OAK RIDGE National Laboratory
# Reporter
Retiree Newsletter
January 2011

SCIENCE

## Supercomputing research opens doors for drug discovery

**A quicker and cheaper technique to scan molecular databases developed at ORNL** could put scientists on the fast track to developing new drug treatments.

A team led by Jerome Baudry of the UT-ORNL Center for Molecular Biophysics adapted a widely used existing software to allow supercomputers such as ORNL's Jaguar to sift through immense molecular databases and pinpoint chemical compounds as potential drug candidates.

"Our research is the missing link between supercomputers and the huge data set available in molecular databases like the Human Genome Project," Baudry says. "We have an avalanche of data available to us, and now we need to translate those data into knowledge."

Such translation is critical for the first stages of drug development, in which researchers look for appropriate chemicals that interact with a target in the body, typically a protein. If the chemical is suitable, it attaches onto the protein and produces a desirable effect in the cell.

But with thousands of known proteins and millions of chemicals as potential drugs, the number of possible combinations is astronomical.

"It is very expensive and time-consuming to measure these interactions experimentally," Baudry says. "But with supercomputers, we can process millions of molecules a day."

The quick and efficient processing of molecules offers scientists an opportunity to take risks on previously unexamined drug candidates, which could lead to diverse and innovative classes of drugs.

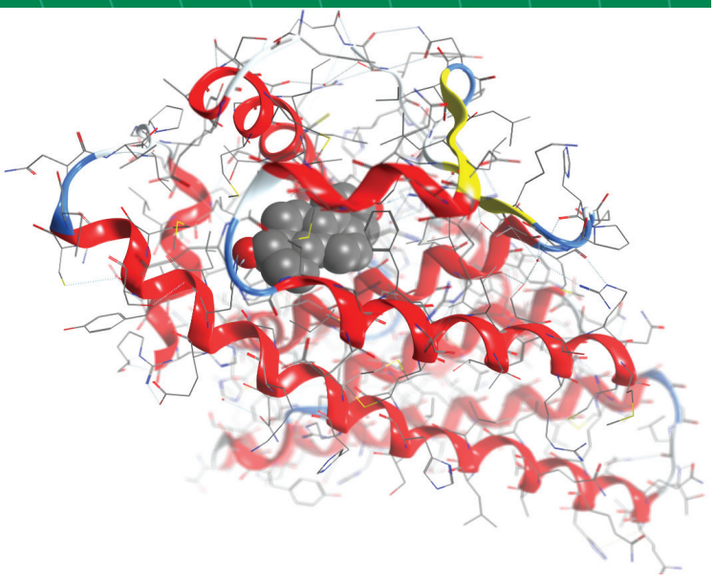
"Before, we threw away a lot of information because molecules did not have a preferred profile," Baudry says. "Now, every molecule can be examined without worrying about wasting resources."

> "Our development work is the computational equivalent of building the Saturn V rocket."

The researchers have already started work to launch the research into reality through a new collaboration supported by the National Institutes of Health. The project team plans to put the computational development to work on ORNL supercomputers to look for chemicals that could treat prostate cancer. The research is funded by an NIH Clinical Translational Science Award, which was awarded to Georgetown and Howard universities and includes ORNL, Med/Star Health and the Washington D.C. Veterans Affairs Medical Center as key partners.

"Our development work is the computational equivalent of building the Saturn V rocket," Baudry says. "Now we want to fly it to the moon."

*—Morgan McCorkle*



*Supercomputers could help speed up the drug discovery process by identifying suitable chemicals (seen as gray spheres) that can dock onto a designated target in the body, such as a protein (seen in red).*

## Table of Contents

# Retiree Joe Setaro helped bring credit union branch to the Lab

*Joe Setaro chats with Ann Murray of ORNL's Nuclear Science and Engineering Directorate during a visit to the ORNL Federal Credit Union branch on ORNL's Main Street. Setaro helped establish the branch following his retirement. (ORNL photo)*


*Joe Setaro talks with ORNL Federal Credit Union employees Donna Caquelin, middle, and Cindy Miller during a visit to the Lab's branch. (ORNL photo)*

**Until a few years ago, when ORNL employees needed to conduct bank business during the day, they spent their lunch breaks driving the approximate 20-mile round trip to and from Oak Ridge.** The opening of the ORNL Federal Credit Union branch on campus made banking both less time consuming and more convenient. The branch is handy for all personal banking needs, provides a quick source of cash for lunch and coffee breaks and offers employees easy ways to save and handle business reimbursements.

Joe Setaro was one of the people who made the credit union campus branch a reality. Joe worked at ORNL 35 years over two different time periods. Following his retirement on Jan. 1, 2000, he joined a group that worked out how to bring the branch to campus.

"I served two terms on the credit union board, and the idea of putting a branch at the Lab was something a lot of people had wanted for some time," Joe said recently during a visit to the branch office located on ORNL's Main Street. "I worked closely with Herb Debban, ORNL's director for facilities and operations and a member of the credit union board, in making that happen."

Joe started his Oak Ridge career in 1960 but spent five years during the 1970s working for General Electric in California. When the opportunity arose to return to Oak Ridge in 1977, Joe was ready to come home.

During his first years in Oak Ridge, Joe was involved in working with and managing various radioisotope programs. Upon his return in 1977, Joe oversaw the ORNL production of a dosimeter to measure power flux for the Fast Flux Test Facility in Hanford, Wash.

During his later years at ORNL, Joe was a technical assistant to Jerry Swanks, who headed the environment, safety and health operations until 2000. Joe became an authority on ORNL facility operations from his office in Building 4500 North.

After he retired, Joe still visited ORNL often. "I came out here for meetings once a month for five years and saw all of these new buildings put up," Joe says. "It is fantastic how the Lab has been transformed over the past 10 years."

Joe became active with the Coalition of Oak Ridge Retired Employees (CORRE), and he served on the ORNL Benefits Advisory Group that periodically met with benefits manager Mark Wagner to discuss benefits issues of concern to employees and retirees alike.

"One of the accomplishments I'm most proud of as a member of that board is that we were able to get vision and dental coverage for retirees, which had not been there before," Joe recalls.

Joe stays active in his homeowners association in Farragut and still avidly keeps up with ORNL news and activities.

"This has always been such an exciting place to work," Joe says. "I've been retired for more than 10 years and associated with the Lab in some way for more than 50 years, but my appreciation continues to grow for all of the accomplishments that have occurred here and all I have witnessed."—*Fred Strohl*

# CORRE issues an information booklet

During the past few months, the Coalition of Retired Oak Ridge Retirees has produced a booklet that gives much information about the organization: who it is, what it does, and why it does it. The purpose of this booklet is to inform constituents and elected representatives, especially the newly elected ones, about CORRE and its programs. A copy of this booklet has been posted on the CORRE website (www.corre.info) under the "Information" tab and "Reports" sub-heading.

*Reporter* is published for retirees of ORNL, which is managed by UT-Battelle for the U.S. Department of Energy.

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## Special basketball ticket pricing for retirees

**As a retiree of ORNL, you have the opportunity to purchase specially priced tickets to UT men's and women's basketball games listed.** Tickets are $7 each, all located in the 300 level of the arena. There is a $1.50 fee on each ticket purchased. Contact Rocky Kundert at rkundert@utk.edu or 865-974-1059.

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| Jan. 26 | Vols – LSU |
| Feb. 5 | Vols – Alabama |
| Feb. 10 | Lady Vols – Florida |
| Feb. 16 | Vols – S. Carolina |
| Feb. 19 | Vols – Georgia |
| Feb. 21 | Lady Vols – Georgia |
| Feb. 26 | Vols – Mississippi State |
| Feb. 27 | Lady Vols – LSU |

## Playhouse kicks off "Have a seat!" campaign

**Following three years of planning and fundraising and led by an early corporate gift from UT-Battelle, the Oak Ridge Playhouse is ready to begin renovations to the lobby, auditorium and exterior of the Playhouse.** The campaign offers contributors a unique opportunity to create a permanent legacy as part of the Ebert Renovation, by honoring someone special with their name, or your own, engraved on a name plate to be placed on one or more of the new theater seats. Recognition is available at $250 per seat. Visit orplayhouse.com for more information or to make a donation.

## Discount tickets to Knoxville Symphony Orchestra Pops Series

**Don't forget to get your tickets through Club ORNL for the KSO Pops Series:** John Williams Spectacular, Romantic Broadway, Tribute to the Music of John Denver, and Chris Botti concert.

KSO Knoxville Symphony Orchestra

## Cirque du Soleil comes to Knoxville March 23 – 27

**Cirque du Soleil's critically acclaimed production *Alegría* will be performed in Knoxville** at the Thompson-Boling Arena, from March 23 – 27, 2011, for eight shows only. Alegría is a Spanish word that means happiness, joy and jubilation. The show features an international cast of 55 performers and musicians from 15 countries and showcases breathtaking acrobatics. Club ORNL is offering ORNL employees and retirees a discount to select performances of *Alegría*. To order tickets and receive the discount, you MUST identify yourself as an ORNL employee or retiree by calling 250-3842 directly.

*Alegría* discount show schedule (March 23 – 27, 2011); there are **no** ORNL discounts for the March 25th 7:30 or March 26th shows:

- Wednesday, March 23 at 7:30 p.m.
- Thursday, March 24 at 7:30 p.m.
- Friday, March 25 at 3:30 p.m.
- Sunday, March 27 at 1:00 p.m. and 5:00 p.m.

## ORNL F&O Directorate earns commitment award


*As part of the cleanup of laboratory space in Building 4500S, members of the lab cleanout team handled some 30,000 samples of unwanted chemicals, which were identified and disposed of through an off-site waste management vendor.*

**A comprehensive effort undertaken by the Facilities and Operations Directorate of Oak Ridge National Laboratory to improve efficiency, security and safety has helped earn an award from the Tennessee Center for Performance Excellence.**

The F&O Directorate has nearly 1,000 employees who are responsible for the physical infrastructure to enable science at the Lab. F&O staff scrutinized virtually every area of the Lab as it completed eight improvement projects in fiscal year 2010.

One of the major challenges involved cleaning out 90 laboratories in Building 4500S, a research facility built in the early 1960s, in preparation for moving these labs into the new Chemical and Materials Sciences Building, under construction. The Lab Cleanout Project Team removed more than 30,000 samples of chemicals, 22,375 pounds of metal, 55,306 pounds of glass and 235 pounds of miscellaneous scrap in fiscal year 2010 at a cost savings of $800,000.

In the area of sustainability, modernization efforts saw the construction of 1.2 million square feet of offices and lab space since 2000, with another 400,000 square feet in the queue. The new high-performance buildings resulted in a 33 percent increase in space with just a 5 percent increase in energy usage. The new buildings enabled ORNL to become the largest Leadership in Energy and Environmental Design-certified facility in the Southeast. In addition, 75 percent of ORNL's vehicle fleet uses alternative fuel, and the Lab won a White House Closing the Circle Award for Green Transportation.

The Commitment Award will be presented at the 18th annual Excellence in Tennessee Awards Banquet, Feb. 23, in Franklin. The award's annual evaluation and assessment process uses the Criteria for Performance Excellence, established by the Baldrige Performance Excellence Program, as the evaluation tool.—*Ron Walli*

## Hefty fuel savings and cleaner air could prompt Tennesseans to turn over new Leaf

*The Nissan Leaf is one of the all-electric vehicle options now available to American consumers.*

**New car buyers who opt for electric vehicles like the Nissan Leaf could be a bit more jolly next December** as they can save more than $1,600 in gasoline and oil changes over the next 12 months.

As gas prices in Tennessee for December 2010 hit an all-time high — up 38 cents per gallon from December 2009 — people who drive less than 100 miles per day may soon choose the electric route.

While the Nissan Leaf has a range of 100 miles, most drivers in Knox County, for example, commute less than 50 miles to and from work, according to statistics provided by a team led by Budhendra Bhaduri of the Lab's Geographic Information Science & Technology Group. Assuming those drivers travel 50 miles per day five days a week, the cost of regular gasoline at $2.82 per gallon would be $155 per month for a vehicle that averages 20 miles per gallon.

Driving the same distance, 1,100 miles per month, the owner of a Leaf would spend about $1.20 per day (four hours charge time, five times a week), or $26.40 per month, to recharge the half discharged battery. So, while annual costs for the gasoline vehicle would total $1,860, the electric vehicle cost per year is about $317, with no oil to change.

In Knox County, on a typical work day, commute trips by nearly 179,000 drivers total about 1.9 million miles, according to Bhaduri. Assuming each vehicle achieves 20 miles per gallon, total fuel consumption is 95,000 gallons. Since each gallon of gasoline when consumed in an internal combustion engine produces 19.4 pounds of carbon dioxide[1], the total $CO_2$ generated in Knox County per day is 1.84 million pounds.

For non-work commutes, assuming that the average vehicle in Knox County is driven the national annual average of about 13,500 miles, the amount of $CO_2$ produced per vehicle is nearly 13,100 pounds per year[2].

In addition to carbon dioxide, automobiles produce carbon monoxide, methane and nitrous oxide from the tailpipe and hydrofluorocarbon emissions from leaking air conditioners. All of these contribute to air quality problems that already challenge East Tennessee residents.

"By choosing an all-electric or plug-in hybrid electric vehicle, drivers can save money at the gas pump and help improve the region's air quality," said Tom King, director of the Energy Efficiency and Electricity Technology program.—*Ron Walli*

[1]Source: "Emission Facts: Greenhouse Gas Emissions from a Typical Passenger Vehicle, U.S. EPA"

[2]U.S. Department of Transportation, Federal Highway Administration

# New year: New routine

## Start 2011 off on the right foot with realistic goals

**Resolutions – many of us will make them but few will keep them.** Studies have shown that by June of the new year, less than half the resolutions made are being maintained. Instead of trying to reach insurmountable goals like losing 50 pounds in a month or giving up a two-pack-a-day habit cold turkey, start with a realistic plan. Below are some tips.

**Set simpler, realistic goals.** It's okay to dream big, but for the short term it's important to think small and be realistic. For most of us, it's unrealistic to expect our bodies to be marathon-ready in a month. Start by listing all your health and fitness goals and consider these to be long term. One by one, make small changes. For example, if you resolve to work out an hour a day yet your job requires long hours, you may not have enough time or energy to meet this ambitious goal. Rather than be discouraged and give up, start with 15 minutes a day and know you are making a daily difference for your overall health.

**Replace one habit with another, better habit.** Willpower and discipline are overrated. Roy Baumeister of Florida State University and his research colleagues have discovered our storehouse of willpower is a limited resource that gets depleted throughout each day, depending on how often you call upon it to override temptation. That means setting too many willpower goals at once—like losing weight, spending less, exercising more—is destined to fail. The best way to ensure you'll make behavior changes is to form new habits, e.g., rituals done without thinking. Habits are better than goals because they persist through time. Support routines by planning ahead. If your goal is to jog to the mailbox each day, make sure running shoes are sitting by the door.

Joan Lawson of ORNL's Wellness Program agrees. "If you execute the plan long enough, then it becomes a habit. Like getting ready to come to work: you get up at a certain time, take a shower, brush your teeth, etc.," says Lawson. "You must plan what you will eat and when you will exercise, and soon it will become a no brainer."

**Assess your progress.** To measure goals, you need to provide a self-assessment tool. It can be a mark on a calendar, a record book, or a sticker chart—whatever will help you track your habit and evaluate consistency. There is a common phrase that whatever you measure will get better. Every star on a chart equals a met goal and provides a sense of accomplishment, and your brain will desire to have that star. Don't give up on your new habit if you miss a day but try to make the best of the rest of the week.

Experts say it takes at least two weeks to form a good habit. Don't add any additional health or fitness goals until you have succeeded for at least two consecutive weeks on your current goal.

Build confidence and don't be so hard on yourself. Successful, confident people typically know and appreciate their own limitations. Too often, the average person tends to focus on failures rather than successes. Remember that no one is perfect. When you are less insecure about personal limitations, you can focus more energy on progress.

## 10 exercise tips for busy routines

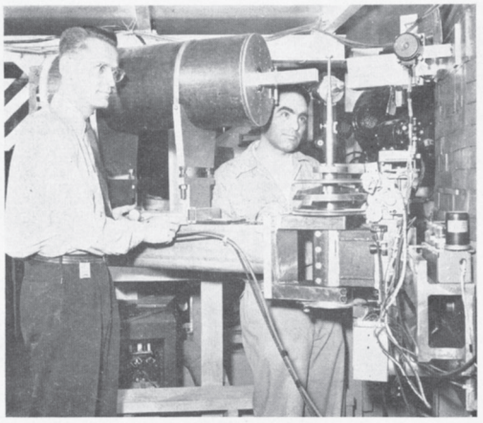
1. **Make an appointment** with yourself – put it on your calendar.
2. **Multitask.** Ride your bike to work or take your dog for a walk.
3. **Join the club.** Start or join a fitness club or group such as a softball team, bowling league or running group.
4. **Move during meetings.** Instead of booking a conference room, invite workers to "walking meetings."
5. **Rethink errands** by biking to the neighborhood store or walking to the post office.
6. **Set your alarm 30 minutes earlier** to take a walk or pop in a fitness DVD.
7. **Travel smarter** by staying in hotels with fitness centers and pools.
8. **Keep it in the family.** Make family time more physical – plan outings that promote exercise like biking, hiking or backyard games.
9. **Do your chores.** Rake the yard, wax your car or do more energetic housework.
10. **Pair up with a friend.** The buddy system is an excellent motivator.

ORNL Wellness Program

THE NEWS
OAK RIDGE NATIONAL LABORATORY

A Publication by and for the ORNL Employees of Carbide and Carbon Chemicals Division, Union Carbide and Carbon Corporation

Vol. 3—No. 28 OAK RIDGE, TENNESSEE Friday, January 26, 1951



*STUDY CHEMICAL BONDING—Dr. H. A. Levy, left, and Dr. S. W. Peterson, both of the Chemistry Division, are shown in their laboratory in the Pile Building as they operate a neutron diffraction spectrometer in investigating the arrangement of atoms in crystals. The object of their study is to obtain a better understanding of chemical bonding in materials—particularly that known as hydrogen bonding. The project has been in its development stages for about a year.*

## Drs. H. Levy, S. Peterson Investigate Properties of Chemical Binding

Many are the age-old problems of science—believed unsolvable—that are now receiving renewed investigation owing to the new scientific tools and instruments which have been made available by the atomic energy program. Such a problem is that of understanding the properties of chemical bonding, the nature of chemical forces that hold the particles of all materials together. Dr. Henri A. Levy and Dr. S. W. Peterson of the Chemistry Division are now working on a project to bring much needed light on this subject.

Members of the Chemical Physics Group of the Chemistry Division, Drs. Levy and Peterson since June, 1949, have pursued an investigation of the structure of crystals. They have carried on their research by means of neutron diffraction, using a spectrometer constructed entirely at the Laboratory by the Research Shops and the Chemistry Division Shop. The basic design of the instrument was produced by Dr. E. O. Wollan of the ORNL Physics Division.

Employment of neutron diffraction constitutes a considerable departure from x-ray diffraction, the older method of studying crystal structure, which had its inception in 1913 when it was developed by a German scientist. About 1945, it was found that a beam of neutrons could be diffracted from a crystal and that its diffraction pattern could be interpreted to give useful information on crystal structure. This technique for determining the relative positions of atoms in materials has been intensively developed by Dr. E. O. Wollan and Dr. C. G. Shull, also of the ORNL Physics Division.

The neutron diffraction method has distinct advantages over those of x-ray diffraction. For ex-

*DR. EUGENE P. WIGNER, ORNL Consultant, who extolled scientific achievements at the Oak Ridge National Laboratory in an address given at the recent AAAS meeting in Cleveland. Dr. Wigner, Professor of Physics at Princeton University, was associated with ORNL as Director of Research and Development from June of 1946 to June of 1947. Excerpts of his AAAS address are printed below.*

## Dr. Wigner Praises ORNL Scientists

Dr. Eugene P. Wigner, ORNL

## Award To Weinberg Honors Laboratory

Dr. C. E. Larson, Director of ORNL, in the following statement to The News expresses the deep gratification felt at the Laboratory for the prominence reflected by the recent honor bestowed on Dr. Alvin M. Weinberg, ORNL Director of Research.

"It is a source of pride to everyone of us and a mark of high honor for the Oak Ridge National Laboratory that our Director of Research, Dr. Alvin M. Weinberg, has been chosen one of the United States' ten most outstanding young men of the year 1950. The national recognition given Dr. Weinberg for eminence in the field of atomic energy, we at ORNL know, is richly deserved.

"The nomination of Dr. Weinberg for the United States Junior Chamber of Commerce award was made by the Laboratory in October. Selection of Dr. Weinberg for the award was made by a committee of distinguished Americans which included such outstanding figures as Dr. Andres Millikin, president emeritus of California Institute of Technology, and a former Nobel prize winner in physics; Otto Seyferth, president of the U. S. Chamber of Commerce; Dean Rusk, Assistant Secretary of State; Cody Fowler, president of the American Bar Association; and Thomas J. Watson, Jr., executive vice president of the International Business Machines Corporation."

### Health Physics Dance Tonite

The third annual dance of the Health Physics Division will be held from 9 p. m. 'till 1 a. m. tonight at the Jefferson Recreation Hall. There will be no tickets sold at the door.

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## Sixty years ago this month
### Taken from *The ORNL News* for January 1951

- Drs. Stockdale and Klepser, two UT geologists, make geological surveys of the Oak Ridge area to determine the best locations for excavating foundations of new buildings at ORNL. They also select areas that have desirable geological characteristics for the disposal of radioactive wastes, contributing to the overall Health Physics effort. Their total efforts entail tracing the upturned strata back 500 million years—early in the Paleozoic Era.
- A ground-breaking ceremony for a new health physics waste research building will be located in the southeast section of the ORNL area. This building will be designated "3504." The research will be concerned primarily with the public health aspects of radioactive waste disposal and removal of radioactive materials from water.
- A new spacious 21,000 square foot instrument laboratory opens on Central Avenue across from the radioisotopes processing area. Its new features include a shielded room with a double metallic shell, which keeps out electrical interference and disturbances, and a standards room for checking and calibrating all precision meters and measuring equipment in the Laboratory.
- Drs. H. Levy and S. Peterson of the Chemistry Division show that neutron diffraction has distinct advantages over the older x-ray diffraction method for investigating and clarifying the underlying principles governing crystal and molecular structures.
- ORNL's Director of Research Dr. Alvin Weinberg is chosen as one of the United States' ten most outstanding men of 1950 for eminence in the field of atomic energy.
- Dr. Eugene Wigner, ORNL consultant and past ORNL director of research and development, praises ORNL scientists for their outstanding scientific accomplishments in the field of atomic energy. Of national importance are the stable isotopes produced at Y-12, the neutron diffraction work of Drs. Shull and Wollan and Dr. Shull's proof of the radioactivity decay of the neutron.

*—prepared by ORNL History Room volunteers*

**January.** Gov. Phil Bredesen announces UT-ORNL energy science and engineering graduate program. Murray Rosenthal returns to the Lab to talk about its history of nuclear reactors. Chestnut Ridge gets a cafeteria.

**February.** ESD researchers help sequence Brachypodium gene. ORNL responds to Haiti quake.

**March.** Energy Secretary Steven Chu visits, announces UT-Battelle contract extension. The Main Street courtyard closes for the Building 5700 addition. Herb Mook receives the neutron scattering Shull Prize. ORNL's atom images featured on *Nature's* cover.

**April.** ORNL plays critical role in discovery of element 117. ORNL and Y-12 separate benefit operations.

**May.** ORNL lands the Nuclear Energy Modeling & Simulation Energy Innovation Hub. UT-Battelle celebrates the contract extension. BioEnergy Science Center researchers identify a key ethanol gene in Z. mobilis.

**June.** Jaguar hangs on to its top spot among supercomputers. Traffic cams installed to help with daily backups. Record number of summer students arrive.

**July.** ORNL wins nine R&D 100 awards. UT-Battelle donates $50,000 to Oak Ridge education. Mike Miller named UT-Battelle corporate fellow.

**August.** Article on doubly magic tin-132 puts Holifield's tandem accelerator on the cover of Physics Today.

**September.** ORNL hosts User Week to showcase the Lab's collaboration opportunities. A $36 million contribution to ORNL's pension fund is among the topics in Thom Mason's Director's Forum.

**October.** New Nuclear S&T Directorate marshals ORNL's nuclear know-how into one organization. Energy & Environmental Sciences Directorate combines energy technology organizations. Neutron science exhibit provides high point in Washington's USA Science & Engineering Festival.

**November.** Little Red Schoolhouse joins outdated facilities torn down as well as the 2000 complex. ORNL has four Presidential Early Career Award winners. UT-Battelle, DOE and UT contribute a meeting place in the ORR woods. Sheng Dai is top researcher at Awards Night. As expected, China takes supercomputing's top spot, but ORNL supercomputing stays in the elite.

**December.** Gov. Bredesen helps dedicate the Joint Institute for Neutron Sciences, ORNL's third state-funded facility. A 1944 memo suggests—actually pretty much proves—that ORNL's E.O. Wollan pioneered neutron diffraction analysis. Overnight snow closes the Lab for first time in years. A few days later, freezing rain sparks a two-hour delay. DOE's Secretary Chu, citing hard times, freezes salaries.

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## DARPA's titanium smashdown

**Researchers from ORNL's Materials Science & Technology Division helped a team of visiting DARPA military officers award a $50,000 prize in December.** The competition involved the fabrication of a couple hundred titanium mesh spheres by a process called electron-beam deposition in Building 5500's recently remodeled high-bay area.

The prize in DARPA's DMACE Challenge went to a University of California at Santa Barbara team, which came up with the most accurate predictive model of the components' properties.

The competition featured spheres made from a titanium-based powder that is fused with an electron beam. The spheres were then smashed to produce the parameters for the competition.

The real aim of the competition, says MSTD's Craig Blue, was to build awareness of new technologies that are reducing the cost of working with materials such as titanium.

The DARPA team—representing the Army, Navy, Marines and Air Force—came up with the DMACE Challenge idea at the beginning of their three-month fellowship, and partnered with ORNL to fast-track the competition to completion. For more information and to view animations of the sphere manufacturing process, visit www.dmace.net.

The $50,000 DMACE Challenge, conceived by participants in DARPA's three-month Service Chiefs Fellows Program, drew 179 entries from 13 countries and 38 universities.


*A titanium-based powder is fused with an electron beam to produce a hollow mesh sphere from a computer-aided drawing.*