Features

EXPANDING RESEARCH PARTNERSHIPS

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During a recent visit to Oak Ridge to break ground for a new Center for Nanophase Materials Sciences, Energy Secretary Spencer Abraham took advantage of the opportunity to see firsthand the progress of the Spallation Neutron Source, one of the world’s largest science projects. Sweltering in the Tennessee heat on a ridge overlooking the massive construction site, the Secretary was provided a glimpse of a $1.4 billion facility that in 2006 will anchor the next generation of scientific discovery at Oak Ridge National Laboratory.

Less apparent but in some ways equally significant, the SNS facility also is symbolic of the collaboration that increasingly defines large-scale scientific research. Joined by Chuck Shank, director of Lawrence Berkeley National Laboratory, the Secretary inspected the $21-million front-end system designed by Berkeley as part of the SNS complex. Berkeley’s system, already installed and operational, is the first of five major SNS components that will be delivered by other Department of Energy laboratories at Argonne, Brookhaven, Jefferson, and Los Alamos. No single laboratory possessed the resources needed to design and construct a project of such enormous scale and complexity. Experience also suggests the political hurdles that stalled previous “big science” projects would have been insurmountable for a laboratory acting alone.

This issue of the ORNL Review is dedicated to a variety of partnerships, both scientific and operational, that are influencing the Laboratory’s research mission and reshaping ORNL’s traditional relationships with a host of university, government, and community stakeholders. Some partnerships, like ORNL’s study of electrical power transmission with the Tennessee Valley Authority, represent new research projects with long-time friends. Others, such as the effort with Cray to design and build one of the world’s largest supercomputers, reflect more recent collaborations between ORNL and the private sector.

In many respects ORNL’s most significant partnership is that between the University of Tennessee and Battelle, the Laboratory’s managing contractors. The inclusion of six “core” universities as primary research partners and a partnership with the state to commercialize Laboratory technologies are but two of the initiatives brought to Oak Ridge by UT-Battelle. As noted in the following pages, the fusion of UT and Battelle’s distinctive cultures may prove over the next decade to be the single most important factor in redefining ORNL’s identity.

While only time will reveal the precise nature of ORNL’s emerging partnerships, we can be certain that the partnerships are changing in fundamental ways the process by which we address the future’s great scientific challenges.
In the eyes of some, the marriage was a strange one.
One of the partners had no experience managing a national laboratory. The other had no presence or history in Tennessee.
The former represented the genteel protocol and heritage of a southern land grant university. The latter was the nation’s largest not-for-profit research corporation with a corporate philosophy more attuned to the pace of the Northeast.
To succeed, the partnership would require a fusion of two very different cultures into a single management team and a single vision.

Despite these differences, the University of Tennessee, with system headquarters in Knoxville, and Battelle Memorial Institute of Columbus, Ohio, in late 1998 hinged their futures to one another. A year later the Department of Energy selected UT-Battelle to manage Oak Ridge National Laboratory. United as a limited liability corporation, UT and Battelle entered the partnership with different goals. For UT, managing ORNL was an opportunity to enhance the university’s research program by expanding a relationship between the two institutions that had existed for more than a half-century. Battelle, which already managed national laboratories in Upton, New York, Richland, Washington, and Golden, Colorado, viewed Oak Ridge as a chance to broaden the company’s portfolio of technologies in a way that provided synergy for Battelle’s long-term research agenda.

The partnership was real, and was reflected in the makeup of UT-Battelle’s senior management. ORNL’s new director was Bill Madia, a career Battelle employee who came to Oak Ridge from his role as director of Pacific Northwest National Laboratory (PNNL). ORNL’s new deputy director for science and technology was Lee Riedinger, professor and head of UT’s Physics Department. Jeff Smith, also from PNNL, became the deputy director for operations. Billy Stair, executive assistant to the UT president and former senior policy advisor to the Tennessee governor, became the Laboratory’s new director of communications.

Numerous other senior management positions were filled by UT and Battelle staff. All had played a part in developing UT-Battelle’s management proposal, meaning that each brought to the Laboratory a clear understanding of the purpose and goals of the new partnership.

An Immediate Challenge

An immediate challenge took the measure of the unique talents brought to the new partnership by both UT and Battelle. ORNL was in the early stages of designing and building the Spallation Neutron Source (SNS), a $1.4-billion pulsed-neutron-beam accelerator and one of the world’s largest science projects. Completing the SNS on time, within budget, and within scope was critical to the Department of Energy’s effort to sustain credibility with Congress, particularly among members skeptical of spending huge sums for basic science research. Indeed, congressional opponents of the SNS in April 1999 had imposed a challenge and deadline some feared would kill the project. The House Science Committee required that any further appropriations for the SNS be halted unless the Tennessee General Assembly repealed by February 1, 2000, the state sales tax on the SNS construction, valued at $28.3 million.

The calendar provided few options. Although UT-Battelle would not assume operational control of ORNL until April 2000, efforts to repeal the sales tax had to begin as soon as the Tennessee General Assembly convened on January 12, only 19 days prior to the February 1 deadline. The SNS sales tax crisis revealed UT’s political currency in Nashville and the university’s untapped potential for ORNL. Both the House and Senate speakers were UT graduates, as were key members of the Governor’s cabinet. For the first time, political assistance for ORNL also meant helping the state’s flagship university. The legislature approved the sales tax exemption for the SNS in 16 days, a record time for legislation of such
In Washington, the House Science Committee received an official copy of the legislation with two days to spare. Congressional opposition to the SNS project subsided, providing UT-Battelle the opportunity to shift attention to critical issues of design and construction.

**Simultaneous Excellence**

Back in Oak Ridge, the strong affinity for UT among political and community stakeholders was complemented by Battelle’s extensive experience in managing research laboratories. Battelle brought to ORNL a belief that successful laboratory management requires that the contractor, in addition to providing excellence in scientific research, also provide a comparable degree of excellence in both operations and community service. Indeed, over the years a number of laboratories have seen their scientific agendas compromised by the failure to exercise operational discipline or, in some instances, to be regarded as a valued member of the community. Known as the philosophy of “simultaneous excellence,” UT-Battelle integrated the three-pronged goal as the core value of ORNL’s new laboratory agenda. The result was a fundamental realignment of scientific, operational, and community outreach strategies.

Developing the management structure and attracting the personnel needed to deliver the SNS on time and within budget dominated UT-Battelle’s early months. As ORNL’s new contractor, UT-Battelle faced the intimidating task of coordinating an extraordinarily complex project design among six national laboratories that in some cases were unfamiliar with collaboration on such a large and highly visible scale. Conducted in parallel with the SNS design were preparations for procurements and construction contracts worth hundreds of millions of dollars. UT-Battelle’s new management team at SNS took on an international flavor. Thom Mason, a 36-year-old Canadian physicist, was selected to direct the project. Mason in turn chose Ian Anderson of Great Britain to head up the project’s Experimental Facilities Division and Norbert Holtkamp of Germany to lead the Accelerator Systems Division.

As UT-Battelle realigned the SNS project, efforts were under way to identify the scientific competencies on which ORNL would build the Laboratory’s future. Over the years a multitude of scientific programs had proliferated within the Laboratory, each competing for a finite amount of financial resources. A lack of focus within the science agenda at times diminished the Laboratory’s ability to articulate funding priorities within the halls of DOE and Capitol Hill. UT-Battelle believed that focusing the science agenda was critical if ORNL wished to take advantage of emerging opportunities, such as nanophase materials and national security technologies, that held potential for substantial research funding.

By 2001, UT-Battelle had determined that ORNL would prioritize the Laboratory’s resources so as to develop and sustain competencies in the six scientific areas of energy, advanced materials, complex biological systems, national security, high-performance computing, and neutron science. Looking at the energy horizon, ORNL made a commitment to allocate additional resources to nuclear and fusion research programs. UT-Battelle undertook a concentrated effort to attract strategic hires and build world-class facilities for high-performance computing. The Laboratory’s research divisions were reorganized to align staff and programs with ORNL’s new scientific agenda. Researchers developed proposals to compete for major new programs in nanophase materials science, national security, and functional genomics. By the end of 2001, UT-Battelle had in place a roadmap for ORNL’s research program.

UT-Battelle sought to implement the new research agenda by first addressing two operational challenges. Drawing upon Battelle’s experience with DOE and UT’s with the state of Tennessee, ORNL undertook a $300-million modernization of the Laboratory’s aging infrastructure. (See ORNL Review, Vol. 36, No. 2, pp. 2-7.) As they planned and designed 11 new buildings, UT-Battelle management also sought ways to reduce the cost of conducting research at the Laboratory. Ultimately, some $30 million in operational costs were eliminated. Although some of these savings were negated by unanticipated costs required to remove legacy wastes, pay for medical benefits, and close a salary gap with other laboratories, UT-Battelle’s operational initiatives proved as aggressive as those in science and technology.

Smaller in scope but often higher in visibility, UT-Battelle’s corporate outreach program allocated more than $1.2 million annually for legacy projects designed to support science education, economic development, and volunteerism in the region. From providing new high school science labs to supporting 30 start-up companies, UT-Battelle pursued a goal of being viewed by its neighbors as a valued partner in the community.

**A Maturing Relationship**

More than three years into the partnership, both UT and Battelle understand the challenges and opportunities that come with running a national laboratory. Each has made a distinctive mark on ORNL’s research agenda and the accelerated pace of the Laboratory’s modernization. As the relationship matures, a further blending of the cultures and styles that each brought to Oak Ridge is likely. While only time will reveal the road’s destination, the partnership undoubtedly will shape in a lasting way the scientific missions of ORNL, Battelle, and the University of Tennessee.—Billy Stair, ORNL Communications and Community Outreach Director
Since the Laboratory’s birth in the 1940s, ORNL has enjoyed a special relationship with the University of Tennessee. Since UT became a partner in managing ORNL in 2000, ties between the two institutions have become closer than ever before. As a result, the two institutions together often are more effective in advancing scientific research and education than each could be working alone.

Among the partnership’s most significant milestones was the creation of the Science Alliance, a Tennessee Center of Excellence opened in 1984 to strengthen research bonds between UT and ORNL. With the 20th anniversary of the partnership on the horizon, Science Alliance advocacy of the ORNL-UT research agenda is stronger than ever. In 2000—the same year UT-Battelle management of ORNL began—the university broadened the center’s research scope beyond Knoxville to include science and engineering programs throughout the UT system.

The Science Alliance’s academic cornerstone is the Distinguished Scientist program, through which prominent, senior-level scientists and engineers are appointed to joint, 50-50 positions at both institutions. The partnership encompasses multiple levels of research, attracting talented scientists and graduate students to work with one or more of the distinguished scientists. Additional appointees are being considered in catalysis, physics theory, and functional genomics and computational biology. Today’s ORNL-UT Joint Faculty program for some 20 ORNL staff and UT faculty evolved from the 1984 model for the Science Alliance, now directed by Jesse Poore.

Science Alliance centers and joint institutes foster numerous external partnerships that bring both national and international research talent to Oak Ridge. The Joint Institute for Heavy Ion Research, established in 1984, and the early Joint Institute for Computational Sciences, created in 1991, served as models for developing large-scale, organized collaborations, enhanced by state-funded facilities sited at ORNL.

Distinguished Scientists

A recent addition to the Distinguished Scientist Program is Jimmy Mays, hired in 2001. A “scientific extrovert,” Mays has a global reputation for establishing highly productive collaborations with leading scientists and engineers. He specializes in creating polymer compounds with well-known structures and architectures. He then works with engineers, physicists, and other scientists to discover how the structure affects material properties.

In one branch of his work, Mays experiments with room-temperature ionic liquids (RTILs) to make block copolymers, chain-like compounds in which a long stretch of one polymer is attached to a similar stretch of another. Using this process, Mays creates patterns of individual units in the chain and examines how the design affects a material’s properties.

RTILs are gaining a reputation for their potential to replace the odorous, toxic volatile organic compounds currently used in making polymers. Mays has developed environmentally benign liquids that provide an economic advantage in making commercially important polymers, such as Styrofoam and Plexiglas. The process is 10 times faster and produces materials with higher molecular weights, which translates into higher quality.
Applied physicist Takeshi Egami, a recent arrival to the Distinguished Scientist Program, says a material’s novelty and usefulness fuel his research. Egami studies unusual local atomic arrangements to learn how atoms control material properties. Through special processing of data from diffraction studies of high-temperature superconducting materials, he has found that under “usual” conditions, actual atomic positions deviate only slightly from those established by traditional crystallographic research. However, they deviate considerably as the material nears its superconducting transition temperature.

Although magnetism is thought by many to be the mechanism behind high-temperature superconductivity, Egami believes “atomic motion,” or vibration, also plays a major role. And material properties, he says, are influenced more by “next-door-neighbor relationships” than by those far away.

Egami’s preference for the untried led him to champion successfully a technique called the “atomic pair-density function,” a method used previously on glasses and liquids but rarely, if ever, to study local atomic structure in reactive crystal materials. Egami will receive the American Crystallography Society’s 2003 Bertram Eugene Warren Diffraction Physics Award in recognition of his use of this technique to analyze data collected on disordered crystals using pulsed neutrons and synchrotron X rays.

Joint Faculty Program

In 2000, the Science Alliance began oversight of the Tennessee Advanced Materials Laboratory (TAML), a new UT Center of Excellence led by ORNL-UT Distinguished Scientist Ward Plummer. TAML conducts science-driven synthesis of complex and artificially structured materials and is dedicated to training a new breed of graduate student, capable of tackling all aspects of materials science, from synthesis to characterization to modeling and design.

TAML has a broad scientific and engineering base, augmented by extensive partnerships with ORNL. The center has assisted with 17 joint faculty appointments, including that of Mike Simpson, whose molecular-scale research bridges the agenda of TAML and UT’s Center for Environmental Biotechnology, led by Gary Sayler.

Hired to ORNL’s scientific staff in 1992, Simpson recently became one of a growing number of scientists with a UT-Battelle-sponsored joint faculty appointment. Like several of his colleagues, he wears several hats.

At ORNL, Simpson is leader of the Nanofabrication Research Laboratory, part of ORNL’s new Center for Nanophase Materials Sciences (CNMS), a Department of Energy user facility scheduled for completion in 2005.

Recently, Simpson donned his UT hat to lead a large group of researchers in a quest for National Science Foundation (NSF) funding to bring a National Nanofabrication Infrastructure Network node to UT. The Massachusetts Institute of Technology is the project’s network leader, with the universities of Illinois at Urbana-Champaign and California at Berkeley serving as co-leaders. If funded, the network will bring the nation’s leading nanoscience experts to Knoxville for collaborative research.

An electron-beam writer, scheduled to arrive at UT in the fall of 2003, will make it possible for the university to be an integral team partner. Although not a funded partner on the NSF pro-

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TWO JOBS FOR THE PRICE OF ONE

One recent benefit of the UT-ORNL partnership is Thom Dunning, the new director of the Joint Institute for Computational Sciences (JICS). Dunning has been making waves for much of his career. He helped develop computational techniques for solving the Schrödinger Equation, also known as the Wave Equation. One of his papers has over 4200 citations—more than most scientists receive for a lifetime of work.

When Dunning was director of the Environmental Molecular Sciences Laboratory (EMSL) at DOE’s Pacific Northwest National Laboratory, he assembled a group that made waves in computational chemistry. The group, led by Jeff Nichols and Robert Harrison—both now at ORNL, developed Northwest Chem, a molecular modeling package to predict the structures, energies, and properties of molecules. NWChem, designed from “scratch” for modern parallel computers, can routinely do calculations once considered intractable.

As Assistant Director for Scientific Simulation at DOE headquarters in Washington, D.C., Dunning was asked to use his EMSL experience to create a new scientific computing program in the Office of Science. The result was “SciDAC,” DOE’s Scientific Discovery through Advanced Computing program that funds teams of researchers to create codes that take advantage of the fastest supercomputers to solve complex scientific problems.

In September 2002, Dunning came to ORNL and the University of Tennessee from the University of North Carolina. Why was he attracted to this appointment?

“The one impression my stay in Washington left with me,” he says, “is the importance of integrating the national laboratories into the U.S. research fabric, especially the universities. JICS directly links ORNL to UT and UT-Battelle’s six core universities.

“JICS will have 30 joint faculty positions in computational science, applied mathematics, and computer science. My challenge is to find university faculty who will work synergistically

TENNESSEE’S JOINT INSTITUTES

In 1981 after the Holifield Heavy Ion Research Facility became operational at ORNL for nuclear physics studies, Professor Joseph Hamilton of Vanderbilt University came up with the idea for what became the first joint institute between ORNL and a university. His idea, called the Joint Institute for Heavy Ion Research (JIHIR), is still being used to provide free housing and office space for graduate students and postdoctoral researchers conducting accelerator research on what is now the Holifield Radioactive Ion Beam Facility.

Hamilton identified the potential of a joint institute when he served on the national policy board for the Holifield facility. He persuaded Vanderbilt, ORNL, and the state of Tennessee to commit the funds necessary to make ORNL’s first joint institute a reality.

When the state in 1984 created the Science Alliance between ORNL and the University of Tennessee, the joint institute became a natural extension of the partnership. “Joint institutes allow university faculty and graduate students access to the resources of Department of Energy user facilities based at ORNL,” says Lee Riedinger, ORNL’s deputy director for science and technology. “The integration of ORNL and UT capabilities in joint institutes provides the two parties resources and research talent at a lower cost than either could gain alone.”

UT and ORNL conducted joint research ventures in energy, environmental effects, environmental biotechnology, computational science, and transportation. In 2000 the UT-ORNL National Transportation Research Center opened, showing that a creative combination of federal, state, and local funding could make such an important joint venture possible.

The outstanding success of JIHIR laid the groundwork for convincing the state legislature in 1997 to pledge $8 million to build a new Joint Institute for Neutron Sciences (JINS), owned...
by UT and located at ORNL. The pledge for the new institute played an important role in leveraging the decision to locate the $1.4-billion Spallation Neutron Source in Oak Ridge.

A similar pledge by the state to construct three new joint institutes was an equally critical element of UT-Battelle’s successful bid in 1999 for the management contract at ORNL. The state committed $26 million to construct, in addition to JINS, the Joint Institute for Computational Sciences (JICS) and the Joint Institute for Biological Sciences (JIBS). The creative plan included the transfer of DOE property to the state of Tennessee, state ownership of the facilities, and shared costs by UT and ORNL for the operation of the institutes located on the ORNL campus.

JICS will be located in a $9-million building on ORNL’s east campus directly across the street from ORNL’s new Center for Computational Sciences. The new JICS facility also will house the Oak Ridge Center for Advanced Studies. JICS’ location will help provide UT faculty and students with access to one of the world’s most powerful unclassified supercomputers.

Planning funds for the Joint Institute for Biological Sciences were included in the 2004 state budget. JIBS will offer expanded opportunities for graduate students from another joint venture—the UT-ORNL Graduate School for Genome Science and Technology, the successor of the UT-Oak Ridge Graduate School of Biomedical Sciences, established four decades ago. JIBS also will be leveraged as part of ORNL’s proposal to house a new DOE genomics research center.

Although the Joint Institute for Neutron Sciences will be built last, probably around 2007, a JINS group led by UT’s Lee Magid has organized numerous workshops for hundreds of university and national lab scientists and engineers who need a powerful neutron source for their research. Attendees have formed teams to design research instruments for the 24 beam lines available at SNS.

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Z. L. Wang played a crucial role in helping Oak Ridge National Laboratory become a site for one of the Department of Energy’s nanoscience centers. He helped an ORNL team write a successful proposal that won initial funding for the design of DOE’s Center for Nanophase Materials Sciences, to be built near the Spallation Neutron Source, now under construction at ORNL.

But Wang is not an ORNL employee. He is a professor at Georgia Tech, one of the six “core” universities that are a formal part of the management structure of UT-Battelle, which manages ORNL for DOE. The other member universities are Duke University, Florida State University, North Carolina State University, the University of Virginia, and Virginia Tech. One of the most innovative partnerships in the national laboratory system, the “cores” have become an integral part of the scientific agenda at ORNL.

Core university faculty have joined with University of Tennessee faculty and ORNL researchers led by Thom Dunning to write a winning proposal to the National Science Foundation to add ORNL’s present and future neutron-scattering resources—High Flux Isotope Reactor and Spallation Neutron Source—to the TeraGrid, NSF’s high-speed network connecting supercomputers and data storage centers across the nation. The proposal calls for DOE’s Center for Computational Sciences at ORNL to become part of the Southeastern TeraGrid Extension for Neutron Science.

Universities generally have easier access to NSF funding than do mainly DOE-funded national laboratories. For ORNL researchers an advantage of collaborations with UT and core university faculty is improved access to federal funding from agencies such as NSF.

ORNL’s partnership with UT and the core universities provides researchers from the Laboratory and the member schools access to greater opportunities for joint research projects, conferences, and academic workshops. The partnership, which includes a number of historically black colleges and universities (HBCU), makes possible a unique opportunity to combine the resources of outstanding research programs into a unified approach to address a variety of high-technology issues.

**Joint Faculty Appointments**

UT-Battelle and the core universities are working in several areas to broaden existing partnerships with ORNL. One fruitful initiative is the joint faculty appointment, which allows a faculty member from UT, a core university, an HBCU, or another university with strong ties to the Laboratory to spend about half his or her time conducting research at ORNL. The cost of the joint faculty position is shared by the two institutions.

According to Lee Riedinger, ORNL’s deputy director for science and technology, “UT-Battelle has signed legal agreements with each of the six core universities to establish a joint faculty program. We’ve established the guidelines with respect to cost sharing, overhead waivers, and intellectual property considerations.”

After three years’ effort, eight joint faculty positions with the core universities will likely be in place by the end of 2003. Two will be from the University of Virginia, four from North Carolina State, and two from Georgia Tech.

The first two joint faculty appointees were postdoctoral researchers at ORNL who obtained faculty positions at the core universities. One joint faculty hire was Gerd Duscher, who completed a postdoctoral program in ORNL’s Condensed Matter Sciences Division and successfully competed for a faculty position at North Carolina State. The second joint faculty hire is Shawn Agnew, a former Wigner Fellow in ORNL’s Metals and Ceramics Division.

Duke University
*Key areas of joint research:* biology and biomedicine.

North Carolina State University
*Key areas of joint research:* nuclear science and physics.
Division, who won a position at the University of Virginia. Both institutions have research competencies that complement ORNL in the areas of materials and nanoscience research.

The universities were happy to share with ORNL the costs of supporting two researchers who know the Laboratory well and want to teach and advise graduate students doing research on campus and in Oak Ridge. “Some joint faculty positions are based at the university and are advertised as a shared position,” Riedinger says. “The general model is that the joint faculty hire will teach only one semester a year and have the other semester and the summer available for joint research, partly done at ORNL.”

An example of a potential joint faculty arrangement involving ORNL, UT, and NC State is in the area of neutron science. The Laboratory’s High Flux Isotope Reactor, combined with the Spallation Neutron Source (in 2006), will make ORNL the world’s foremost center for neutron science. A new UT-ORNL joint faculty member is Geoff Greene, a former Los Alamos National Laboratory scientist who is developing two instruments for an SNS beam line to measure a neutron’s lifetime and other fundamental physics characteristics. Because NC State has a research reactor used for neutron science, the university seeks to pair one of its faculty with Greene in a joint faculty arrangement.

The core universities represent six of the nine seats on the UT-Battelle Board of Governors’ Science and Technology Committee, giving them an important voice in shaping ORNL’s science agenda. The advisory committee provides high-level scientific direction to the Laboratory, including rigorous reviews of major scientific initiatives. The core university principals also sit on the ORNL Corporate Fellows Selection Committee. Len Peters, former Virginia Tech vice provost for research who chaired the committee in 2002, is now director of DOE’s Pacific Northwest National Laboratory.

The Board of Governors subcommittee reviewing ORNL’s complex biology research is chaired by Jim Siedow, vice provost for research at Duke University. “The marriage I’m trying to arrange is between ORNL and Duke, which has a well-known medical center,” Riedinger says. Duke worked with ORNL and non-core universities such as Vanderbilt, Emory, and the University of Alabama at Birmingham on a proposal to the National Institutes of Health to create a Southeast Center of Excellence on Biothreats and Emerging Infectious Diseases.

Oak Ridge Center for Advanced Studies

In spring 2004, another new building will open on the ORNL campus. The facility will house the Oak Ridge Center for Advanced Studies (ORCAS), as well as the UT-ORNL Joint Institute for Computational Sciences. According to Riedinger, “ORCAS was a proposal idea that came from the core universities in 1999 during the development of UT-Battelle’s proposal to manage ORNL. The concept of a joint institute staffed in part with joint faculty evolved from a 20-year emphasis at UT on building special joint programs at ORNL.”

ORCAS is conceived as a policy center that will offer graduate education to students at UT and the six core universities, as well as challenging intellectual opportunities for faculty. Riedinger calls it a new experiment of trying to combine 10 institutions—UT, Battelle, ORNL, six core universities, and Oak Ridge Associated Universities—into a single center for the study of large scientific challenges.

“ORCAS is fueled by the collective intellectual firepower of the tenants,” Riedinger says. “ORCAS’s mission is to provide a variety of research perspectives to science and technology issues of importance to DOE and the country. Each of the 10 member institutions has submitted initial three-year operating support that will allow UT-Battelle to hire a director, get us started, and provide a revenue stream. An active search for a new director of ORCAS began in the summer of 2003.” By the time a new director is in place, ORCAS will be among the most creative of ORNL’s partnerships, and it will greatly boost the Laboratory’s ability to raise scientific understanding to the next level.
NEW PARTNERSHIPS WITH HISTORIC INSTITUTIONS

Lee Riedinger, ORNL’s deputy director for science and technology, is determined to build better bridges between ORNL and historically black colleges and universities (HBCUs) and other minority education institutions (MEIs).

“I am firmly committed to helping form stronger relations with HBCUs,” he says. “There are 103 HBCUs in the country, mostly in the Southeast, because of the historical misfor-
tune that until recently prevented black students from attending majority universities.

“We have too few African-American scientists and engineers. I’m convinced we can encourage more black science students to follow paths to scientific careers by enabling them to spend time here working in science. That’s why the summer program we operate through the Oak Ridge Institute for Science and Education is so important. ORNL participates in the summer program called SULI, or Science Undergraduate Laboratory Internships, funded by DOE’s Office of Science and operated under the direction of ORISE’s Linda Holmes. Riedinger encourages promising HBCU seniors who work at ORNL in the summer to attend graduate school at one of UT-Battelle’s core universities. “They then can come back to ORNL to do research as graduate students,” he says. “If they do well, they may be future ORNL staff researchers.”

“Another way we can help is to nurture more relationships between our researchers and HBCU faculty—to improve their chances of winning their own grants. We want to help them build a pipeline to enable their best science students to be accepted by graduate schools at the University of Tennessee and the UT-Battelle core universities.”

Ron Townsend, president of ORAU, says that ORISE has played a role in enabling about a dozen faculty members from HBCUs and MEIs to conduct research at the Laboratory in the summer. “I endorse Lee Riedinger’s emphasis on building relationships between Lab scientists and university researchers,” Townsend says. “We believe in the program enough to help the Lab fund these summer research programs.”

ORNL is poised to announce in the fall of 2003 a “joint faculty hire” with an HBCU. Dhananjay Kumar, a faculty member at North Carolina A&T State University’s Center for Advanced Materials and Smart Structures, will spend half his time teaching and performing research at the university and the other half conducting research at ORNL. In the summer of 2002, Kumar collaborated with ORNL Corporate Fellow Stephen Pennycook, whose laboratory has one of the world’s most powerful electron microscopes. “It was one of the best scientific experiences of my life,” Kumar asserts. “ORNL’s summer research program is a very useful program for people who need opportunities.”

Scientific Research

From a science perspective, ORISE has a historic partnership with ORNL’s Physics Division that has evolved into the use of radioactive ion beams (RIBs) to study the basic structure of matter. The collaboration benefited from the leadership and vision of Vanderbilt University’s Joe Hamilton and Lee Riedinger, then with UT and now ORNL’s deputy director for science and technology. The partnership expanded after ORNL’s Holifield Heavy Ion Research Facility opened in 1980. The facility is now used for research with RIBs instead of stable ion beams.

ORAU manages the University Radioactive Ion Beam (UNIRIB) Consortium, a group of eight universities that includes UT, Vanderbilt University, and more recently, Rutgers University. In April 2003, the National Nuclear Security Administration announced the award of $2.96 million for three years to a Rutgers team and Ken Carter, an ORAU scientist who manages the UNIRIB Consortium and works in ORNL’s Physics Division. The team represents co-principal investigators in a study that uses the capabilities of RIBs at the Holifield Radioactive Ion Beam Facility for stockpile stewardship science. The participants will conduct basic nuclear science research on the characteristics of unstable isotopes of atomic nuclei. The research is designed to produce nuclear physics data needed to help DOE accurately predict the performance of aging nuclear weapons.

“The ORAU-ORNL partnerships together made this grant possible,” Townsend says. “None of these institutions alone would likely have won this project.”

Increasing Scientific Users

Looking forward, ORAU seeks to expand university participation in new scientific facilities under construction in Oak Ridge. Specifically, ORAU is developing plans to increase the number of graduate students and faculty at ORNL’s Spallation Neutron Source. ORAU will undertake similar efforts as the Laboratory brings on line new facilities in supercomputing, nanoscience, genomics, and electron microscopy. According to Townsend, “As UT-Battelle builds the next generation of user facilities, ORAU’s goal will be to build the next generation of users.”
Atmospheric carbon dioxide is taken up by vegetation and converted by photosynthesis into carbon-containing material that is eventually deposited in the soil. This organic material is decomposed by bacteria, fungi, and soil animals, which can return carbon to the atmosphere by respiration. Soil carbon retention could be increased by advanced farming and forestry practices, but extensive research, including data collection and computer modeling, is needed to determine which measures best promote carbon sequestration. Carbon sequestration could help deter climate change attributed to the buildup of carbon dioxide and other greenhouse gases in the atmosphere.

The Consortium for Research to Enhance Carbon Sequestration in Terrestrial Ecosystems (CsiTE), comprising a wide-ranging network of partners, was created in 1999 to provide the science-based understanding to support development and assessment of terrestrial carbon sequestration strategies.

CsiTE includes three Department of Energy national laboratories—ORNL, the Pacific Northwest National Laboratory (PNNL), and Argonne National Laboratory (ANL); seven universities—Colorado State, Cornell, North Carolina State, Ohio State, Texas A&M, Virginia Tech, and Washington; a research institution—the Joanneum Institute for Energy Research in Austria, and several U.S. Department of Agriculture (USDA) facilities. ORNL CsiTE researchers include Gary Jacobs, Gregg Marland, Mac Post, Tristam West, Phil Jardine, and Chuck Garten, all of the Environmental Sciences Division.

“By choosing only a few field sites to focus on, the consortium brought in and integrated different scientific disciplines from across the partners,” says Jacobs, co-leader of CsiTE with PNNL’s Blaine Metting. “A key site has been DOE’s FermiLab Accelerator Ring in Illinois, where prairie grasses are growing instead of corn. Some previous cornfields have been restored to prairie longer than others, so the site offers a variety of information.”

The consortium partners have been determining the chemical composition of the soil, as well as the types and amounts of microorganisms and carbon compounds present (e.g., from decayed roots). They have characterized the above-ground vegetation and measured boosts in soil carbon content after tilled agricultural land morphed into natural prairie.

“We are using discoveries and data at that site to guide experiments and improve the accuracy of our computer models,” Jacobs says. “The results could lead to new ideas on how to manipulate terrestrial ecosystems to increase carbon accumulation in the soil.”

Two other sites being studied by the CsiTE partners are the USDA’s North Appalachian Experimental Watershed at Coshocton, Ohio, and DOE’s Oak Ridge Reservation. The partners are developing a concept to work at a larger regional scale in the Midwest and to computationally predict future soil carbon concentrations if advanced land management methods are used.

Options that could reduce releases of carbon from the soil include no-till agriculture (made feasible with the advent of advanced pesticides); additives that help tie up the soil carbon with clay particles, protecting it from microbial action; and manipulation of moisture levels to cycle the soil’s oxygen content, promoting the formation of carbon compounds that better resist microbial degradation.
BUILDING ONE OF THE WORLD’S LARGEST SCIENCE PROJECTS

Six DOE national laboratories are building the ORNL-led Spallation Neutron Source project.

The Department of Energy’s Spallation Neutron Source (SNS) at Oak Ridge National Laboratory will be an extraordinary tool for exploring matter. But the SNS is extraordinary in other ways, too.

It’s one of the world’s largest science projects under construction, and it’s the first DOE project to be designed and built by six DOE national laboratories, making it a potential model for future multilab projects. Because almost every research university and national lab in the country is or will be involved in designing or using the research instruments on the neutron beam lines at the SNS, the SNS has broad scientific support.

The SNS will include an ion source, a linear accelerator (linac) to speed up the ions, an accumulator ring to compress the ion-derived proton pulses, a liquid mercury target for the protons, and beam lines to transport neutrons produced in the target to experimental samples for measurements by scientific instruments. The six DOE labs responsible for the pieces of the SNS puzzle are the Argonne, Brookhaven, Lawrence Berkeley, Los Alamos, and Oak Ridge national laboratories, as well as the Thomas Jefferson National Accelerator Facility.

How, for the first time, did six national labs become involved in the design and construction of a large DOE science project? According to Thom Mason, ORNL’s associate laboratory director for the SNS, in the mid-1990s DOE decided that the next neutron source would be an accelerator-based machine sited in Oak Ridge. But ORNL did not possess sufficient accelerator design expertise. The technical know-how and experience in designing and operating large accelerators resided at other national labs.

“The multilab arrangement was a way to draw on that broader pool of expertise in the DOE complex,” Mason says. “Each of the partner labs has responsibility for areas of the SNS in which it has special expertise.”

Thus, Berkeley is responsible for the ion source; Los Alamos, the warm linac and high-power radiofrequency systems; JLab, the cold linac; Brookhaven, the ring, magnets, and power supplies; and Argonne, the research instruments. ORNL is taking the lead on the civil construction of the SNS buildings, development and construction of the mercury target system, and the overall integration of the SNS components.

The six-lab partnership, which has involved up to 800 people, has benefits and challenges. “Because of the expertise that exists at the DOE labs, we don’t have to go out and hire and relocate experts,” Mason says. “The challenge at Oak Ridge has been to coordinate the design and construction of hardware in a very complicated machine and to deal with interfaces between the highly technical hardware components.

“The bolt holes have to line up and the beam physics has to match up. The people who do the designs of the SNS components have to transfer that expertise to the people who will run them. Our staff of 400 will have to get it all to work when the SNS becomes operational in 2006.”

To develop the mercury target, ORNL received quality assistance as a result of its involvement in an international collaboration on high-power target development. “This partnership has been extremely useful,” Mason says. “A lot of important results that have helped underpin the design of the SNS mercury target came from this collaboration among American, European, and Japanese researchers. ORNL’s target developers benefited from important measurements done at Los Alamos and Brookhaven and in Japan.”

In addition to construction partnerships with the national labs, which also involve numerous procurements from industrial firms, the SNS will have scientific partnerships with the participating DOE labs. The reason: They have scientists who want to use the SNS for their research.

“We also will have partnerships with the academic community, industry, and other research enterprises, including those in other countries,” Mason says. “All these organizations—DOE labs, hundreds of universities, industrial firms, and foreign institutions—have scientists interested in conducting research at the SNS. For example, IBM and Seagate researchers are interested in using an SNS reflectometer to help them improve magnetic data storage.

“We’ve already begun interacting with these organizations through Joint Institute for Neutron Sciences workshops that form teams who develop instruments. So far we have approved instruments for 16 of the 24 neutron beam lines.”

Have these partnerships helped ensure the SNS Project a stable flow of federal funding? “We draw upon a fairly broad base of support for that funding because of the eventual user community,” Mason says. “Just about all U.S. research universities and national labs have research programs that will make use of the SNS.”

Chuck Shank, director of Lawrence Berkeley National Laboratory, inspects part of the front-end system LBNL designed and built for the SNS. Photograph by Renee Manning.
In contrast to the early years, when the Laboratory was cloaked in mystery and top-secret security, ORNL today actively seeks research partnerships with a broad variety of American industries. These partnerships, which include a long-standing alliance with the nearby Tennessee Valley Authority (TVA), provide funding for specialized research that is beyond the ability of most companies to conduct on their own. Together, the partnerships represent a conscious effort to integrate ORNL’s resources into the nation’s economic activity.

Taking advantage of the Laboratory’s unique suite of competencies, research with industrial partners is funded primarily through cooperative research and development agreements (CRADAs), work-for-others agreements, royalties from ORNL-patented technologies, and copyrighted software licensed to private companies. Other partnership mechanisms include subcontracting, guest research assignments, and user agreements that permit industrial partners to access the Laboratory’s national user facilities. For ORNL, industrial partnerships play an important role in supporting the Laboratory’s larger scientific agenda. In return, industrial firms and utilities gain access to world-class research and development that can provide the critical margin needed for increased quality and productivity.

A Powerful Partner

Over the years, ORNL and TVA, America’s largest public power company, have collaborated in a broad spectrum of research, including nuclear reactor operations, carbon sequestration, hydropower systems, and energy-efficient electric technologies. Most recently, ORNL and TVA have expanded their joint ventures into the important new field of advanced conductors for electricity transmission. Through ORNL’s National Transmission Technology Research Center, the two parties are teaming with industry to develop the next generation of cable technologies, to reduce power congestion, prevent blackouts on the electric grid, and increase power transmission security.

ORNL-TVA collaborations focusing on energy-efficient electric technologies include one with Babb Industries to develop autoclaved aerated concrete (ACC) walls containing flyash from TVA coal-fired power plants. Buildings made of these walls would use less energy than buildings with concrete walls because flyash ACC walls have superior insulating properties.

Another collaboration involving ORNL’s Buildings Technology Center, TVA, and industry is working to build and demonstrate the Habitat for Humanity “Net-Zero-Energy” Home. The goal is to show that low-income homes equipped with structural insulated panels, energy-efficient appliances (such as the ORNL-industry-developed heat pump water heater and the frostless heat pump), and power-producing solar photovoltaic collectors consume no more electricity than they generate. TVA is also spearheading an effort to support greater market adoption of ORNL’s frostless heat pump technology. This technology overcomes the limitations of conventional heat pumps by providing frostless heating and advanced defrosting, thus minimizing indoor “cold blow” and offering greater operational efficiency and reliability.

“ORNL and TVA have worked together closely for years to improve energy efficiency in buildings,” says Marilyn Brown, manager of the Energy Efficiency and Renewable Energy Program at ORNL. “Thanks to ORNL-TVA partnerships, power consumers will soon have access to super-efficient appliances, heat pumps, and lighting.”
Sharing The Power

On April 10, 1996, at the spring meeting of the Materials Research Society in San Francisco, ORNL researchers rolled out a new high-temperature superconductor. The prototype was a tape 15 millimeters long and 3 millimeters wide, made using ORNL’s new rolling-assisted biaxial textured substrates (RABiTS™) process. The tiny tape caused a big stir among materials researchers. Today ORNL’s industrial partners can produce 10-meter RABiTS tapes almost 1000 times longer than the original sample of a high-temperature superconducting wire.

As they get longer and stronger, RABiTS tapes are inching closer to commercialization. Commercial RABiTS tapes should be produced in 2 years, less than 10 years after ORNL researchers applied for the first patent on the process, which continues to be further developed and improved. Spliced-together RABiTS tapes may soon be found in commercial transmission cables and electromagnets for transformers, motors, and generators because of their ability to carry up to 100 times as much current as copper wires with half the energy loss.

The RABiTS technology received an R&D 100 Award in 1999 from R&D magazine for being one of 100 top innovations of the year. The RABiTS process has been licensed to companies such as American Superconductor, Oxford Superconducting Technology, and MicroCoating Technologies. “The partnership among ORNL researchers, program managers, industrial researchers, and ORNL’s Technology Transfer and Economic Development (TTED) Office is vitally important to the progress we made in the development and scaleup of RABiTS,” says Bob Hawsey, director of the High-Temperature Superconductivity Program at ORNL. “ORNL has received more than $1 million in funds for superconductivity research from its CRADA partners and licensees. Sustained support has also come from the Department of Energy.

“Companies appreciate that our researchers stand behind them after the license deal is complete. Our researchers provide technical support to the companies and try to make the technology work so it can be marketed. We are helping the companies improve the performance of the coated conductors while lowering their cost.”

A good example is the close relationship between ORNL and American Superconductor Corporation in Massachusetts, the longest-running partnership in the superconductivity field. The chief executive officer of American Superconductor is a former ORNL staff member, and a former ORNL postdoctoral fellow is now in charge of American Superconductor’s CRADA with ORNL. American Superconductor, which is providing funds to the RABiTS research program, recently purchased a clean room for a new rolling mill, located in a building used by ORNL’s Metals and Ceramics (M&C) Division. “Both parties continue to benefit from the partnership,” says Hawsey.

In the RABiTS technology, texture is introduced into a tape made of a nickel alloy by rolling and annealing it. The texture is transferred to a superconductive oxide coating through buffer layers deposited on the metal substrate.

One way to help industry reduce the cost of fabricating the coated conductor is to apply the buffer layers chemically rather than by the originally used laser deposition technique. Parans Paranthaman and co-workers in ORNL’s Chemical Sciences Division have developed a chemical process that simplifies the buffer layer application, lowering the cost. The process involves a solution-based dip coating in which the metal tape is run through a bath of special chemicals and heated in a furnace. All RABiTS licensees are studying this process.

Another way that industry could cut production costs is to use copper instead of nickel alloy for the substrate, because copper costs one-third as much. The problem with copper is its rapid oxidation after exposure to many gases. ORNL’s Claudia Cantoni and Amit Goyal seek to discover ways to cover the copper with a buffer layer quickly enough to prevent oxidation of the substrate.

Hawsey says that the R&D 100, Federal Laboratory Consortium, and industry awards that the RABiTS technology has received “reflect our responsiveness to industry and recognize the favorable way we treat companies from a business standpoint.”

Materials For Microturbines

Microturbines, which typically burn natural gas and supply 30 to 500 kilowatts of electricity for use in buildings, operate most efficiently at temperatures approaching 1200°C. Unfortunately, some metallic components, such as rotors, do not survive long in that environment. One solution may be ceramic rotors developed to tolerate heat well, turn at speeds greater than 80,000 revolutions per minute, and last 11,000 hours.

Matt Ferber and Hua-Tay Lin, both of the M&C Division, take a unique approach to the problem. In work for United Technologies, Ingersoll-Rand, and General Electric, all of which manufacture microturbines, the ORNL researchers examine the effects on microturbine ceramic components after they have been in use for hundreds of hours. Their findings will guide improvements in ceramic rotor development.

ORNL researchers in collaboration with the Caterpillar Technical Center have developed a new, modified cast austen-
itic stainless steel for advanced diesel exhaust components that is also potentially useful to manufacturers of microturbines and other devices. They have shown that this material performs significantly better and is more durable and reliable when exposed to high temperatures than the common commercial grade of this stainless steel.

The new cast steel, called CF8C-Plus, was engineered using an ORNL alloy design method based on studies of changes in a material’s microstructure and microcomposition when alloying elements are added and when the altered material serves at high temperatures and pressures. The steel’s development was motivated by the need to improve the performance and reliability of high-temperature exhaust components for advanced diesel engines used in heavy-duty trucks.

This alloy received an R&D 100 Award in 2003 from R&D magazine as one of 100 most significant innovations of the year. The award was made possible through a partnership involving Phil Maziasz and Bob Swindeman (researchers from ORNL), Caterpillar, Bradley University, and Solar Turbines.

The new steel resists failure during creep, mechanical fatigue, and thermal fatigue at up to 850°C, a 200-degree improvement in performance and reliability over the common grade of such cast steel. In addition to structural components in diesel engines and microturbines, the steel could be used in parts for marine diesel engines, industrial gas turbines, automotive gasoline engines, natural-gas–reciprocating engines, advanced land-based gas turbines, and ultra-supercritical steam turbines.

Designing Lighter Vehicles

Reducing the weight of automobiles by 60% to help them use fuel more efficiently is a goal of the U.S. automotive industry. ORNL researchers at the National Transportation Research Center (NTRC) are working toward this goal with the Automotive Composites Consortium (ACC)—a research arm of the Big Three automakers.

Three brands of automotive vehicles on the road today are lighter and sturdier than previous models. Thanks partly to ORNL research, durability research by ORNL and the ACC is providing a better understanding of how to design vehicle components made of glass-fiber and carbon-fiber composites so they are durable and crashworthy. Automotive engineers have applied these design guidelines to the construction of a glass-fiber composite truck bed for the Ford Explorer SportTrac vehicle and the GM Silverado pickup truck. The research results were also applied in DaimlerChrysler’s use of a carbon-fiber sheet-molding compound in nine components of the 2003 Dodge Viper, to enhance structural performance and reduce vehicle weight. According to DaimlerChrysler engineers, ORNL’s durability research, combined with efforts to reduce the cost of producing carbon fibers, is increasing the feasibility of using carbon-fiber composites in numerous automotive applications.

ACC persuaded DOE to provide NTRC with a new $1-million experimental apparatus dubbed the TMAC (for “test machine for automotive crashworthiness”). This physical and virtual test machine will be gleaning data to help researchers predict how well lightweight materials for future fuel-efficient cars will hold up in a crash.
of cost-competitive, composite-intensive automotive body-in-white vehicles (assembled, unpainted shells without parts such as doors and bumpers). The multi-year, multimillion-dollar effort includes numerous industry and university partners. Boeman also works with ACC to support the development of a composite pre-forming process for the manufacture of lightweight automotive materials. His work uses ORNL's capabilities in materials science and technology, as well as modeling and simulation.

Adding It Up

ORNL has established a number of critical partnerships to enable advances in high-end computing research. Computational science places stringent requirements on supercomputer design that are often quite different from those for commercial applications. Major improvements in scientific simulation and analysis can be obtained through advances in the design of supercomputer architectures. To meet the need for effective computing performance in the 100-teraflop range and beyond, DOE’s Center for Computational Sciences (CCS) at ORNL is partnering with Cray, IBM, and SGI to enable the evaluation, installation, and application of new, very high-end computing architectures for computational science.

The CCS has moved into a new, world-class, 170,000-square-foot facility that includes a 40,000-square-foot computer center. The facility is connected to the DOE ESNNet at 622 megabits per second and the NSF Internet2 at 10 gigabits per second. According to Thomas Zacharia, ORNL’s associate laboratory director for Computing and Computational Sciences, the state-of-the-art facility would allow deployment of leadership-class computers for open scientific computing in support of the Laboratory and the academic community.

Specific collaborations through DOE’s Scientific Discovery through Advanced Computing initiative include partnerships ORNL has with 13 laboratories and 50 universities. These partnerships will address a wide variety of high-end software needs to manage and fully exploit applications for solving grand-challenge scientific problems on petascale and beyond computing systems. ORNL’s partnerships with academia include the UT-Battelle core universities and the UT-ORNL Joint Institute for Computational Sciences (JICS). JICS will also be located in a new, state-of-the-art building with distance learning capabilities that will attract top research faculty, facilitate appointments and collaborations, and educate and train the next generation of computational scientists.

Nuclear Futures

ORNL is involved in partnerships that support the development of a new generation of nuclear reactors for power production. One of these is a partnership with Westinghouse Electric Corporation to develop IRIS (International Reactor Innovative and Secure), an advanced, passively safe light-water reactor supported by DOE’s Nuclear Energy Research Initiative. Westinghouse is now interested in expanding a partnership with ORNL to include technical support for the development and deployment of the South African pebble-bed modular reactor, in which British Nuclear Fuels Limited, the parent company for Westinghouse, is an investment partner.

ORNL software is improving the productivity of fabricators of semiconductor chips.

The United States Enrichment Corporation (USEC), a private company that manages the Paducah and Portsmouth gaseous diffusion plants, formerly operated by DOE, is planning to build an advanced gas centrifuge plant that will produce enriched uranium fuel for nuclear power plants economically. ORNL has a CRADA with USEC to help the company develop smaller, more robust centrifuges that will increase the plant’s efficiency. The CRADA should bring ORNL $28.5 million between 2002 and 2007.

Searching For Profits

Using an algorithm that sorts through digital images quickly by comparing their digitized pictorial content in a decision tree, an ORNL search engine groups images of layers of semiconductor chips marred by defects similar in color, shape, size, and texture. As a result, tens of thousands of images can be indexed so that visually similar images can be rapidly retrieved.

“We demonstrated that we can search 80,000 images and find 128 similar defect images in 7 seconds,” says Ken Tobin, leader of the Image Science and Machine Vision Group in ORNL’s Engineering Sciences and Technology Division. “Our content-based image retrieval method works.”

ORNL licensed this award-winning Automated Image Retrieval (AIR) system to Applied Materials, Inc., of Santa Clara, California, which makes chip manufacturing and inspection equipment. This ORNL system has been integrated into the company’s Defect Source Identifier product (DSI™-AIR). The new software is ramping up the yield and profits for companies that fabricate chips dotted with increasingly smaller, more closely packed features, to enable computers, cell phones, and signal-processing devices to run faster.

This is the second technology transfer success story for Tobin’s team, which includes Regina Ferrell, Shaun Gleason, and Tom Karnowski. Since 1999 ORNL has licensed the team’s spatial signature analysis (SSA) software tool to 18 companies, half of which are semiconductor manufacturers and half equipment suppliers. SSA has helped the semiconductor industry rapidly recognize defect patterns on silicon wafers, such as long scratches, and trace them to a manufacturing problem, such as an errant robot handler.

Thanks to ORNL research in collaboration with industry, software tools have been made available to the semiconductor industry that will reduce production waste and increase the yield of saleable chips, boosting the industry’s profits. For ORNL, the collaboration shows the value of technology transfer, which represents an increasingly important part of the Laboratory’s research agenda.
In 1992-93, the buildup of atmospheric carbon dioxide slowed, and the effect was attributed to aerosols from the 1991 volcanic eruption of Mount Pinatubo. Many scientists at the time believed that the earth's land surfaces released less carbon dioxide because the aerosols' cooling effects lowered the temperature, reducing plant and soil respiration. But in a paper published March 28, 2003, in *Science* magazine, the authors offered evidence that the dramatic slowdown was at least partly due to an increase in diffuse sunlight as a result of volcanic aerosols. The diffuse sunlight boosted photosynthesis because normally shaded leaves in the forest were illuminated.

The lead author of this fascinating study is Lianhong Gu, a researcher in ORNL’s Environmental Sciences Division (ESD). The study was made possible because of both the ORNL work by Gu and one of his co-authors, fellow ESD researcher Tom Boden, as well as the contributions of five other co-authors from three universities—University of California at Berkeley, Harvard University, and the State University of New York at Albany.

Many of today’s scientific problems, such as understanding what makes a living cell tick, are so complex and difficult that no one person or team from a single institution can solve them. Increasingly, to solve the tough problems for which funding is available, scientific teams comprise researchers from a handful of universities, national labs, or, in some cases, the private sector. Although these partnerships require a significant amount of trust and cooperation, they make possible research that none of the institutions alone would have the resources to conduct.

Some ORNL research could not be done without universities and other partners.

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**THE SUM OF THE PARTNERSHIPS**

**Life and Medical Sciences**

ORNL researchers are involved in numerous projects that could not be completed without the contributions of the Laboratory’s partners. Some of the largest projects involve an array of partnerships in life and medical sciences.

One key Laboratory partnership is the Joint Genome Institute, which provides the genomic sequences of microorganisms for computational annotation of genes by ORNL researchers. According to Barry Berven of ORNL’s Life Sciences Division, many national laboratories, universities and colleges, and private-sector organizations serve as collaborators in gene-finding projects involving ORNL’s specialists in computational biology.

ORNL has established an extensive network of partnerships for its current activities in DOE’s Genomes to Life program. Participants include both universities and other national laboratories. The research involves developing rapid methods of identifying microorganisms, determining quickly the response to stress of bacteria that digest radionuclides of interest to DOE, and ascertaining why certain ocean bacteria are limited in their ability to take up and sequester atmospheric carbon dioxide.

Another example of an ORNL partnership is the *Shewanella* Federation, a multi-investigator and cross-institutional consortium devoted to understanding the biology of the metabolically versatile bacterium *Shewanella oneidensis* MR-1 at a whole-system level. According to ESD’s Gary Jacobs, this project involves more than 30 scientists representing different governmental, academic, and private research organizations, including ORNL, two other national labs, Michigan State University, the University of Southern California (USC), Baylor College of Medicine, the Institute for Systems Biology, and Genomatica.

The Tennessee Mouse Genome Consortium pools expertise and resources for analyses of complex biological systems and promotes the mouse as a biomedical research model. This partnership supports ORNL collaborations with Meharry Medical College, St. Jude Children’s Research Hospital, the University of Memphis, the University of Tennessee, East Tennessee State University, and Vanderbilt University Medical Center. The consortium provides ORNL mouse biologists with complementary capabilities (e.g., medical centers) and medical expertise. A five-year grant from the National Institutes of Health, which began in late 2001, supports the consortium’s neuromutagenesis program. According to Berven, this grant is being increased from...
$12.7 million to $13.7 million to cover expanded ORNL involvement.

A collaborative project between the USC Doheny Eye Institute and five DOE national labs (including ORNL) is aimed at developing an artificial retina to restore the sight of legally blind patients afflicted with retinitis pigmentosa or age-related macular degeneration. The other four labs are Argonne, Lawrence Livermore, Los Alamos, and Sandia national laboratories. A prototype design of a high-density sensor was recently inserted into a canine and tested successfully, according to ORNL’s Eli Greenbaum. Future goals include improvement of the prototype design of the retinal device and its eventual implantation into the eye of a blind person.

Scientists at ORNL and USC have developed a cancer-detecting microchip that works as a sensitive assay for prostate cancer. The device, which uses microcantilever technology pioneered at ORNL, is 20 times more sensitive than currently used assays. The technology also can be adapted to measure other clinically important molecules at high levels of sensitivity.

Climate Change Research

ESD is involved in climate change research that includes contributions from scientists at ORNL in collaboration with many partner institutions. (See p. 12 for an article on one major example.) Although university and private-industry participation is critical to the success of many ORNL initiatives, international partnerships are also important, as ORNL seeks to provide a leadership role in areas of interest to DOE and the nation. In the International Populus Genome Consortium (IPGC), scientists from ORNL and other institutions throughout the world have joined together in research associated with the DOE-sponsored sequencing of the first tree genome (*Populus*). More than 250 scientists from 24 countries are building upon the unprecedented opportunity afforded by DOE’s investment in sequencing the poplar genome. The IPGC will formulate a comprehensive science plan that should help plant biologists exploit this tremendous genetic resource.

According to Jerry Tuskan, co-leader of the IPGC and an ESD plant geneticist, “the information generated through this work should help scientists determine which genes in poplar trees are linked to carbon storage, possibly enabling them to genetically design trees that possess an improved ability to sequester carbon from the atmosphere and, thus, mitigate potential greenhouse warming. This would not have been possible just a few years ago.”

Probing the Nanoscale

The Transmission Electron Aberration-corrected Microscope (TEAM) development project is a collaboration among electron beam microcharacterization facilities at ORNL, three other national labs, and the University of Illinois at Urbana-Champaign. These facilities are sponsored by DOE’s Office of Basic Energy Sciences. ORNL already has two of the world’s first aberration-corrected electron microscopes, with a third to be delivered next year. The TEAM project is designed to combine the expertise of multiple institutions to take this technology to the next level of performance, enabling new scientific questions to be addressed in nanoscale science and technology. ORNL’s Advanced Materials Characterization Laboratory, which will be built by 2005 and will be open to users from universities and other institutions, will house some of the world’s most powerful electron microscopes.

Computational Astrophysics

Obtaining a detailed understanding of how a star explodes and creates and disseminates elements in the midst of this violent process that lasts only a few hours is the goal of the Terascale Supernova Initiative, led by Tony Mezzacappa of ORNL’s Physics Division. This computational astrophysics project is supported by $9 million in funding from DOE’s Office of Science initiative called Scientific Discovery through Advanced Computing (SciDAC). The partners are ORNL, the National Center for Supercomputer Applications at San Diego, and eight universities—UT, the State University of New York at Stony Brook, the University of Illinois at Urbana-Champaign, the University of California at San Diego, the University of Washington, Florida Atlantic University, North Carolina State University, and Clemson University. The project represents one of many model national lab-university partnerships that are pushing the frontiers of science.
HELPING PATIENTS WORLDWIDE

IAEA enables an ORNL device to help treat heart and cancer patients on four continents.

The Atomic Energy Commission (AEC) Act of 1949 called for the use of the unique facilities at the AEC’s national laboratories to provide radioisotopes for medical, research, and industrial applications. When Alvin Weinberg was director of Oak Ridge National Laboratory, he observed: “If at some time a heavenly angel should ask what the Laboratory in the hills of East Tennessee did to enlarge man’s life and make it better, I dare say the production of radioisotopes for scientific research and medical treatment will surely rate as a candidate for the very first place.”

Today, thanks to partnerships with hospitals, universities, private firms, and the International Atomic Energy Agency (IAEA), ORNL’s Nuclear Medicine Program can claim enormous success in transferring radioisotope technology to clinical trials throughout the world.

Russ Knapp, manager of ORNL’s Nuclear Medicine Program in the Nuclear Science and Technology Division (NSTD), has been finding ways to apply ORNL isotopes to medical uses for over two decades. His research has ensured that some of the Laboratory’s new technologies and the radioisotopes produced at ORNL’s High Flux Isotope Reactor (HFIR) are used for medical diagnoses and treatment, particularly for heart disease and cancer.

Using funds from the Department of Energy’s Offices of Biological and Environmental Research and Isotopes for Medicine and Science, Knapp’s team (including NSTD’s Arnold Beets and Saed Mirzadeh) invented a radioisotope delivery system called the tungsten-188/rhenium-188 radioisotope generator. The team also designs, develops, and conducts animal tests of new radiopharmaceutical agents (such as rhenium-188–labeled agents for cancer therapy) and has active medical cooperative programs in which new agents are evaluated in patients at collaborating hospitals in the United States and abroad.

Aiding Developing Nations

Rhenium-188, which emits beta particles that kill cells, is being used on heart patients to prevent restenosis, or reclogging of coronary arteries, after balloon angioplasty has cleared fatty deposits. Because rhenium-188 also relieves inflammation, the isotope has proven useful for reducing the pain of arthritis, bone cancer, and liver cancer.

“Our radioisotope delivery system gives clinics in developed and developing countries a broad range of medical uses,” Knapp says. “It also offers a low-cost capability for treating cancer patients.” A collaboration that Knapp established with A. J. Padly, head of IAEA’s Nuclear Medicine Section, enables ORNL to supply the radioisotope delivery system to developing countries. ORNL’s rhenium generator is being used for restenosis therapy in a 10-clinic multi-center trial and for liver cancer therapy at 13 clinical sites supported by IAEA. Liver cancer, which often develops in hepatitis patients, is a major cause of death in the developing world.

Many patients with inoperable liver tumors need palliative therapy to decrease their pain. Rhenium-188 is chemically attached to a lipid-soluble, “embolitic” agent or particle later injected through a catheter into the hepatic artery that provides blood to the tumor; the radioisotope becomes trapped in the tumor’s small blood vessels. This “radioembolization” procedure decreases pain by providing radiation that reduces both inflammation and tumor mass.

Radioisotope Generator

The ORNL generator—a portable cylinder packed with an aluminum oxide powder—is loaded at the top with tungsten-188, a radioisotope obtained from HFIR. The tungsten-188 binds tightly on the powder. The tungsten-188 has a half-life of 69 days, so the useful shelf life of the generator is several months. As the tungsten decays, it is transformed into rhenium-188, which is released from the powder. By washing the radioisotope down from the top with saline, a solution of rhenium-188 is obtained. Thus, the generator is easy to use, has a shelf life of several months, and is very cost effective.

“A highly concentrated rhenium-188 solution is of particular importance for restenosis therapy,” Knapp says. “Our new patented technology provides a highly concentrated radioactive liquid used to inflate the angioplasty balloon at low pressure following high-pressure balloon inflation with saline to unclog the artery. The radiation produced by decay of the radioisotope inhibits the growth of smooth muscle cells that cause restenosis.”

More than 500,000 patients in the United States undergo coronary balloon angioplasty procedures each year, but reclogging may occur in as many as 40% of these patients. Several years ago, Knapp arranged patient studies of the rhenium-188 treatment at Columbia University in New York and Cedar Sinai Hospital in Los Angeles. The studies showed that treatment with balloons filled with the radioactive rhenium-188 liquid effectively decreased the probability of reclogging. Patient studies are now being conducted outside the United States at more than 30 clinical sites in Europe, the Far East, and the Pacific Rim, including the IAEA trials.
Rhenium-188 generators from ORNL also offer low-cost pain relief for cancer patients. When cells from cancerous tumors of the breast, prostate, and lung spread to the skeleton, significant bone pain can result. Knapp and his colleagues have found that rhenium-188-labeled agents, which are taken up by bone, reduce bone pain in many patients. A new agent developed by the University of Bonn, Germany, and ORNL is being used in clinical trials at more than 10 sites worldwide.

Rhenium-188 also holds promise as a cancer treatment. Recently, Diatide, Inc., of Londonderry, New Hampshire, devised a technique that chemically attaches rhenium-188 to its new synthetic peptide—a synthetic compound containing several amino acids—that specifically binds to small-cell and non-small-cell lung tumors. Knapp helped Diatide incorporate the ORNL generator technology into the procedures used by the company for the rhenium-188 labeling of its peptide. Recent results of the research show that rhenium-188 linked to the peptide effectively destroys lung tumors in mammals and targets lung tumor cells in human patients. A dose escalation trial will be conducted using a larger patient group.

Studies in Germany have shown that a rhenium-188-labeled antibody targets and selectively destroys the “sick” bone marrow of leukemia patients. Additional research is being performed to determine whether the rhenium therapy is safer, more effective, and less costly than procedures used today. Researchers are currently engaged in ongoing discussions with Vanderbilt University Medical Center about the use of this technique.

Heart Imaging Agent

A heart attack will damage part of the heart muscle—either reversibly or irreversibly—as a result of a blockage in a coronary artery, reducing or preventing the flow of blood that carries oxygen and nutrients to the heart. When the amount of oxygen available to regions of the heart is reduced, the heart switches over to a different energy source for these regions and metabolizes glucose instead of fatty acids. With DOE support, Knapp’s group developed a radioactive imaging agent called BMIPP—a fatty acid labeled with radioactive iodine-123—that efficiently detects how much heart muscle is still alive after a heart attack. Medical scanners detecting the injected agent’s radioactivity help physicians identify changes in metabolism, to locate damaged regions of the heart. They also can determine whether bypass surgery or balloon angioplasty successfully restores full blood flow to the heart.

Researchers worldwide have conducted more than 350,000 patient studies using the BMIPP agent. In fact, BMIPP has been commercialized in both Japan and Russia. A new partnership with Mallinckrodt Medical/Tyco in St. Louis will support the development of the next generation of a fatty acid heart-imaging agent by Knapp’s team.

For almost 60 years, medical radioisotopes from ORNL have provided diagnoses and treatments for heart and cancer patients, as well as pain relief. The work of ORNL’s Nuclear Medicine Program and the Laboratory’s partners should be pleasing to that heavenly angel.
Glenn Young is the first native Tennessee and University of Tennessee graduate to become both a Eugene Wigner Fellow and division director at Oak Ridge National Laboratory. His parents worked in Oak Ridge during the Manhattan Project — his father is a physical chemist and his biologist mother, he says, "worked for Manhattan Project security, keeping an eye out for security breaks and any suspicious activities that might be of interest to the intelligence forces." The Young family grew to nine members after the parents migrated to Kingsport, Tennessee. His youngest sister, Joan Young Martin, works in ORNL's Engineering Science and Technology Division. In September 1978 Glenn joined ORNL's Physics Division. He became division director in July 2002.

Q. What got you interested in science?
Our parents encouraged us to be interested in science but didn’t insist upon it. I joined a math club and became involved in state-level math competitions; one year I got third in the state. I took chemistry and physics in our new high school that had great new science labs. Tennessee Eastman, where my dad worked, ran a science seminar I attended. Doctors, chemists, and professors of science would tell us what they did on their jobs.

Q. Why did you decide to go to UT for your undergraduate education?
We all went to UT. We couldn’t get large scholarships because our family had no financial need. I just about paid my way through college, thanks to my summer jobs at Tennessee Eastman, one of which allowed me to run a nuclear magnetic resonance rig and learn NMR theory. I had a National Merit scholarship for one year for $1000. I had a $100 corporate scholarship from UT.

Q. Did UT faculty encourage you to like science?
My favorite subject was math, but I ended up majoring in both math and physics. In my junior year I took a course in experimental nuclear physics from Professor Robert Lide. When you turned in a lab report, he would return it and you’d see he had written more than you had. He had a wonderful museum in the building where he worked. He taught us how to run gamma-ray counters and other scientific equipment he stored there. The late Dick Present, who had worked with Eugene Wigner, encouraged me. Lee Riedinger (ORNL's deputy director for science and technology), then a new assistant professor of nuclear physics at UT, was looking for people to help out in his Oak Ridge lab. At ORNL I was shown an active cyclotron experiment with state-of-the-art computers and cathode-ray displays. Riedinger and Lide gave me a key to a UT lab and let me fiddle around with germanium gamma-ray detectors and learn how they work.

Q. Why did you choose to attend MIT for graduate school?
After my interview at MIT, a professor sent a letter back trying to recruit me because he knew I was looking at other schools with nuclear physics departments. His letter rattled off an enormous list of people in nuclear physics at MIT. I took the letter over to Lee Riedinger and he just stared at it and said, “Good heavens, why would you go anywhere else if there’s that many people working in that many parts of nuclear physics?” That just sort of made up my mind for me.
Q. How did you get a Wigner Fellowship at ORNL?

In October 1977, six months after I became a Chaim Weizmann postdoctoral fellow at MIT, I saw Lee Riedinger again at a nuclear physics meeting in Rochester. He invited me to come to Oak Ridge to give a talk, so I did. Later John Pinajian, head of Ph.D. employment at ORNL, offered me a Eugene P. Wigner Fellowship. Pinajian said the magic phrase: “After two years, if it all works out, you’ll have a regular job.”

Q. What did you do during your two years as a Wigner Fellow?

I worked with Frank Plasil’s group on studying nuclear reactions that don’t lead to fusion or fission but are somewhere in the middle.

Q. What research did you do first after you got a permanent position at ORNL?

In the early 1980s at the Holifield Heavy Ion Research Facility, we showed that pions (short-lived particles that serve as the “glue” in the nucleus) can be emitted from nuclear reactions at unexpectedly low energies, triggering revisions in nuclear physics theory.

Q. For many years, you have been involved in the quest to find the quark-gluon plasma, the primordial soup of the early universe. How did you get involved in this work?

I learned to design big detectors to collect and measure the energy of high-energy particles for neutron oscillation experiments, and in 1983, I learned how accelerators work by visiting other national labs. While attending “accelerator school” at Brookhaven, I heard a cultural lecture by Tom Ludlum on calorimetry—detection technology used at big particle-physics colliders. When we heard eight months later that CERN’s international quark-gluon plasma project needed a group to work on calorimetry, we signed up. It helped that an ORNL group led by Tony Gabriel was among the world’s experts in simulating detector technology for calorimeters using Monte Carlo codes. We proved we could engineer these devices, build them, and put them to work.

Q. And then you started traveling frequently to the Relativistic Heavy Ion Collider (RHIC) at Brookhaven to continue this quest?

In early 1991 we got involved in defining the physics program and in designing detectors and electronic components for the RHIC quark-gluon experiments. This was a 450-person collaboration to build the $100-million PHENIX, one of two large arrays of particle detectors at RHIC. The lead-glass spectrometers we built for CERN are still in operation in PHENIX. We are at high enough energies at RHIC when gold nuclei collide with other gold nuclei or deuterons that we can “see” the debris—jets of particles running off together—that occur when two quarks, or a quark and a gluon, hit each other directly and scatter before the very violent main reaction. We believe we are close to seeing what happened 10 microseconds after the Big Bang.

Q. When were you appointed director of the Physics Division at ORNL?

I thought I would spend another 10 to 12 years working on the RHIC experiment where I had been deputy project director and deputy spokesman since 1991. But when Fred Bertrand told us he would retire as division director in June 2002, ORNL Associate Laboratory Director Jim Roberto met with me and other people. About a month later, Jim asked me if I would be the new director, and I said, “yes.”

Q. What’s the outlook for the Physics Division?

We are upgrading the Holifield Radioactive Ion Beam Facility (HRIBF) and starting work on a beam line at the Spallation Neutron Source (SNS). We are working on a proposal to get funding to build a neutrino detector for the SNS target, called the Supernova Neutrino Study on the SNS, or SNS squared. The SNS produces neutrons in the same energy range as supernovas, so it could be a good source of data for our supernova simulations on supercomputers led by Tony Mezzacappa. It could be a great project for graduate students. We are also excited about talking with the Naval Research Laboratory about building a gamma-ray detector that NASA could place in a satellite and launch to get data on gamma rays from nova and supernova.

Q. What’s the future for HRIBF?

Our facility is training future experimenters for DOE’s Rare Isotope Accelerator, which may be built in 10 or more years somewhere else. DOE may then want a big, stable ion beam machine so Holifield could be converted to that purpose.
A thin film made of randomly oriented semiconducting polymer molecules is luminescent for a few seconds. But after exposure to oxygen in the air, this light-emitting property vanishes, as shown in high-resolution images in an epifluorescent microscope.

Now, using ink-jet printing techniques in which nozzles spray extremely small droplets of ink on paper to create dot-filled images, an ORNL-university team has coaxed the single-protein-sized molecules of polyphenylene vinylene (PPV), a well-studied semiconducting polymer, to stand up straight and shine. These oriented nanostructures can remain luminescent for as long as a few hours.

Mike Barnes, a researcher in ORNL's Chemical Sciences Division who led a six-man team in developing these PPV-oriented nanostructures, compares the structure of PPV molecules in thin films to old-fashioned wooden carpenter's rules that are stretched out and bent in different directions, producing randomly oriented tangled masses. Using ink-jet printing techniques, Barnes's team induced the stretched-out, micron-sized carpenter's rule molecules to collapse in compact cylindrical structures—much like a folded carpenter's rule. High-resolution fluorescent images of these molecules show the distinct “doughnut” intensity patterns characteristic of “antennas” oriented perpendicular to the glass substrate. In a sense, these molecules form a group of “glowing antennas” at the nanoscale.

“We achieved an extraordinary uniformity in orientation of these nanoscale PPV particles, which are 7 to 10 nanometers high,” Barnes says. “In August 2001, a month before our LDRD funding from ORNL ran out, we discovered a surprisingly easy way of preparing oriented nanostructures from single molecules of semiconducting polymers.

“First, we selected the right solvent and dissolved the right concentration of PPV in the solvent. Then, using an ink-jet technique to produce droplets of the PPV solution, we induced molecules of the solvent to evaporate at a rate that caused the chain-like PPV molecules to collapse and pick up electrical charges. As a result, the folded-up single molecules were aligned and oriented perpendicular to the support.”

The ORNL team used a combination of atomic force microscopy and novel optical probes to determine the size, orientation, and intramolecular structure of the molecules “printed” onto the substrate. The team found that the oriented nanostructures have properties profoundly different from those of the bulk PPV thin films.

“These species were two to three orders of magnitude more stable photochemically than polymer materials widely used in light-emitting diodes; tiny lasers; and displays for laptop computers, cell phones, and personal digital assistants,” Barnes says. “And they emit light in a much more narrow wavelength range with different colors that appear to be correlated with structural details of the polymer chain.”

Ultimately, these nanostructures might be used to form optical or molecular wires. When pumped with light, they could conduct an electrical current, and when injected with charge carriers, they could emit light.

Barnes thinks it may be possible to deposit these nanostructures in a compact pattern to create a nanoscale laser diode with a tunable color. Such a device might be used for quantum information processing in which photons, rather than electrons, carry bits of data. Because such a device would be useful for transmitting and receiving ultra-secure, encoded data, Barnes’s team has received funding from the National Security Agency (NSA) to continue this research.

Barnes’s team members are Adosh Mehta and Thomas Thundat, both of ORNL’s Life Sciences Division; Pradeep Kumar, a University of Tennessee graduate student; Bobby Sumpter and Don Noid, researchers in ORNL’s Computer Sciences and Mathematics Division who have performed molecular dynamics simulations; and Robert Dickson, professor of chemistry at Georgia Tech. In addition to the LDRD Program and NSA, the Department of Energy’s Office of Basic Energy Sciences provided funding for this project.
Thanks to neutron-rich beams in an energy range available only at the Department of Energy’s Holifield Radioactive Ion Beam Facility (HRIBF) at ORNL, researchers have performed several tour de force experiments that provide insight into the atomic nucleus.

In one set of experiments, a team led by David Radford of ORNL’s Physics Division bombarded a beryllium-9 target with a high-energy beam of tellurium-134 ions. “We expected to detect gamma rays but we were surprised to detect alpha particles also,” Radford says. “Beryllium nuclei in the target were each emitting two helium nuclei. “Then we realized that a neutron had been transferred from the beryllium-9 target nucleus to the tellurium beam nucleus, leaving behind a beryllium-8 nucleus. Beryllium-8 is unstable so it broke up immediately into two helium-4 nuclei, or alpha particles.”

In this and other pioneering experiments, Radford’s team has demonstrated the value of measurements of gamma-ray emissions and detection of residual target-like nuclei from beam-target collisions. The team can show that a neutron or proton has been transferred from a beam nucleus to a target nucleus, or vice versa.

The HRIBF is the only facility in the world that can produce neutron-rich beams of high enough energies to overcome the natural Coulomb repulsion between the positively charged nuclei in both the beam and the target. As a result, the beam and target nuclei get close enough for neutrons and protons to cross over.

These measurements by Radford’s team shed light on the relative energy of the transferred neutron or proton in the orbit it enters inside the nucleus. Using germanium gamma-ray detector arrays to measure the position, time, and energy of each emitted gamma ray, nuclear physicists determine the energies of the various neutron and proton orbits, or shells, which make up the nuclei of different atoms. They then report whether these measurements agree with predictions by theorists.

ORNL has produced a beam of tin-132 ions, as well as tellurium-134 and other beams in this mass region—a major achievement. Tin-132 is doubly magic because both its proton number and neutron number correspond to “full” shells—orbits that have their allowable limit of these nuclear particles. Some doubly magic nuclei—such as oxygen-16 and lead-208—are stable, like the inert gases, which have full electron shells. Other doubly magic nuclei, such as tin-132 and tellurium-134, have been difficult to study because their unfavorable ratio of protons to neutrons makes them unstable.

Teams led by Radford and Jim Beene, HRIBF director, have conducted experiments using tin beams with even mass numbers in the range of 126 through 134. These radioactive beams were formed by ionizing atoms extracted from fission fragments produced by bombarding a thick uranium carbide target with protons from the Oak Ridge Isochronous Cyclotron. The tin ions, which have lifetimes of under a minute, were then accelerated using the HRIBF tandem accelerator. Radford’s tin beam experiments use carbon as a target and Beene’s experiments use titanium and zirconium. The tin beams are accelerated at low enough energies that the ions come close to, but never contact, the nuclei in the carbon and titanium targets.

Radford and Beene are measuring the probability that tin nuclei will pick up energy as they pass the target, despite the natural repulsion between beam and target nuclei. Each excited nucleus returns its donated energy as a gamma ray. Beene found that tin-134 nuclei have the same probability of emitting gamma rays when excited by the target as do the tin-130 nuclei, reflecting the expected symmetry with respect to the doubly magic tin-132.

“Doubly magic nuclei are harder to excite because their closed shells must be broken,” Radford says. “Our experiments reveal some details of the internal structure of the doubly magic nucleus. So far what we have found agrees with theory.”
A tissue perfusion sensor, about the size of the famous cream-filled Oreo cookie, may someday be implanted in a human body. ORNL is developing the sensor for the Department of Energy's Office of Biological and Environmental Research to measure changes in blood circulation within transplanted organs.

“Our goal is to get an early indication of circulatory deficiency so surgical or pharmaceutical action can be taken to improve patient outcome,” says Nance Ericson, principal investigator and senior research and development staff member in the Monolithic Systems Development Group of ORNL's Engineering Science and Technology Division (ESTD).

Increasing a patient’s chance for recovery and good health after a procedure such as a liver transplant has long challenged doctors, who traditionally rely on blood analyses and other methods that do not assess circulatory health instantly. Only after the blood work indicates a problem do they know something has gone wrong. Because of this sort of delay in detecting a circulatory deficiency, appropriate action may not be taken in time. As a result, the patient might lose the use of the transplanted organ and have to undergo another surgical procedure.

“Our implanted sensor could prevent such complications because it will provide real-time information on whether blood is circulating normally in the transplanted organ,” Ericson says. “If the sensor reports a problem, there is a greater chance that the physician can take action to save the organ.”

The sensor, which can be placed directly on the organ of interest or just beneath the skin, uses three different wavelengths of light to measure circulation. Some of the light is absorbed by the hemoglobin in the arterial blood. The light that is not absorbed is picked up by the detector.

The implanted instrument also uses direct sequence spread spectrum technology to transmit these measurements to a local receiver in the form of radio waves. Because radio waves travel through the body, additional incisions are not needed to get readings, unlike with other methods.

“Inserting the sensor in the patient is minimally invasive,” Ericson says. “The surgeon implants it when the patient is already open.”

To ensure that the implanted sensor does not invoke a dangerous immunological response when placed in the human body, the device must be encapsulated in biocompatible materials. The sensor must also be designed to remain immobile and to take into account the optical density of tissue. To meet these challenges, Ericson is collaborating with his co-principal investigators, Mark Wilson of the University of Pittsburgh and Gerard Coté of Texas A&M University. Ericson’s ESTD collaborators Chuck Britton, Mike Emery, Mike Hileman, Mike Moore, Miljko Bobrek, John Wilgen, and Roberto Lenarduzzi are helping them solve these problems, as well.

“One polymer being investigated for its viability in this research is a cross-linked hydrogel of poly(ethylene glycol), PEG for short, which has been shown to be stable, nontoxic, and non-antigenic in vivo,” Coté says.

By the summer of 2004 Ericson and his colleagues at Pitt hope to begin biocompatibility testing on large animals such as pigs, which are excellent models because they are physiologically similar to human beings. How a pig’s tissue reacts to the sensor and its material casing will likely indicate how human tissue would respond.

These tests and others must be done before the tissue perfusion sensor is ready for its first trial in a human patient. Regardless, Ericson and his colleagues are optimistic about the technology’s ability to perform well in the human body, even in surgical areas outside of organ transplants.

“The device’s potential clinical applications extend beyond transplantation,” Wilson says. “Critically ill patients who need operations for traumatic injury would be ideal candidates to monitor with such a sensor, to assess their responses to therapies for shock.” Ericson concedes, however, that the length of time the medical world must wait for a fully operational sensor depends on funding.—Erin DeMuth, ORNL Communications Group intern.
Attention, Guinness Book of World Records. Two ORNL researchers claim to have weighed the smallest amount of material ever measured, using a microelectromechanical system (MEMS) sensor. The sensor is a million times more sensitive than a dog’s nose.

Panos Datskos and Nickolay Lavrik, both in ORNL’s Engineering Science and Technology Division, have achieved this nanoscience feat. They deposited a single layer of 10 million molecules of a sulfur (thiolated) compound on a gold-coated silicon cantilever and detected and measured their presence.

A dog can smell a mass of chemical particles equivalent to a few billionths of a gram, according to Datskos. But the ORNL cantilever, which is 2 microns long and 50 nanometers thick, recorded the weight of a thiolated compound as light as 5.5 femtograms. A femtogram is a millionth of a billionth of a gram.

The cantilever was one of an array of silicon bars of different lengths, like a comb with broken teeth. Each cantilever has a unique vibration rate, or resonant frequency, when heated by the appropriate wavelength of laser light. But when coated with different amounts of gold and thiolated compound, each of the laser-heated bars vibrates at different rates.

To measure the variations in the resonant frequency of each cantilever, the ORNL researchers heated the gold-coated array with pulses of light from a diode laser. As a result, each silicon bar moved up and down about two million times a second, with the lighter bars vibrating more times per second than the heavier bars. The frequency variations indicated the additional mass of each coated bar.

“We used a diode laser to heat the cantilevers, causing them to bend, because the silicon in each bar and its gold coating expand at different rates,” Datskos says. “We pulsed the laser to get different frequencies close to the resonance frequency of the cantilever. Pulsing allowed us to controllably actuate the cantilever and measure its resonance frequency by determining the number of times per second that the cantilever bends, as a function of laser modulation.”

The researchers first measured the frequency of an uncoated cantilever. Then they deposited on the cantilever a monolayer of a thiolated compound (11-mercaptopoundecanoic acid) that binds to the gold coating. They measured the frequency again and found a shift of about 2 kilohertz out of a vibration rate of 2 megahertz. In other words, because the cantilever was heavier, it vibrated about 1,998,000 times a second, instead of the approximated 2 million times a second.

“We calculated the change in the cantilever mass to be about 5 femtograms—close to the mass we deposited,” Datskos says. “Because we knew beforehand how much mass was added, we verified the accuracy of our experimental measurements and calculations.”

“We used a helium-neon laser and a photodetector to measure the rate of cantilever vibration,” says Lavrik. “Laser light reflected by the vibrating bar combined with the reference laser beam forms an interference pattern that appears and disappears, indicating bar deflection with an accuracy as high as a millionth of a micron.”

Datskos believes the most amazing result of the experiment is that he and Lavrik proved that very small mass changes can be measured in the air. Such a measurement is difficult, however, because the cantilever experiences friction when it displaces air molecules during vibration.

One goal of the ORNL researchers is to detect single molecules by improving their MEMS sensor. “We must first fabricate smaller, stiffer silicon bars so we can raise the vibration frequency from 2 to 50 megahertz,” Datskos says. “Then, theoretically, we should be able to measure the mass of a single molecule captured by a cantilever’s coating.”

The researchers hope to build a MEMS sensor even more sensitive than a dog’s nose—and smaller, too. It would have a tiny laser like that used in a portable CD player.

An optical microscope image of three cantilevers, used in the femtogram mass detection experiment, appears on the monitor.
ORNL has received four R&D 100 awards from R&D Magazine, which, since 1963, has given awards for the 100 most significant innovations of the year. ORNL now holds 116 awards, making it second only to General Electric in the competition and first among Department of Energy laboratories. ORNL researchers winning R&D 100 awards for 2003 are Tuan Vo-Dinh, Joel Mobley, Brian Cullum, David Stokes, Alan Wintenberg, and Steven Frank, for RAMiTS (Raman Integrated Tunable Sensor), a compact, “point-and-shoot,” fully integrated, battery-operated Raman monitor that can identify and quantify hundreds of substances, including toxic chemicals, by-products from explosives, biomedical markers, pharmaceuticals, and illicit drugs, for such uses as environmental monitoring, medical diagnostics and homeland security; Michael Ramsey, William Whitten, Peter Reilly, and Oleg Kornienko, for MicroTrapMS, a highly miniaturized, low-cost ion trap mass spectrometer that can be used for on-line screening for toxins in municipal watersheds and detection of drugs, explosives, and hazardous substances at airport checkpoints; Philip Maziasz and Robert Swindeman, for CFSC-Plus, a new cast stainless steel based on ORNL’s unique engineered microstructure alloy development methodology that can be used at the higher temperatures found in advanced diesel engines for heavy trucks and gas-fueled microturbines for power production; Panos Datskos, Slobodan Rajic, Lawrence Senesac, Nickolay Lavrik, and James Corbell, for UMIR-Cam (Uncooled Micromechanical Infrared Camera), a sensitive, miniature imaging and infrared photodetection device that operates at room temperature and can be used for night vision, industrial process monitoring, and medical imaging, as well as to help firefighters see through smoke.

Because they have 14 or more patents, 11 ORNL inventors have been designated “distinguished inventors” by Battelle. On March 26, 2003, the 11 ORNL inventors and 18 others from Battelle and other Battelle-managed institutions were honored in Columbus, Ohio. ORNL’s honorees are Tuan Vo-Dinh, Amit Goyal, Don Kroeger, Vinod Sikka, Michael Ramsey, C. T. Liu, Terry Tieg, Rodney McKee, Thomas Thundat, Tim Burchell, and Mariappan Parans Paranathan.

Gene Ice of ORNL’s Metals and Ceramics Division, Ben Larson of the Condensed Matter Sciences Division, and Kenneth Tobin of the Engineering Science and Technology Division have been named UT-Battelle corporate fellows. UT-Battelle corporate fellows are selected for their significant contributions over many years that have been acknowledged by their peers throughout the United States and other nations. Ice was recognized for his research in X-ray optics, microdiffraction, and diffuse X-ray scattering. His pioneering work on wide-angle and microfocusing of synchrotron X-rays has earned numerous awards, including two R&D 100 awards. Ice and Larson (who received the 1985 Bertram Warren Diffraction Physics Award for pioneering nanoscale time-resolved X-ray diffraction studies of laser melting) co-developed three-dimensional X-ray microscopy technology for investigating the microstructure of materials. Larson also pioneered work in calculations to determine the real-band structure of materials, resolving a 20-year difference of opinion among researchers studying the issue. Tobin has led a group whose work prompted significant advances in the field of applied computer vision research, addressing important national issues in industrial and economic competitiveness, biomedical measurement science, and national security. Tobin has received an R&D 100 Award and six Federal Laboratory Consortium awards for his technology transfer efforts. He was the Tennessee Academy of Sciences Industrial Scientist of the Year and is a fellow of the International Society for Optical Engineers.

Thomas Maier has been named a Eugene P. Wigner Fellow. He works in ORNL’s Computer Science and Mathematics Division.

Edgar Lara-Curzio received the 2003 Richard Fulrath Jr. Award from the American Ceramic Society “for his outstanding contributions to ceramic science and engineering.” He is leader of the Mechanical Properties and Mechanics Group in the Metals and Ceramics Division.

Pengcheng Dai has been selected as a co-winner of the 2003 Outstanding Young Researcher Award of the Overseas Chinese Physics Association.

Tuan Vo-Dinh (left) and Michael Ramsey both received R&D 100 Awards and were named “distinguished inventors” by the Battelle Memorial Institute.
Renowned ORNL geneticist and member of the National Academy of Sciences whose research on mice led to radiation protection standards for humans.