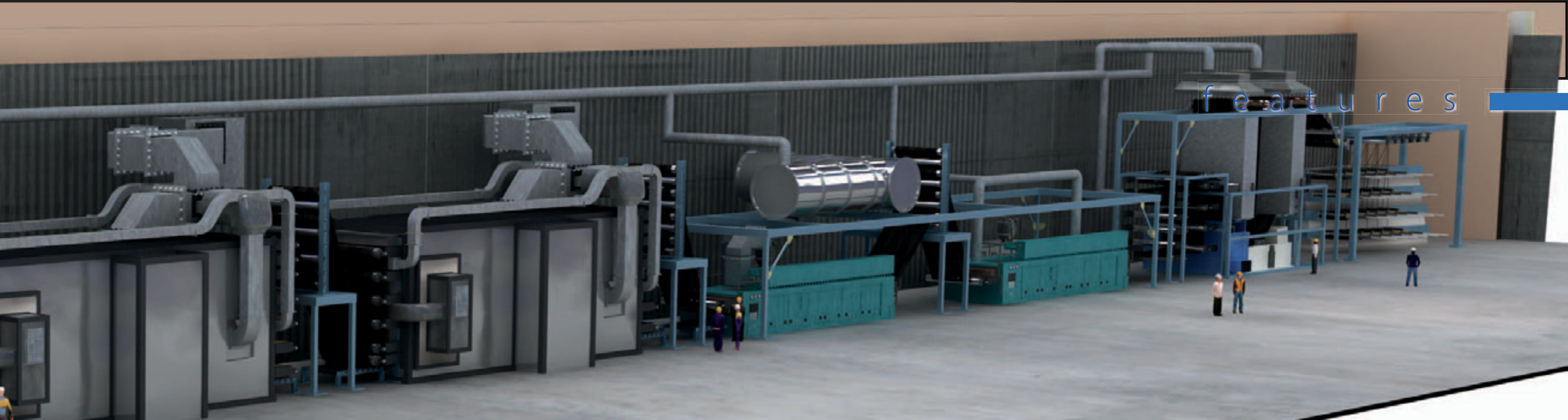
As plans to build this pilot plant began to take shape, Rogers noted that quite a few companies showed an interest in the facility's progress. He knew some of them from their connections to past CF research at the laboratory but was surprised by the number of calls the lab was getting from other organizations interested in investigating new materials, testing CF processing equipment, and developing new products using CF produced by the facility.

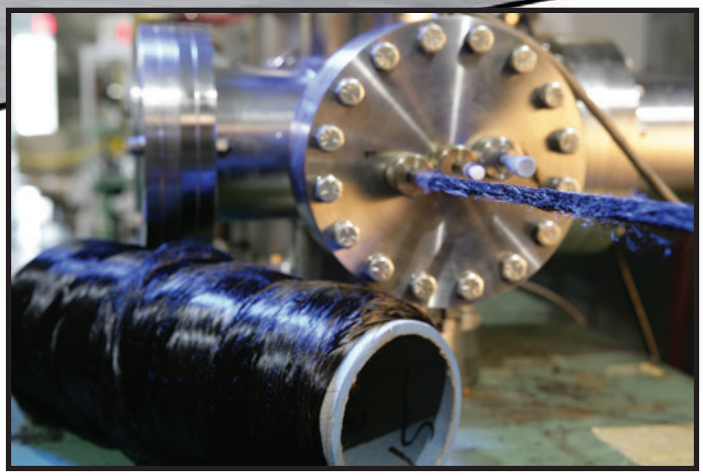
"We decided to capitalize on that interest," Rogers recalls, "by sponsoring a group to help private industry and government agencies work together to accelerate CF technology." The Oak Ridge Carbon Fiber Composites Consortium now has several dozen members, like industrial heavy hitters, including Dow, Ford and Volkswagen.

"We're partnering with a number of those companies," Rogers says, and in June the Department of Energy announced a $9 million award in support of Dow and Ford's efforts to develop a lower-cost carbon fiber production process.

"Our goal is to build what we call a regional manufacturing 'cluster' around this activity." A successful cluster includes not only manufacturers, but also a trained workforce, so the laboratory has worked with Roane State Community College to create the Advanced Materials Training and Education Center on the ORNL campus.

"AMTEC is training people for the jobs we hope to create," Rogers says. "Our challenge is not only to use our research and development resources to attract new companies to the area, but also to make sure we have a trained workforce to fill the jobs that new businesses will create. When a manufacturer decides to locate in the region, by the time they have a plant built, we will have a trained





ORNL's 400-foot-long Carbon Fiber Technology Facility is scheduled to be in production by early 2013. Photo: Jason Richards

workforce ready to go. ORNL has a clear R&D lead in this area, and we can use it to benefit the entire region."

Pilot plant

Materials scientist Cliff Eberle emphasizes that the Carbon Fiber Technology Facility represents the fruition of decades of research by dozens of ORNL researchers. The pilot plant will eventually house two separate production lines. The first production runs will be used to test new CF "precursors"—the raw materials for CF production. To date, most CF has been made using a petroleum-based material called PAN (polyacrylonitrile). The pilot plant will work with PAN, but it will also add some newer materials into the mix, including polyethylene, the material plastic grocery bags are made of, as well as lignin, a plant-based by-product of paper manufacturing.

Initially, all of the testing will be done using tried and true processing techniques. "Because we are working with several new precursors that are not well understood, we want to use processes that are well understood, so we can control the quality of the product and the process," Eberle says.

Similarly, when ORNL's carbon fiber R&D team begins to apply advanced processing techniques, such as using microwave-created plasmas to heat materials, they will try them out first using PAN because the behavior of this time-tested material is better understood than that of newer precursors.

"Once we understand both the precursors and the advanced processing techniques fairly well," Eberle says, "we'll put them together on a production line. However, right now, we're doing those kinds of experiments on a smaller scale in the laboratory. For example, we're seeing how polyethylene behaves in a microwave chamber and what happens to lignin in a plasma field."

The price is right

The answers to processing-related questions like these are critical to promoting wider use of CF in manufacturing. If CF processing costs can be reduced, so can the cost of the finished product. Obviously, manufacturers will use more CF at $5 a pound than at $7 a pound, so processes that are faster, less expensive or less energy-intensive are likely to spur manufacturers to incorporate more CF into their products.

By the same token, the cost of raw materials also affects manufacturing practices. "Basically the more affordable the raw material becomes, the more companies show an interest in picking it up. That's why we're looking at polyethylene and lignin," Eberle says. "This is true both for structural products for cars, planes and bridges, as well as for CF used in nonstructural applications, such as thermal insulation for high-temperature industrial furnaces."

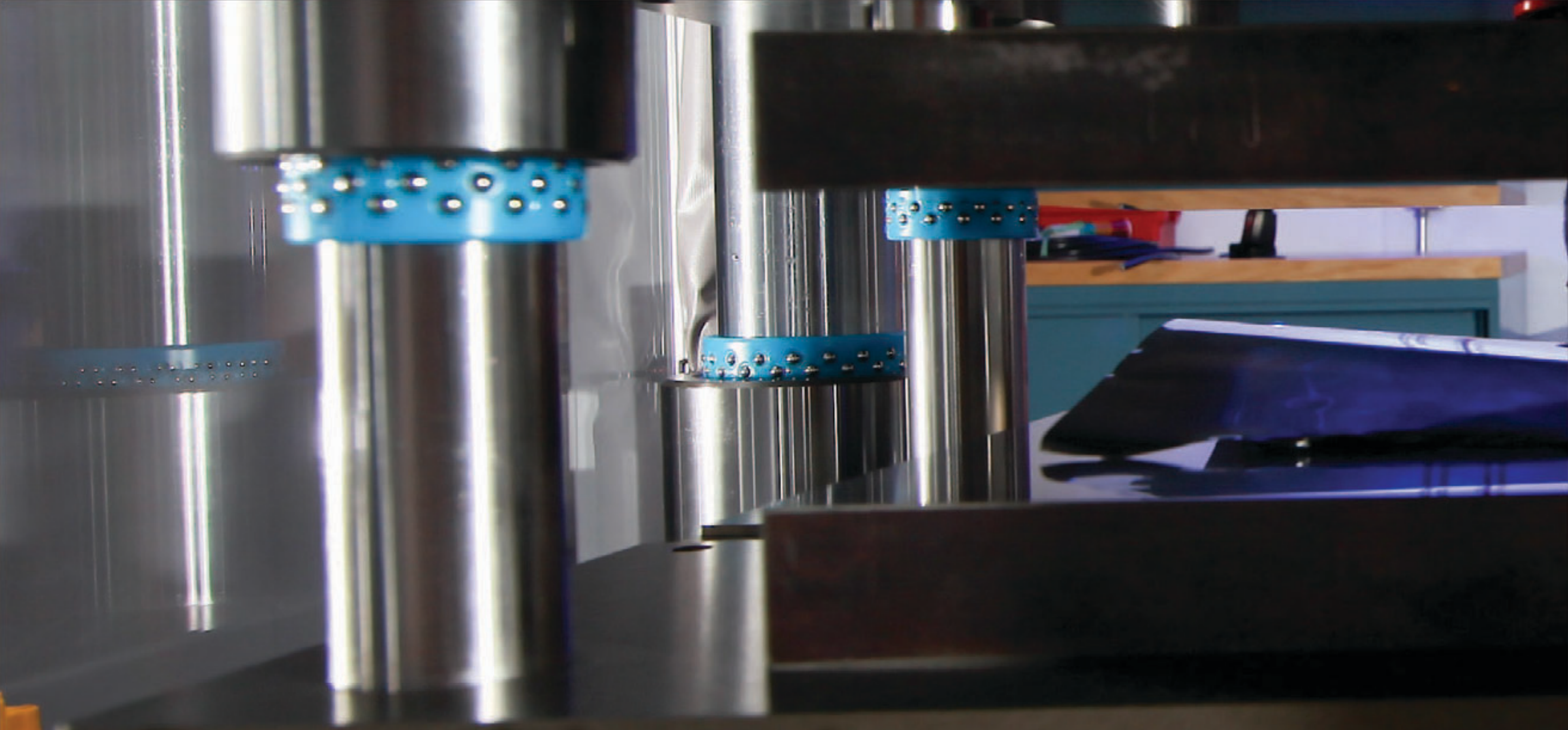
Recapturing the lead

The ultimate goal of ORNL's efforts in the area is to significantly reduce the cost of CF and to put thousands of pounds of new, low-cost materials into the hands of American manufacturers, so they can explore how this technology can be applied in the broader market. "This will cause the market to grow," Rogers says, "and that means more American manufacturing jobs will be created."

Eberle points out that carbon fiber technology was invented in the United States.

"We didn't capitalize on that advantage," Eberle says, "so Japan took the lead in CF manufacturing and still dominates the market today. Now, if we leverage our R&D and business resources, we have the opportunity to recapture the lead in an industry that is important both to our economy and our energy independence. If we want to put this technology to work for the nation, we have to deploy it in the commercial arena." Ⓡ

—Jim Pearce



Competitive advantage

Manufacturing R&D facility accelerates battery technology

We live in a battery-powered world, and the competition to produce reliable, longer-lasting batteries for phones, computers and electric vehicles is fierce. Fortunately, US manufacturers are getting a boost from ORNL in the form of the country's largest open-access battery manufacturing research and development facility. The Battery Manufacturing Facility is strategically collocated with both the lab's Manufacturing Demonstration Facility and National Transportation Research Center. The MDF is a state-of-the-art research and development center designed to advance manufacturing technology and give American business a competitive edge in the global market. The NTRC houses much of ORNL's transportation research, from engine development and power electronics to fuel cells and other alternative fuel technologies.

The BMF adds tremendously to ORNL's existing energy storage material processing capabilities, providing scientists with the ability to analyze every aspect of battery production, from raw materials to finished product.

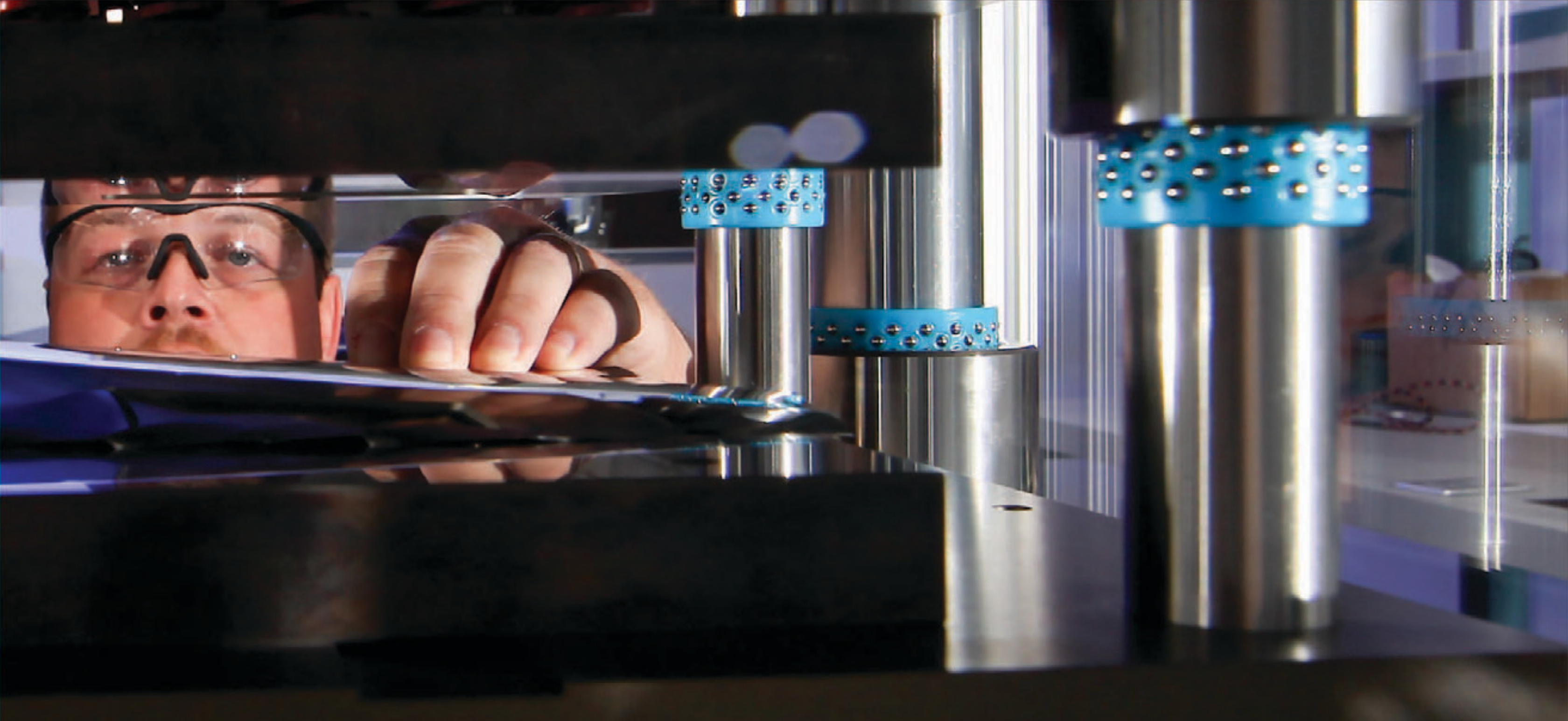
The facility is available to any US battery manufacturer, material supplier or battery user. "The advantage we offer," says Claus Daniel, deputy director of ORNL's Sustainable Transportation Program and scientific head of the facility, "is the ability to integrate any component into a complete battery, analyze the results, and determine how the components can be further improved." The battery manufacturing equipment is modular, so users can "plug-and-play" individual processes, and BMF staff can provide help and guidance every step of the way. "The idea," he says, "is to showcase the user's material or process improvements and to quantify the advantage they provide."

Through the battery facility, Daniel and his colleagues are involved in collaborative R&D with a number of companies, including efforts with battery manufacturer Dow Kokam to develop next-generation materials manufacturing and processing technologies as well as a project with A123 Systems to save energy by reducing heat treatment temperatures and times.

The manufacturing facility can produce batteries with capacities up to 7 ampere-hours—about seven times that of a cell phone battery. Daniel explains that his group chose that size because it's small enough that a company with limited amounts of material can demonstrate the impact of its innovations, yet large enough to make manufacturing decisions about making larger devices. "If a battery works at that size," Daniel says, "it can be scaled up to whatever size you want—the physics of the battery will be more or less the same."

Not surprisingly, there has been no shortage of interest in the new facility. Daniel explains that, normally, if materials suppliers want to test a new material in a battery, they either have to stand up their own manufacturing facilities—which is cost-prohibitive and takes years—or ally themselves with a specific battery manufacturer, which often means giving the manufacturer exclusive rights to use the material being tested. "This kind of arrangement limits the supplier's ability to disseminate the innovation broadly in the marketplace," Daniel says. "Our facility allows them to keep control of their intellectual property, demonstrate their technology in a complete battery, and benchmark its performance against other commercially available materials. It's all about growing the domestic supply chain for energy storage devices."

Several companies are working on projects at the facility, and procedures are in place to ensure that companies can work at the facility without running the risk of leaking proprietary information to a competitor.



From the ground up

ORNL researchers already had a detailed vision for how they could impact battery manufacturing when they began working with the Department of Energy's Vehicle Technologies Program and Advanced Manufacturing Office sponsors to establish the BMF. The new facility enables scientists and engineers to access every aspect of battery manufacturing with an eye toward improving performance and reducing cost. As a result, many of the facility's projects involve analyzing each step in a battery's production process, looking for the opportunities to boost efficiency.

For example, because certain battery components need to be moisture-free when they are assembled, they are dried once after they're manufactured and again just before they're assembled. Because drying is an expensive, energy-intensive process, researchers are studying alternative methods of removing moisture that could be implemented more quickly and cheaply. Daniel says the goal in all of these efforts is twofold: to improve the science behind the materials that go into the battery and to improve the battery production process.

The biggest challenge for battery researchers is that there is no single item or step in the process that has enough cost-saving potential to meet the overarching goal of making battery-powered vehicles competitive with other vehicles in terms of cost. Despite this challenge, Daniel believes that, working in partnership with industry, the research being done at the battery facility can significantly influence three aspects of battery production: cost, energy density, and production yield. "These things combined will get us to the goal," he says.

Part of the reason for Daniel's optimism is that, currently, batteries are about four times bigger than they need to be. This supersizing helps to ensure that as a battery's ability to store energy lessens over the predicted 15-year life of the vehicle, it will always be able to provide the necessary power. Daniel believes ORNL scientists working with industry will be able to produce a smaller, more cost-efficient battery with greater energy density that will allow vehicles to be driven farther between charges.

Daniel is also confident that production yield—a measure of the quality of the final product—can be significantly improved. He notes that manufacturers know how to judge the quality of the raw material used to produce the battery parts, but once a battery component is assembled, they don't have effective ways to test it until the final product is produced. "If there is a problem with an early step in the production process," Daniel says, "the manufacturer doesn't know about it until the finished battery fails to work."

To address this potentially costly problem, David Wood, a scientist in Daniel's research group, is heading the development of in-line quality-control procedures to detect flaws as early as possible, quantify them, and even repair them—improving both the quality of the final product and the manufacturer's bottom line.

The ultimate goal

In the short term, Daniel expects that research and development collaborations at the battery center will help manufacturers reach DOE's battery cost target of $250 per kilowatt-hour. That's about a half to a third of the cost of producing batteries today. The DOE cost target reflects both the level at which the cost of electric vehicles becomes competitive with other modes of transportation and the price point where US battery manufacturers can compete in a global marketplace dominated by Korea, Japan and China.

In the longer term, Daniel expects that the research partnerships being developed at the battery facility will contribute to developing a viable alternative to internal combustion engines for light-duty vehicles. "Right now," he says, "electric vehicles are not drop-in replacements for gasoline-powered cars. The problem is that our whole society runs on fossil fuel, and the volatility of the price of oil is crippling our economy. If we can provide the science and manufacturing technology needed to create a battery that allows us to drive 400 miles on a single charge, then electric vehicles will become a viable option."

"That is the ultimate goal." R

—Jim Pearce

Keeping it fresh

Partnering with industry keeps new tech flowing


Optical fibers sprout from photomultiplier tubes in a cross-fiber neutron detector. Photo: Jason Richards

ORNL is teaming up with PartTec, an Indiana-based scientific equipment manufacturer, to make the most of the world's premiere neutron scattering research facility, the laboratory's Spallation Neutron Source.

SNS researchers use the phenomenon of neutron scattering to reveal the inner structure of a range of materials, from metals to microbes. They do this by aiming a beam of neutrons at a sample of material and then measuring exactly how the direction and speed of these minute particles change as they strike and pass through the sample.

The key to recording, analyzing and ultimately understanding the results of these collisions lies in a piece of equipment called a scintillation detector, which intercepts neutrons shortly after they exit the sample. When a neutron strikes the detector, it produces electric signals that are fed into a data collection system. Analysis of the information enables researchers to determine where the neutrons struck the detector, and the pattern and intensity of the impacts tell them quite a bit about the internal structure of the sample material. Thoroughly investigating the structure of a sample in this way can involve collecting data from many millions of neutrons.

Partners in science

PartTec's role in supporting the laboratory's neutron scattering inquiries has been to help the SNS ramp up production of detectors needed for experiments on two of the spallation source's key instruments.

According to SNS instrument development scientist Richard Riedel, PartTec originally specialized in building detectors for high-energy physics research facilities but eventually branched out into neutron detectors as well. Several years ago, when a team of ORNL researchers was running experiments on the University of Indiana's pulsed neutron source, they got to know the PartTec staff members who were working on the facility's detectors.

At the time, the SNS detector development group was building prototypes for the detectors that would be installed on the spallation source's POWGEN and VULCAN instruments. However, the number of detectors that would be needed to fully equip these instruments was greater than the small group could handle. "When we saw PartTec's work at UI, we decided to ask them to help us manufacture these units," Riedel says. "We knew the level of subtlety required to build this sort of instrument was very high—not just any manufacturer could do it."

PartTec is currently involved in manufacturing two different detectors for the SNS. One of these, the latest addition to the facility's analytical repertoire, is a next-generation cross-fiber detector. "Originally PartTec provided only a portion of each detector," Riedel says, "but that worked out so well that they now manufacture the whole instrument."

The cross-fiber detector uses a woven optical fiber assembly to carry light created by neutron strikes from the scintillator to a bank of photomultiplier tubes for amplification and analysis. Riedel notes that the optical fiber assembly on this detector is "more sophisticated, but less complex," than that of similar detectors—using one-tenth as many fibers, to achieve similar results. The detector's "woven" arrangement of fibers combined with the sophistication of the software that interprets the data they gather, enables it to do more with less.

Partnering with industry on manufacturing frees up scientists to push technology beyond the state of the art

The other focus of the ORNL-PartTec detector collaboration is an updated "Anger" detector, named after its inventor, University of California scientist Hal Anger. The Anger detector, which has a much higher resolution than the cross-fiber instrument, detects incoming neutrons using a scintillating glass plate. As is the case in the cross-fiber detector, light resulting from neutrons striking the scintillator is boosted and analyzed by photomultiplier tubes and then passed along to a data collection system.

Although they both employ scintillators to detect incoming neutrons, the two detectors are designed for use with different kinds of samples. Anger detectors are often used when a tightly focused pattern is anticipated—like those that result from the analysis of a single crystal. The cross-fiber detector, on the other hand, is tailored to detect the more diffuse, ring-shaped patterns that are characteristic of analyses of powders and larger samples.

Riedel recalls that, at first, PartTec was involved only in making the electronic circuit boards for the Anger detector. "Each detector contains about 20,000 components," he says. "PartTec started out providing just the circuitry, but now we're talking about having them manufacture the entire detector for us."

Keeping it fresh

Partnering with industry on detector manufacturing helps to ensure that a fresh stream of technology flows into the private sector. This also frees up laboratory scientists to concentrate on pushing detector design beyond the state of the art.

An example of this sort of innovation can be seen in the improvements the collaboration has made to the design of the cross-fiber detector—particularly to the woven optical fiber assembly. "Similar detectors designed in Europe to serve the same purpose are much more complex," Riedel says. "We refined the design, and now some European neutron scattering facilities are interested in buying PartTec detectors. PartTec has been instrumental in helping improve the manufacturing process as well as providing improvements in key parameters such as detector efficiency."

Riedel notes that the detector development group handed off the technology behind their previous generation of gas-filled detectors to General Electric, their manufacturing partner at the time. The laboratory's collaboration with PartTec has been similarly beneficial.

"The relationship with PartTec has been good for us because it allows us to focus on advancing the technology, rather than on manufacturing," Riedel says. As a result, the latest generation of instruments produced by this collaboration is faster, more accurate, and integrates better with state-of-the-art computer hardware.

The relationship has also paid dividends to PartTec. Interest in their detectors has come from both international research facilities and the US military as well as from organizations that monitor the transportation of fissionable material.

"This is been a good partnership," Riedel says. "PartTec is easy to work with, and they're very interested in building collaborative relationships." Ⓡ —*Jim Pearce*

10,000 feet down

Extreme bacteria provide an unexpected boost to manufacturing

Ten thousand feet below Vicksburg, Virginia, bacteria lurking in the hot, dark recesses of ancient rocks spend their lives transforming metal into magnetic nanoparticles. Some folks think that's a little creepy. Tommy Phelps thinks it could be the start of a new industry.

Phelps, an ORNL biologist, has spent decades studying extremophiles, organisms that have adapted to life under difficult conditions. The Vicksburg bacteria, recovered from gas drilling core samples, are called *Thermoanaerobacter ethanolicus* and live under millions of tons of rock in total darkness and in temperatures as high as 70°C (158°F).

These extreme bacteria produce magnetic excretions on the outside of their cell membranes through a process known as nanofermentation, which converts salts, metals (iron in this case), and other nutrients into metal-containing nanoparticles. Scientists think these bacteria, which also excrete ethanol and acetic acid, produce the nanoparticles as part of a chemical balancing act that prevents levels of the other two waste products from becoming toxic.

Metal-containing nanoparticles are used in a variety of manufacturing processes, from battery and solar cell production to electronics. However, while these particles are useful and versatile, they can also be fairly expensive to produce. Enter *T. ethanolicus.*

Industrially relevant

Phelps and a cast of collaborators that numbers in the dozens are trying to make "industrially relevant" nanoparticles using biological processes that work not only in the laboratory but also on an industrial scale. "Some of our production models suggest we might be able to generate this material at less than one percent of the cost of existing commercial processes," he says. "That's a result of the scalability issues and high energy demands associated with current industrial processes."

T. ethanolicus requires only food and warmth. In fact, as it is grown in larger and larger volumes, less energy is required because, as the bacteria become more numerous, they begin heating their environment themselves.

Phelps and his colleagues didn't initially see anything too remarkable about *T. ethanolicus*—it's not all that unusual for extremeophiles to produce nanoparticles. However, when they determined that the particles were magnetite, a magnetic form of iron oxide, they took a closer look. Magnetism is a quality that is in high demand for a range of existing and hypothetical nanoparticle applications. The particles produced by *T. ethanolicus* were unusually numerous. "It's not unusual to wait a couple weeks to see a significant amount of magnetite form on an organism," Phelps says. "We were seeing copious amounts form within a couple of days."

Eventually, other researchers began to suggest ways to persuade *T. ethanolicus* to produce additional materials. By adding metals besides iron to the bacteria's diet of metal-containing salts, Phelps and his colleagues found that they could incorporate them into the nanoparticles as well. They were surprised that, when they added zinc to the mix, the resulting magnetite was 30 to 50 percent more magnetic than magnetite produced using iron alone. "From there," Phelps says, "we set out on a couple tangents. One of our big successes was producing cadmium sulfide nanoparticles—the kind used to make thin films for use in solar cells. Next year we will begin replacing this process with one that produces zinc sulfide, which is more environmentally friendly."

Once researchers recognized *T. ethanolicus*' distinctive qualities, they began thinking seriously about the implications of the organism's qualities for industry. "We realized we could make kilogram-size and larger batches of these particles," Phelps explains. "That's something that isn't seen much in nanotech research. A lot of nanoparticle processes look like they have potential in the laboratory, but when people consider producing them in larger quantities, they see they have scalability issues. We think nanofermentation gets around many of those problems."

Scaling up production

The nanoparticles Phelps and his group cultivate are easily harvested. Because they are made on the outside of microorganisms, they spontaneously break loose and settle to the bottom of the fermentation vessel. Phelps notes that as production of the bacteria was scaled up from test tubes to 30-liter vessels, researchers noticed an increase in particle production per liter of culture. "Unlike many other processes," he explains, "when this simple biological process is scaled up, production increases because there are fewer potential sources of problems. For example, if you put a drop of something into a test tube, you might kill everything in the container; however, if you put the same drop into a 30-liter vessel, you might kill everything within a centimeter, but that's all. So, in some respects, it's easier to control this kind of process on a larger scale. We think that's why we have seen better results."

The next step will be to move production to ORNL's Manufacturing Demonstration Facility (MDF), a facility supported by the Department of Energy's Energy Efficiency and Renewable Energy Advanced Manufacturing Office. The MDF will house an 800-liter pilot plant designed to produce kilogram-scale quantities of materials for industrial, academic and laboratory partners. "There are lots of people who have ideas about potential uses for nanoparticles but don't have a way to produce enough product to test on an industrial scale," he says. "We will be able to provide that capability."

Genetic tweaks

Phelps foresees that as researchers refine their ability to produce nanoparticles from naturally occurring bacteria, the next step will be to look beyond the natural cells.

"We are still learning what the bacteria can do," he says. "It has a lot of potential as well as limitations. At what point do we start changing the organisms? I think that will happen soon. If some of our potential research opportunities come to fruition, we'll be looking at genetically modifying some of the machinery within the cells to enhance their capabilities and scalability."

Some of these opportunities include developing nanoparticles for medical purposes. Phelps and his colleagues have had conversations with medical investigators about, among other things, producing nanoparticles for use in enhancing various types of medical scans by improving medical tracer materials and targeting the delivery of medicines to specific parts of the body.

The iron oxide nanoparticles produced by T. ethanolicus *are magnetic—a quality that interests both scientists and their industrial partners.* Photo: Jason Richards

Tailored to processes

In the near term, Phelps says the biggest challenge is ensuring that the products that come out of ORNL's nanofermentation effort can be incorporated easily into recognized industrial processes. "As we design the industrial-scale system at the MDF, we're asking industry what nanoparticle characteristics are most important to them," he says. "Is it size? Is it shape? Is it chemical reactivity? It's critically important that we reach out to industry and other researchers to see what they want, as well as talk to people who have developed similar processes, so we can learn from them in a collaborative fashion rather than reinventing the wheel."

As the laboratory's nanofermentation research grows, it is focused on three goals: manufacturing quality nanoparticles, expanding the range of particles that can be made using *T. ethanolicus* or a similar organism, and scaling production up to the point that ORNL can provide kilogram-size quantities of these materials for its industrial and laboratory partners. Phelps emphasizes that this effort continues to rely heavily on materials scientists, chemists, engineers and others researchers from across the laboratory. "No single person could have taken this idea and run with it," Phelps says. "It has taken a team. This is the kind of research national laboratories are here for." Ⓡ —*Jim Pearce*

Waterproof warriors

Adapting super-water-repellent materials for national security

Superhydrophobic materials are being considered for national security applications ranging from unmanned aerial vehicles to battleships. Photo: Jason Richards

Nature often exhibits the very characteristics that scientists are trying to create. For instance, a lotus leaf found in the swamps of southeast Asia has a nanoscale and microscale structure that, combined with its waxy chemistry, makes water bead up and roll off its surface. These naturally occurring features are exactly what John Simpson aimed for when he fabricated a super-water-repellent, or superhydrophobic, material.

Rather than starting with a hydrophobic material, making it superhydrophobic, and then improving upon the results, John Simpson, an ORNL materials scientist, and Brian D'Urso, of the University of Pittsburgh, decided to make the most superhydrophobic material theoretically possible and then use that as a basis for a set of water-repellent materials with desirable characteristics, including self-cleaning, anti-icing, thermally insulating, anti-biofouling and anti-corrosive properties.

Wide-ranging applications

Suggested civilian uses for these versatile materials have ranged from clothing to electronics to solar panels. Now they're being considered for national security applications as well

Unmanned aerial vehicles – Simpson and his colleagues originally developed superhydrophobic coatings that could be sprayed or painted onto high-tension power lines to reduce ice accumulation during freezing rain events and ice storms. However, the US Air Force has also expressed an interest in applying these coatings to the wings of unmanned aerial vehicles to prevent ice from forming. Having ice-free wings means UAVs can fly faster, longer and more fuel-efficient missions.

Water-repellent clothing and equipment – Dry clothing and equipment is a boon to servicemen and women in every branch of the military and extends and improves combat readiness, especially in cold, damp conditions. When ORNL researchers apply nanotextured superhydrophobic coatings to clothing, the coated cloth exhibits remarkable water-repelling properties. These coatings amplify the effects of water's surface tension, causing water and water-based solutions to roll or bounce off treated fabric. This effect is so strong that a layer of air is maintained on treated clothing, even while it is submerged in water. Because superhydrophobic coatings rely on a layer of air to repel water, instead of the impermeable polymer barrier used in traditional waterproofing, air is free to move through the fabric, making treated clothing "breathable" as well.

Drinkable water – Evaporation is a simple way to convert salt water or contaminated water into fresh water, but this approach creates salt deposits on the desalination equipment that are corrosive and expensive to remove. As a result, evaporative desalination has all but been abandoned commercially, although interest in a workable desalination process remains high in several regions of the world facing an increasing scarcity of fresh water. "People are predicting that the next war will be over water," Simpson says. "In 10 or 20 years, we could be fighting over water, so we need an inexpensive and efficient way to turn relatively abundant salt water into drinkable water."

When applied to desalination equipment, the superhydrophobic coatings produced by Simpson and his colleagues can greatly reduce the amount of energy and fresh water needed to remove salt deposits, while also reducing their corrosive effects. Initial, small-scale tests have shown these superhydrophobic coatings to be effective at mitigating the effects of salt because of their ability to pin a layer of air on the coating's surface. This pinned air layer reduces the number of evaporated salt crystals that can bond to or corrode the coated surface. Successfully demonstrating this effect on a large scale would fundamentally change the commercial viability of evaporative desalination. Simpson notes that this technology has the potential to substantially reduce the energy needed to convert salt water to fresh water.

In the area of national security, this technology is being considered for portable desalination units that could be used by the military to provide drinking water in areas where fresh water is scarce and where transporting water is dangerous, difficult or expensive. "Imagine where soldiers could go if they knew they would have drinkable water available," Simpson says.

Corrosion resistance – Corrosion due to salt costs the US Navy millions of dollars every year. Currently the best way to prevent or reduce corrosion on buildings and ships is to paint vulnerable surfaces. The problem with paint is that it eventually forms micro-cracks that allow moisture to seep under it and accelerate the corrosion process.

As noted earlier, superhydrophobic coatings have a unique ability to pin a layer of air on treated surfaces. This phenomenon can limit corrosion by maintaining a layer of air between the surface and surrounding water. Simpson notes that, while the treatment slows the interaction between surface and water, it doesn't eliminate it. Treated surfaces can still be reached by water vapor and condensation.

To solve this problem, Simpson and his colleagues developed a superhydrophobic coating that can pin oil or air on its surface. Pinning oil on a surface not only slows down corrosion, but it also reduces "biofouling," the accumulation of plants and algae on wet surfaces.

"Pinning oil on a superhydrophobic surface blocks condensation by acting as a barrier to both liquid water and water vapor," Simpson says. "The oil can be pinned so well that these surfaces won't even look or feel oily."

The upshot of this development could be that, instead of taking ships out of service for 18 months every five years to strip barnacles off their hulls and repaint them, the US Navy could conceivably save tens of millions of dollars by applying an anti-corrosive superhydrophobic coating to the undersides of its vessels.

Wide-ranging potential

By analyzing, enhancing and applying the natural water-shedding abilities of a plant that thrives in a soggy environment, Simpson and D'Urso have developed materials and treatments that enable people and machines to operate more safely, effectively and efficiently under similarly sodden conditions. In a national security setting, these advantages could mean the difference between life and death.

The potential applications of these water-repellent materials and surface treatments are wideranging, both inside and outside the national security realm, and are just beginning to be explored. Simpson predicts that any one of these materials could have considerable impact on manufacturing if applied on a large scale. R

—Emma MacMillan

Lonnie Love

is a senior research scientist in the laboratory's Automation, Robotics, and Manufacturing group. His work at ORNL and in the local community runs the gamut from robotics to prosthetics to science education. We asked him about the impacts of his work and the challenge of working in an increasingly interdisciplinary research environment.

Your research interests include robotics, biology and engineering. Is there a common thread that runs through these projects?

That would be fluid power. I started working with hydraulics and pneumatics when I came to ORNL in 1995 (as a postdoctoral researcher). My advisor had his doubts about that choice. However, after 17 years, every project I've worked on has had fluid power as its foundation.

You collaborate with scientists from a variety of disciplines. How does this "cross-pollination" affect the scientific process?

It gets chaotic—but in a good way. When you're part of a collaborative project, you can't predict where you'll end up. Everyone comes at the problem with a different perspective and a different set of skills. Of course, it's helpful if they share some of the same personality traits. Researchers who are confident, open minded, entrepreneurial, and who see their work as an adventure, instead of a job, are more likely to succeed in collaborations. I've been blessed to work with people from all different scientific backgrounds at ORNL. It's what makes the laboratory special to me.

Additive manufacturing has a lot of people excited. Where do you think this technology will have its biggest impact? [Note: Additive manufacturing is a process that enables custom-designed three-dimensional parts to be "printed" using relatively low-cost equipment—see the article on page 6.]

No one knows—and that's what's exciting. Right now, most of the attention in this field is directed toward aerospace and biomedical applications. However, the technology screams for creativity. I think we're seeing the first indications of this now. The opportunity for innovation in this field reminds me of when I was a kid and personal computers were being introduced. I remember in the late 1970s you could buy a computer as a kit, but you had to put it together, write your own software, and create your own drivers. This is happening again with additive manufacturing. You can buy a 3-D printer for $500. People are sharing models, coming up with modifications for the printers, and even generating new businesses based on the technology. Think back to 1975. Could you have predicted the impact the personal computer has had over the past 35 years?

Could you describe how your hydraulics research has impacted the field of prosthetics?

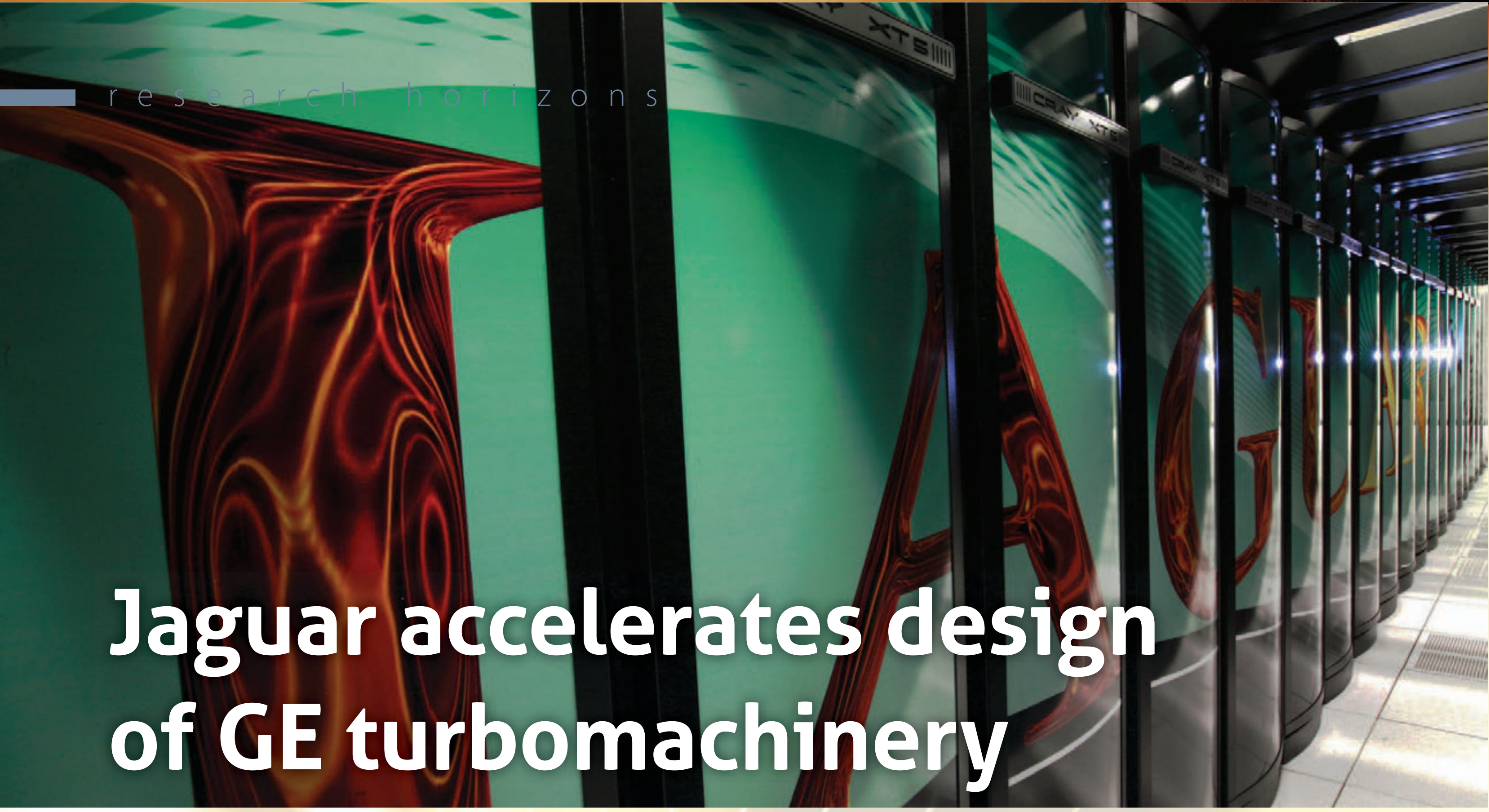
Commercial prosthetics are very limited. While there have been great advancements, cost is a big problem. That's why most upper limb prosthetics today are limited to an elbow, a wrist and a claw. My group has been working on miniaturized hydraulics. The goal is to enable greater dexterity and strength at a lower weight and cost. The latest twist has been the addition of additive manufacturing to the manufacturing equation. We're able to make things today that I couldn't even imagine 5 years ago. We can blend the hydraulics directly into the structure of the prosthesis, much as is done in nature. The big advantage of using additive manufacturing is that we can make structures more complex without making them more expensive. We can create intricate designs that dramatically reduce the weight of various components. As we reduce weight, we require less material and less energy. Less material and less energy means lower cost. This is a true paradigm shift. This technology also makes it much easier to customize every device for every patient. While functionality is important, patients have routinely given up functionality for the sake of aesthetics. They want their prostheses to look natural. Additive processes can easily make lifelike prosthetic limbs that also function well.

A lot of your research has implications for industry. What do you see as the nation's biggest challenge in the manufacturing arena?

Education, on many different levels. I really admire the work Dean Kamen has done with FIRST Robotics. He came up with a way to get everyone—K–12, community colleges, universities, industries, laboratories—working together to make fundamental changes in science education when he established the FIRST Robotics competition for high school students. This really struck a nerve with me. There's a group of researchers at ORNL who see this competition as a perfect platform for introducing the next generation of engineers and scientists to next-generation manufacturing, and it seems to be working. This year, ORNL supported eight FIRST Robotics teams. One of the teams built their entire robot using additive manufacturing. Dean Kamen saw pictures of the robot and asked if he could use them in a presentation he's giving on the future of manufacturing. Is that cool or what?

We also need to come to the understanding that manufacturing is important to the nation. It is also critically important that the United States is able to create new products, manufacture them locally, and still be competitive globally. This is an area in which ORNL can have a tremendous impact. Ⓡ

You can buy a 3-D printer for $500. Think back to 1975. Could you have predicted the impact the personal computer has had over the past 35 years?



Jaguar accelerates design of GE turbomachinery

Researchers at General Electric looked to Jaguar to simulate the design of next-generation turbines. These turbines, used in both aviation and power production, represent an extremely competitive global market. With their flagship code known as Tacoma, GE engineers ran their largest-ever computational fluid dynamics simulation on Jaguar, an achievement that helps pave the way for the design and production of next-generation turbines and uniquely positions GE in the international turbomachinery marketplace.

Few technologies are more vital to modern day life than turbomachines, the bladed devices used to convert fluid power to and from mechanical power to drive propellers, wind turbines, gas turbines, steam turbines, fans, and compressors. These engineering marvels are literally responsible for keeping the lights on given most of the world's electricity is generated by various kinds of turbines. And jets couldn't stay aloft without them to drive a plane's large-diameter fans.

General Electric (GE), the iconic technology, service, and finance company and American industrial leader, has been building turbomachines for nearly a century and is currently a major producer for the electric power generation and aircraft engine industries. Recently, however, GE took its turbomachinery research and development to the fast lane with the help of one of the fastest computers in the world.

Due to the amount of research invested in today's turbomachinery and the sophisticated nature of its engineering, companies have repeatedly grabbed the low-hanging fruit to achieve increased efficiencies, and competition is quite fierce.

"It's a very competitive business," said Principal Engineer Graham Holmes of GE Global Research, noting that the company is up against Rolls Royce and Pratt & Whitney in the aviation market and Siemens and Alstom in the power generation arena. "If you could achieve a 1 percent increase in efficiency for a turbomachine, the market would be yours." That 1 percent fuel-burning advantage would, over time, add up to enormous energy and cost savings for GE's customers and provide GE with a business-critical advantage, according to Holmes.

Enter Jaguar, a Department of Energy (DOE) high-performance computer (HPC) located at Oak Ridge National Laboratory (ORNL). Through ORNL's HPC Industrial Partnerships Program, GE recently harnessed Jaguar's power to study the unsteady fluid flows in turbomachines in greater detail than ever before accomplished. Understanding these flows is essential to achieving greater efficiency, and for GE to gain an edge in an intensely competitive global marketplace.

It's all in the blades

The basic physics of turbomachinery operations have been well understood for years—jet engines and gas turbines go back to the mid-twentieth century. Essentially, turbomachines feature alternating rows of stationary and moving blades either expanding or compressing gas. The design process has evolved from experimentation and highly simplified analytical models to increasingly sophisticated simulations, carried out on increasingly powerful computers. Engineers typically shape blades, run a combination of simulations and experiments, tweak the design, and repeat, which is an expensive path to production by any measure. GE runs these simulations on its in-house Linux clusters. But even with these systems, turbomachinery designers have had to assume that the velocity of air around and across the blades remains steady in the reference frame of the blades, or as seen from the point-of-view of the actual blades.

Turbomachinery designers have always understood that this air flow is unsteady and that it has to be unsteady for a turbomachine to work. But the assumption that the flow, as seen by each blade row, can be approximated as steady has proven to be remarkably powerful. The designs of all the most efficient turbomachines, such as the turbines that drive the large-diameter fans in modern jet engines, have been created using this paradigm.

Any future efficiency improvements will likely depend on deciphering the unsteady nature of the fluid flow. For example, in jet engines low-pressure turbines drive increasingly larger diameter fans, rotating at lower revolutions per minute to increase efficiency. But running low-pressure turbines at lower speeds presents a severe technical challenge—the lower the relative velocity between the blade rows, the harder it is to extract energy to drive the fan, requiring more rows of blades. Unfortunately, as more rows of blades are added, the turbine becomes heavier and therefore less efficient. Understanding the unsteady flows should allow designers to make needed adjustments without adding to the weight of the turbine, resulting in overall greater fuel efficiency.

Unsteady flow analysis is also essential to understanding other phenomenon like blade flutter, or the blade vibration induced by the fluid flow. Blade flutter can be catastrophic in an aircraft engine if it results in damage to one or more blades and turbine failure.

Ready to ramp up

GE was eager to compare its longstanding steady flow assumptions with real-world unsteady flow calculations, but this posed a major computational challenge. Unsteady simulations are orders of magnitude more complex than simulations of steady flows, and beyond the capability of GE's Linux clusters. So GE applied for and received access to Jaguar, one of the most powerful computers in the world.

Holmes was joined by Branden Moore of GE Global Research's Advanced Computing Lab to make the most of this opportunity. They further expanded the collaboration with senior engineer Stuart Connell on the visualization front, to better decode the mountain of data being produced in action.

"We definitely have the benefit of cross-discipline work at GE," said Moore, adding that this collaborative nature ultimately helps GE's HPC applications run faster. And running faster is a key metric in HPC. The faster a code runs, the more simulations can be run in a given timeframe. And more simulations increase the opportunity for new insights and new scientific discovery. GE used its flagship code Tacoma, which features specialized computational fluid dynamics (CFD) for turbomachinery. When they paired Tacoma with Jaguar, GE researchers ran their largest-ever CFD calculation and were able to investigate for the first time the unsteady flows in turbomachinery. Simulations were then ramped up from three to four dimensions, and researchers were able to look at the time-resolved unsteady flows in the moving blades.

Ultimately, said Holmes, GE's goal is to make better machines. The suite of simulations, which will benefit GE Aviation and GE Energy, was "an attempt to explore a better way of analyzing flow in those machines," he said. "Designers want to know how to shape the blades in a turbine to improve performance. With Jaguar our team did just that, investigating various blade interactions and the unsteady flow around them to see how the overall machine performed."

Tomorrow's turbine

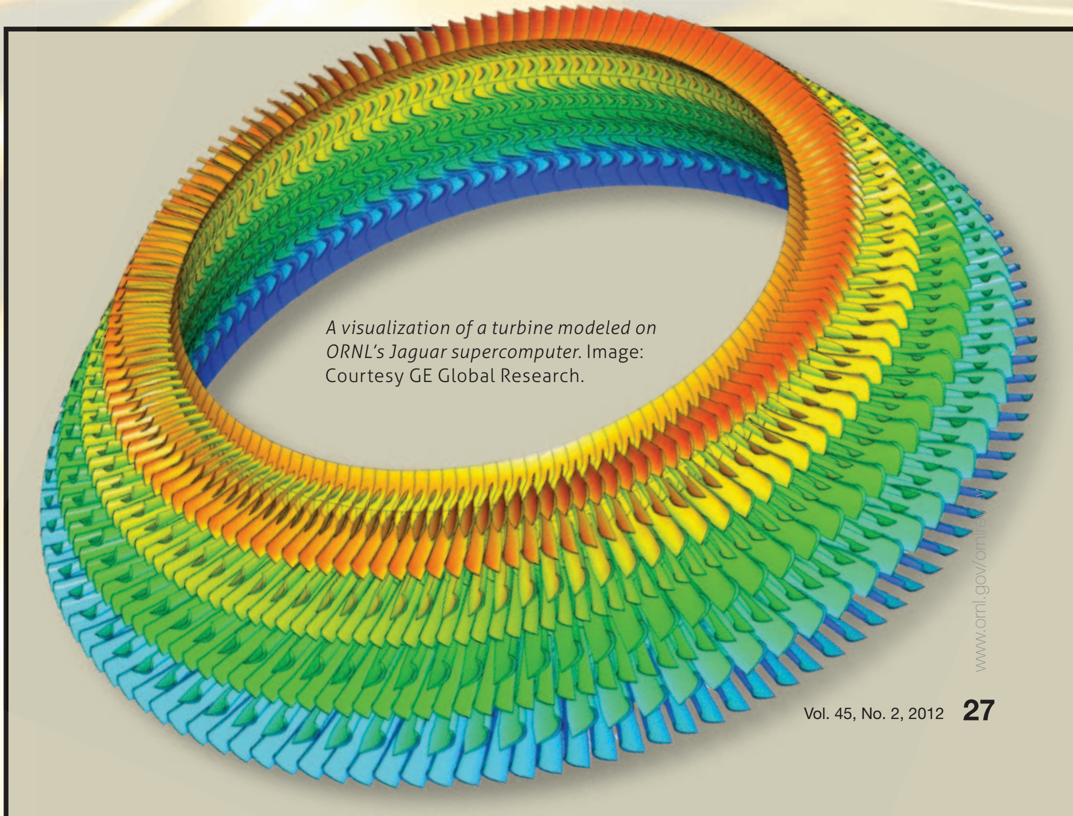
With access to Jaguar, the team was able to examine a turbine test rig and compare steady and unsteady flows. In the two analyses, the efficiency remained the same, which is "an extremely valuable piece of information," said Holmes. Furthermore, the team found plenty of interesting unsteady phenomena occurring throughout the device. For instance, the interactions between the blade and hub created unsteady secondary flows, which behaved differently than those witnessed in the steady analysis.

The team does not yet know why the secondary flows appear unique, but they definitely want to, said Holmes. "We need to dig in and use this information to improve our visualization skills," he said, adding that the team needs to develop a deeper comprehension of the differences in flows and decipher whether the environment or various test factors are to blame. After all, in a global industry chasing a 1 percent increase in efficiency, every little bit counts.

Overall, said Holmes and Moore, GE's simulations on Jaguar advanced the company's R&D in the turbomachinery arena and are providing it with a distinct competitive advantage as the company pours over the simulation results.

The team believes that GE and its competitors will move farther into unsteady flow analysis to achieve the final point in efficiency, a move that will require substantial HPC resources. In fact, largely as a result of these calculations, GE recently purchased its own Cray system, a move that significantly ramps up its in-house HPC capability.

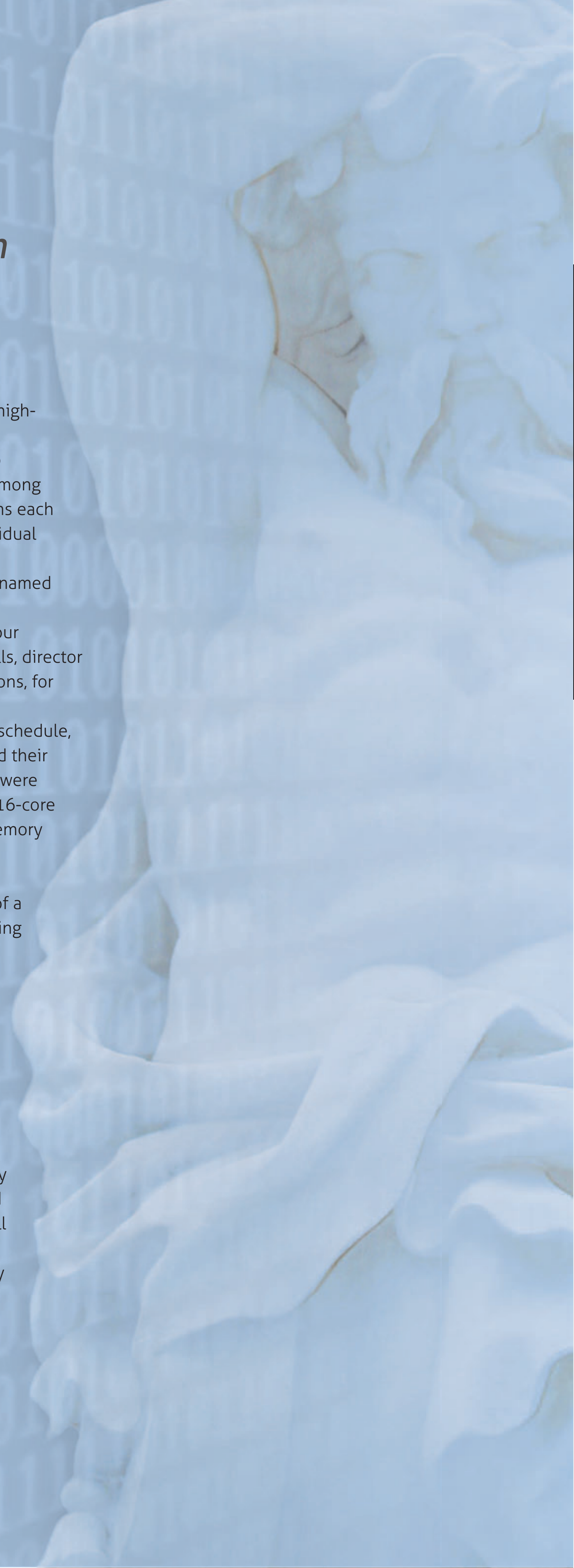
According to Holmes, "we simply could not design a competitive turbine or jet engine without these CFD tools. We would have exited the business a long time ago on both aviation and power generation." ®
—*Gregory Scott Jones*



A visualization of a turbine modeled on ORNL's Jaguar supercomputer. Image: Courtesy GE Global Research.

Titan rising

ORNL completes the first phase of the Jaguar-Titan supercomputer transition



ORNL's Jaguar supercomputer has completed the first phase of an upgrade that will keep it among the most powerful scientific computing systems in the world.

Acceptance testing for the upgrade was completed in February. The testing suite included leading scientific applications focused on molecular dynamics, high-temperature superconductivity, nuclear fusion, and combustion.

Jaguar, manufactured by Cray Inc., is operated by the Oak Ridge Leadership Computing Facility. Even before this month's upgrade to 3.3 petaflops, it was among the world's most powerful supercomputers, capable of 2300 trillion calculations each second, or 2.3 petaflops. The same number of calculations would take an individual working at a rate of one per second more than 70 million years.

When the upgrade process is completed this autumn, the system will be renamed "Titan" and will be capable of at least 20 petaflops.

Users have had access to Jaguar throughout the upgrade process. "During our upgrade, we have kept our users on Jaguar every chance we get," said Jack Wells, director of science at the OLCF. "We have already seen the positive impact on applications, for example in computational fluid dynamics, from the doubled memory."

The DOE Office of Science–funded project, which was concluded ahead of schedule, upgraded Jaguar's AMD Opteron cores to the newest 6200 series and increased their number by a third, from 224,256 to 299,008. Two six-core Opteron processors were removed from each of Jaguar's 18,688 nodes and were replaced with a single 16-core processor. At the same time, the system's interconnect was updated, and its memory was doubled to 600 terabytes.

In addition, 960 of Jaguar's 18,688 compute nodes now contain an NVIDIA graphical processing unit. The GPUs were added to the system in anticipation of a much larger GPU installation later in the year. The GPUs act as accelerators, giving researchers a serious boost in computing power in a far more energy-efficient system.

"Applications that were squeezing onto our earlier nodes can now make full use of the 16-core processor and increased memory. Doubling the memory can have a dramatic impact on application workflow," Wells said.

"The new Gemini interconnect is much more scalable," Wells added, "helping applications like molecular dynamics that have demanding network communication requirements."

GPUs will add a level of parallelism to the system and will allow Titan to reach 20 petaflops or more within the same space as Jaguar and with essentially the same power requirements. While the Opteron processors have 16 cores and are therefore able to carry out 16 computing tasks simultaneously, the GPUs will be able to tackle hundreds of computing tasks at the same time.

With nearly 1000 GPUs now available, researchers will have an opportunity to optimize their applications for the accelerated Titan system.

"This is going to be an exciting year in Oak Ridge as our users take advantage of our new architecture and get ready for the new NVIDIA Kepler GPUs in the fall," Wells said. "A lot of work by many people is beginning to pay off." Ⓡ

—Leo Williams

next issue

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