More than a year after completion, the Spallation Neutron Source is steadily ramping up toward its eventual 1.4 megawatts of power. In its experimental hall, workers are busily installing its suite of state-of-the-art analytical instruments.

Researchers are lining up with experiments that will take advantage of the unprecedentedly bright neutron beams.

ORNL researcher Jeremy Smith refers to a wealth of “challenges” awaiting the powerful DOE Office of Science neutron source when it arrives at its full power and capability. His own challenge for the SNS: Verify the first-ever atomic-detail computer simulation of the lattice dynamics of a protein crystal.

All he and his colleagues are waiting for are the neutron-rich beams to propel their studies into a new realm of experimental capabilities.

“We have extended an invitation to the next generation of neutron scattering instruments at the SNS to demonstrate their capabilities,” says Jeremy, who directs ORNL’s Center for Molecular Biophysics.

There is a noticeable tinge of impatience in his voice. Like a number of researchers, he has an atom-scale theory he eagerly wants to put to the neutron test.

For example, the recent computational studies of molecular-scale lattice dynamics—how protein molecules vibrate in relation to each other—may shed light on how proteins in living cells interact with one another. It is a key question in biological sciences. The SNS and its arsenal of specialized analytical instruments may be able to confirm—or contradict—what the simulations indicate.

“Lattice dynamics calculations have not been possible before, and now we will have a tool—the SNS—that will have the capability to confirm our calculations,” Smith says, humbly adding, “Hopefully, the calculations won’t be too painfully off the mark.”

The study, just published in Physical Review Letters, is a collaboration among Jeremy, who also holds a University of Tennessee-ORNL Governor’s Chair at the University of Tennessee, and researchers from the California Institute of Technology and the National Institute of Chemistry, Ljubljana, Slovenia.

Jeremy says the PRL paper predicts existence and forms of these lattice modes.

“In doing so it throws out a challenge to next-generation neutron science to finally make the breakthrough and determine the dispersion relations experimentally,” he says. In other words, having overcome their computational hurdle, the lattice dynamics team is now ready for the SNS to test their work and see if what is predicted is really there.

Long before SNS, memories of farm life pleasant for Chestnut Ridge resident

When he was only five or six years old, James Brennan delivered a pail of water to a farm worker near the site where the Spallation Neutron Source’s water tower is now. The worker took a drink, pulled out a pipe, removed his eyeglasses and lit the pipe by focusing light through the glasses.

Brennan remembers being profoundly impressed by that feat. Long before the Spallation Neutron Source took up residence on Chestnut Ridge, the land was home to James Brennan. Brennan’s family lived on the property before the government seized it in 1942. His father’s old barn stood where the main office complex at SNS is now.

Brennan, 89, visited ORNL in late August and could still recognize many sites, although the changes over 60 years were sometimes drastic. His directions to the visitor’s center mentioned the Conference Center pond. He remembers that pond as a small stream where he used to come for a drink after services at New Bethel Baptist Church.

Brennan was born in Bear Creek Valley in 1918. His father purchased the farm on Chestnut Ridge in 1915. One of Brennan’s favorite memories of life there is when his father got his 1922 Model T Ford truck stuck on a muddy road.
The Nuclear S&T Division’s Saed Mirzadeh, whose work at ORNL has led to development of new treatments for cancer and other diseases, is the recipient of the American Nuclear Society’s 2007 Seaborg Medal Award.

Saed is internationally known for his contributions to the development of radioisotopes, which are routinely used for the diagnosis and treatment of cancer and other diseases. In the United States, more than 10 million procedures using radioisotopes are performed on patients each year.

Saed recently developed the chemical processes to provide actinium-225 and its decay daughter bismuth-213 for treatment of a type of leukemia. Actinium-225 is a by-product of uranium-233, which currently is not being used for energy or weapons programs but is of great interest for medical applications. The work directly resulted in advanced clinical trials now under way to treat leukemia at New York’s Memorial Sloan-Kettering Cancer Center.

His research also focuses on the use of ORNL’s High Flux Isotope Reactor—one of the world’s most powerful research nuclear reactors—to produce useful medical and industrial radioisotopes.

The award is named for Glenn T. Seaborg, the Nobel-prize-winning nuclear chemist who co-discovered plutonium and many transuranium isotopes and chaired the U.S. Atomic Energy Commission from 1961 to 1971.

“Through the Nuclear Medicine Program, Saed and HFIR have played important roles in making ORNL the leading or sole U.S. supplier of many of the medical radioisotopes in use today,” ORNL Director Thom Mason says. “Winning the Seaborg Medal is an exceedingly appropriate recognition of his outstanding accomplishments.”

He also has worked as a scientist for the National Institutes of Health, a visiting scientist for the Australian Nuclear Science and Technology Organization and an adjunct faculty member at Long Island University.

Saed collaborates extensively with colleagues at other national labs and in industry and academia, including the University of Tennessee. He has supervised a number of postdoctoral fellows, Ph.D. candidates and M.S. students, and mentored numerous undergraduate and graduate students, many of whom have made significant contributions of their own in the field.

Saed will be recognized in November at the ANS Winter Meeting in Washington, D.C.

—Mike Bradley

ORNL welcomed its latest crop of Wigner Fellows at an annual reception on September 25. The two-year postdoctoral fellowships, named for Nobel laureate and first ORNL scientific director Eugene Wigner, have for years attracted top early career researchers to the Laboratory.

Chris Mann received his doctorate in 2006 in applied physics from the University of South Florida. Chris also earned an M.S. and B.S. in physics with astrophysics from the University of Birmingham, U.K. Chris’s dissertation won the outstanding dissertation award from the University of South Florida. His honors include the Frank E. Duckwall Optics Graduate Fellowship and the Fred L. & Helen M. Tharp Physics Graduate Fellowship. Chris joins the Image Science & Machine Vision group, Engineering Science & Technology Division, under Ken Tobin. His research plans focus on biomedical imaging and digital holography.

John Canik received his doctorate in electrical engineering this year from the University of Wisconsin, Madison. He received several awards as a student, including the Samuel F.B. Morse Medal and the David W. Grainger Distinguished Graduate Fellowship, and has nine publications, with two as first author. John joins the Experimental Plasma Physics Group, Fusion Energy Division, under the direction of Don Hills. His research plans focus on the plasma edge in fusion experiments, modeling the particle and power exhaust from magnetic confinement devices and developing the 3D geometry of these experiments.

Michael McGuire received his doctorate in physics from Cornell University in 2006. During his academic career he received the Michael A. McGuire Award for Academic Excellence, a Taylor Medal and a Graduate Achievement Award from the University of Mississippi, and a Cornell University Fellowship. Michael’s research has focused primarily on the discovery and characterization of new, inorganic, solid-state compounds, with particular emphasis on bulk thermoelectric materials.

Michael is now a member of the Correlated Electron Materials group in the Materials Science & Technology Division, supervised by David Mandrus, where he will continue pursuing his interest in bulk materials for thermoelectric conversion as well as exploratory syntheses targeting new materials with interesting electrical, magnetic and structural properties.

Peter Maksymovych received his doctorate in physical chemistry from the University of Pittsburgh. He earned his B.Sc. in chemistry from the Kiev Taras Shevchenko University in Ukraine. He has received two awards for his work on single molecule chemistry and physics on metal surfaces: the Morton M. Traum Award from the American Vacuum Society in 2006 and the Wayne B. Nottingham Prize from the Physical Electronics Conference in 2007. Peter joins the Materials S&T Division and the Center for Nanophase Materials Science under the supervision of J. F. Wendelken. His research focuses on the nanoscale phenomena in ultrathin ferroelectric and multiferroic oxide films as well as advanced scanning probe microscopy for functional imaging at the nanoscale.

Paul Snojders, also working the the Materials S&T Division under John Wendelken, joined the Lab this past spring.
Mason: Deliver the science

It’s time to start cranking out the science. That was a main element of Lab Director Thom Mason’s message in his first Director’s Forum on Sept. 24. He reiterated the Lab’s plans and prospects in a Friends of ORNL community lecture on October 4. “We’re over the hump in modernization,” Thom said at the forum. “Now it’s time to execute the science.”

Thom also emphasized “striking the right balance” in applying the Lab’s world-class facilities toward its scientific output, which entails recruiting top talent, continuing to upgrade Lab facilities and maintaining operational excellence with a strong emphasis on safety.

Major thrusts of the Lab’s continuing modernization will be a new laboratory building to replace 4500 complex facilities slated for renovation, the start of construction on the Oak Ridge Science & Technology Park and the central campus cleanup, which could gain momentum in FY 2010.

Thom also commented on the re-emergence of the energy mission, comparing its momentum in FY 2010.

Momentum in FY 2010.

“Now it’s time to execute the science.”

“With any safety incentive, our primary objective is to increase our awareness of safety in the work place, and remind us to work together to alleviate accidents and injuries,” says ATLC Vice President Carl Wright. “We’ve made great strides in improving our safety numbers, but the statistics are almost beside the point.” says Facilities & Operations Director Herb Debban. “The real benefit is that fewer people are getting hurt in the work place.”

UT-Battelle and the ATLC are sharing the cost of the giveaway pickup.

Truckin’ for safety

“Now it’s time to execute the science.”

The only other paper cited more often was on the human-health topic of colorectal cancer. “There were more than 2,000 papers in Science last year,” Stan says. For biology, this is a bullet.”

Creative thinking on display, Nov. 7

The Laboratory Directed Research & Development Office is reprising its successful LDRD Projects Poster Session, following on last year’s initial symposium and offering Lab staff members and visitors an opportunity to see and discuss some of ORNL’s most creative thinking.

The special session, where researchers will be available to discuss their projects and answer questions, will be from 10 a.m. until noon on Wednesday, November 7, on Main Street. Posters will be on display November 6-8.

LDRD manager Terry Sjoreen says 70 seed money and LDRD projects are finishing up this year, which sets the stage for a bustling Main Street.

“Our objectives are to showcase the results of individual projects and the overall program, stimulate discussions among researchers and introduce the LDRD program to those who are not familiar with it,” Terry says. “This is an opportunity to explore ideas that are at the forefront of science and technology at the Laboratory.

The LDRD program, which consists of small Seed Money Fund grants and larger Director’s R&D Fund projects, provides researchers an avenue to develop innovative ideas toward the DOE mission.

For more information on the session, contact Terry, 574-4174, sjoreentp@ornl.gov.

Reported by Bill Cabage

Leroy Sims belts out a soulful tune at September 26’s International Festival. The food, culture and entertainment event, always one of the Lab’s best attended, raised more than $4500 for the United Way.

The ATLCC’s Carl Wright (left) and F&O’s Herb Debban with the giveaway pickup.
BioEnergy Science Center gets nearly $10M jumpstart

The state-funded Joint Institute for Biological Sciences is taking shape on the west campus. It will be the home of the BioEnergy Science Center, one of DOE’s three bioenergy centers.

“We are anxious to begin the research.”

Lattice dynamics occur when the repeating units of a crystal vibrate relative to each other. These “phonon dispersion relations” relate the frequencies to the wavelengths of the oscillations. Phonon dispersion relations can, in principle, provide information on how proteins interact with each other that could be useful for understanding protein-protein interactions in the living cell. Until now, researchers have lacked the computing power to allow atomic-detail lattice dynamical calculations.

“The calculations, which were on ribonuclease crystals, are in good agreement with all existing experimental measurements,” Jeremy says. “However the most informative experimental technique for measuring crystal vibrations is inelastic neutron scattering, but trials with previously existing neutron facilities failed to provide useful information for protein crystals, due possibly to neutron flux and instrumental limitations combined with the difficulty of working with large and complex molecules.”

Challenge

Continued from page 1

The new and advanced neutron analysis tools at the Spallation Neutron Source can test equally cutting-edge computational simulations aimed at understanding how proteins interact with each other, as visualized above.

With SNS instruments expected to be in some cases hundreds of times improved over currently existing facilities, Jeremy thinks those breakthroughs are within reach.

An added bonus to a confirmation of the business of developing ways to economically make transportation fuel from plants such as switchgrass and poplar trees, Jeremy says. “We are anxious to begin the research.”

Researchers also will focus on development of consolidated bioprocessing using a single microorganism or group of organisms to break down plant matter through a one-step conversion method.

The new building is slated for occupation by December with operations fully under way in January 2008.

BioEnergy Science Center partners Mascoma and the University of Tennessee are also developing a state-funded, $40 million bioethanol pilot plant, which has been sited about 40 miles from ORNL in Monroe County, Tenn.

The plant will be built and operated by Mascoma, with construction scheduled to begin by the end of this year. Plans call for the facility to be operational in 2009.

The Office of Science program in Biological and Environmental Research is in the process of establishing three basic science research centers in bioenergy this year. A second center, under the leadership of Lawrence Berkeley National Laboratory, will be located near Berkeley, Calif., while a third center, run by the University of Wisconsin-Madison in partnership with Michigan State University, will be based in Madison, Wisc.

See the BioEnergy Science Center Website at www.bioenergycenter.org.

—Larisa Brass

October 2007
James’ father gave his mother, who had never driven a car, a crash course in driving while he pulled it out of the mud with a team of mules. She successfully drove to a field near their house but didn’t know how to stop.

Brennan remembers standing on the porch with his brother watching his father run around trying to instruct his mother on how to stop the car while keeping a team of mules under control. James doesn’t remember the conclusion exactly, but somehow his father got the truck stopped.

In December 1941 the Brennans moved to a 64-acre farm near Scarbrough to get electricity but still owned the property on Chestnut Ridge. He says his parents planned to stay there for the rest of their lives, but by fall 1942 events beyond their control dictated otherwise. The family finished moving out near Christmas that year. James had already left for World War II.

During the war, Brennan worked in telephone communications, laying and maintaining telephone wires. He served in the Pacific Theater early in the war—including Guadalcanal and Bougainville—and later in Europe, including the latter part of the Battle of the Bulge and a memorable trip to Paris. “The French government gave us $17. I still don’t understand the reason why exactly, but we accepted the $17 anyway. That’s what we went to Paris on,” Brennan says.

He remembers the beautiful buildings he saw, but his strongest memory is of the Parisian subway system. He and his Army buddies got on the subway not altogether realizing that the stops would be announced in French, that none of them understood French and that they could not see where they were going.

When he returned from the war, Brennan worked at the water treatment plant at Y-12 for a few years. He later did contract work at several sites on the Oak Ridge reservation, including the High Flux Isotope Reactor.

Brennan enjoys researching the history of this area and has many old photographs, news articles and documents that chronicle life here before atomic energy. He has the original land grant for 100 acres near Chestnut Ridge that the state of Tennessee issued to Thomas Hagler on July 12, 1831. He also owns an old dinner bell that they used to ring to call workers in the field to lunch.

Although many things have changed since Brennan lived there, even before the SNS came to Chestnut Ridge science was wowing observers.

Despite hardships, pre-war ridge and valley were productive

James Brennan remembers farm life on Chestnut Ridge as typically hard but pleasant. Because the area was remote and roads were poor, farm families and communities had to be fairly self-sufficient.

But the land was productive, and the Brennans combined farming with a small business to live comfortably.

“Dad had a rolling store, a wagon he pulled with a team of gray mules,” he says. “There were no stores around. He sold the basic goods—sugar, coffee and salt.”

Brennan’s father bought the Chestnut Ridge farm in 1915 and was able to pay it off in just 10 years. He says his father liked the Chestnut Ridge tract mainly because as a farmer he knew the value of water, and the land was unusually endowed with three springs.

“It was productive farm land. We had three tenant families and a sawmill that provided work for a lot of people,” he recalls.

The Brennans raised cattle and crops, marketing their produce in nearby towns. Brennan enlisted in the Army almost immediately after Pearl Harbor. By the next Christmas, the remaining family was uprooting for the Manhattan Project.

“I don’t know how my father was able to get rid of what he had in such a short time,” he says of the move.—B.C.
October is Energy Awareness Month

The Facilities Management Division is highlighting the Energy Star Change a Light, Change the World Campaign, a national call to action to encourage individuals to help change the world, one light—one energy-saving step—at a time.

“We are asking ORNL associates to identify one or more incandescent bulbs in your work area that can be replaced with an Energy Star-qualified compact fluorescent light bulb. The bulbs use 75 percent less energy than incandescent bulbs and last up to 10 times longer,” says Greg Palko of ORNL’s Energy Management Team.

Greg points out that besides saving the Lab money in energy costs, the bulbs, by reducing power demand, help reduce the greenhouse gas emissions that contribute to global climate change.

East Tennessee residents received a harbinger of the potential future during August and September when daily high temperatures soared into the 90s and stayed there. The heat generated peak power demands during one of the driest summers in recent memory.

Lab Director Thom Mason called on staff members to pitch in with the resulting power conservation effort by turning off unnecessary lights and drawing blinds to keep sunlight from heating up offices. F&O Director Herb Debban estimates that ORNL cut its power demand by about a megawatt during the heat wave.

Herb also credits improvement made in the 4500 complex, such as installing variable speed fan motors on fume hoods, with cutting up to $2 million off the Lab’s light bill.

The Environmental Protection Agency cited ORNL’s work with the Green Buildings Council’s LEED program, facility upgrades and recycling efforts with a WasteWise Gold Achievement—Green Buildings award, which will be presented at its November conference, titled, Building Community and Business Partnerships.—B.C.
**Diffraction researcher Gerry Bunick dies**

Former ORNL researcher Gerry Bunick died Sept. 19 in Oak Ridge after a long battle with cancer. He was 60.

Bunick’s main area of study was molecular structure by diffraction methods using X rays or neutrons with crystalline specimens. His work helped establish how the packaging of DNA and proteins occurs.

His protein crystal experiments flew on the space shuttle and on the MIR space station for studies on the effects of microgravity.

He is survived by his wife of 34 years, Dr. Elaine M. Bunick; his son, Dr. Christopher G. Bunick and wife, Lilia Urquiza, of Nashville, Tenn.; and his daughter, Dr. Elissa Bunick-Fleming and husband, Dr. Scott D. Fleming, of Birmingham, Ala.

**Rhoda Frank Grell, geneticist, dies**

Former Biology Division researcher Rhoda Frank Grell died of complications from Alzheimer’s Disease on Sept. 14 in California. The Grell family lived in Oak Ridge from 1958 until 1985, during which time she and her husband, Ed, both worked in the Biology Division.

She was a noted *Drosophila* geneticist and the first researcher to propose distributed pairing as the mechanism for chromosome pairing during meiosis.

Grell edited two scholarly books, authored chapters in another four such works, and published 61 scholarly articles and abstracts, most in leading journals, including *Chromosomes, Genetics, Nature* and the *Proceedings of the National Academy of Sciences*.

**Service Anniversaries**

**October 2007**

**40 years:** Dan Reed Glandon, Fabrication; Wilbert D. Minter, Asset Mgt & Small Business Programs; Lester M. Petrie Jr., Nuclear Science & Technology

**35 years:** Nancy M. Larson, Nuclear Science & Technology; William H. Rose, Facilities Management

**30 years:** James Allen Mullens and Dennis Wayne Heathery, Nuclear Science & Technology; Terry L. Heathery, Information Technology Services; Cindy Ross Lundy and Donald G. Sharp, Communications & External Relations Dir.; Lynn A. Boater, Materials Science and Technology; Dewey M. Williford and Arnold J. Beal, Campus Support & Instrumentation; Brian Patrick Spalding, Environmental Sciences; Terry L. Gray, Nuclear & Radiological Protection; Jackie Price Nelson, Logistical Services; Ronald L. Taylor, Fabrication

**25 years:** Jeanette W. Early, Logistical Services; Dan T. Fehling, Fusion Energy; Patricia M. Presley and Lorie J. Hickey, Business & Information Services Dir.; Marc Livingstone Simpson, Engineering Science & Technology

**20 years:** Gwen A. Green, Fusion Energy; Gary R. Coffey, Utilities; Linda L. Farr, NScD Research Accelerator; Odie Costanzo, Logistical Services; Robert A. Tannert, Jr., and Gregory Carl Hinkel, Information Technology Services; Dane Brashear and Karen Yvonne Kaldenbach, Nuclear Science & Technology; Brian Alan Tatum, Physics; Paul Newsome Leiby, Environmental Sciences; Rick C. Griffin, Facilities Development
Peter Cummings, principal scientist at the Center for Nanophase Materials Sciences and John R. Hall Professor of Chemical Engineering at Vanderbilt University, has been selected to receive the 2007 AIChE Nanoscale Science and Engineering Forum Award. The award recognizes outstanding contributions to the advancement of nanoscale science and engineering in the field of chemical engineering. Peter will deliver a nanoscale science and engineering award lecture during the AIChE Annual Meeting next month.

Nature Nanotechnology recently featured research using slices of rat brain and a carbon nanofibre array to simulate electrical activity in the brain. The work was a collaboration among researchers at Columbia University and the NanoScience Center’s Tim McKnight, Nance Ericson, Anatoli Melechko and Mike Simpson.

Don Palmer has received the 2007 Honorary Fellow Award from the International Association for the Properties of Water and Steam. The award was given in recognition of Don’s outstanding contributions in the field of thermodynamic and transport properties of aqueous solutions of interest in the water-steam cycle, information that has been used in plant chemistry.

The Chemical Sciences Division’s Radu Custelcean has won the 2008 Margaret C. Etter Early Career Award. This award recognizes outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early independent career stage. The award is named for Margaret C. Etter (1943-1992), a major contributor to the field of organic solid-state chemistry. As a winner of this award, he will present a lecture at the American Crystallographic Association Annual Meeting.

Energy Secretary Samuel Bodman cited ORNL’s work at last month’s National Historically Black Colleges and Universities Week Conference in Washington. ORNL received an award from the White House Initiative on HBCUs for its support of administration educational programs. Bodman also recognized the mentor-protégé agreement between Morehouse College and ORNL and cited Lab Director Thom Mason and HBCU coordinator Will Minter, who led the way for this first for the Office of Science. Deputy Director for Science & Technology Jim Roberto participated in the conference opening session. Dr. Houssain Kettani, a professor at Jackson State University, and Lionet Lovett, a Jackson State student, spoke in a session about their work in ORNL’s summer faculty research program.