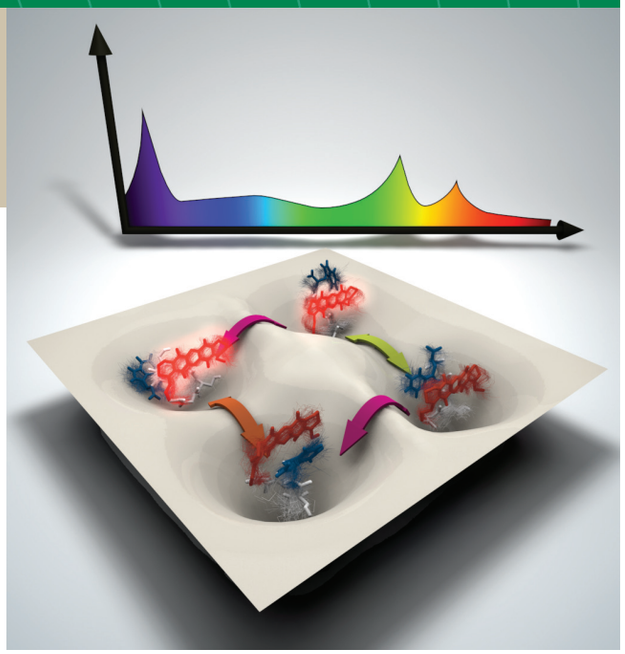
OAK RIDGE National Laboratory
Reporter
Retiree Newsletter
April 2011

SCIENCE

'Fingerprints' match molecular simulations with reality



As a molecule jumps between structural states (lower image), it creates "dynamical fingerprints" (top spectra) that can tie high-performance simulation with experiments.

A theoretical technique developed at ORNL is bringing supercomputer simulations and experimental results closer together by identifying common "fingerprints."

ORNL's Jeremy Smith collaborated on devising a method — dynamical fingerprints — that reconciles the different signals between experiments and computer simulations to strengthen analyses of molecules in motion.

"Experiments tend to produce relatively simple and smooth-looking signals, as they only 'see' a molecule's motions at low resolution," says Smith, who directs ORNL's Center for Molecular Biophysics and holds a Governor's Chair at the University of Tennessee. "In contrast, data from a supercomputer simulation are complex and difficult to analyze, as the atoms move around in the simulation in a multitude of jumps, wiggles and jiggles. How to reconcile these different views of the same phenomenon has been a long-standing problem."

> "We want to create movies of molecules in motion and check experimentally if these motions are actually happening."

The new method solves the problem by calculating peaks within the simulated and experimental data, creating distinct "dynamical fingerprints." The technique, conceived by Smith's former graduate student Frank Noe, now at the Free University of Berlin, can then link the two datasets.

Supercomputer simulations and modeling capabilities can add a layer of complexity missing from many types of molecular experiments.

"When we started the research, we hoped to find a way to use computer simulation to tell us which molecular motions the experiment actually sees," Smith says. "When we were finished, we got much more – a method that could also tell us which other experiments should be done to see all the other motions present in the simulation. This method should allow major facilities like ORNL's Spallation Neutron Source to be used more efficiently."

Combining the power of simulations and experiments will help researchers tackle scientific challenges in areas like biofuels, drug development, materials design and fundamental biological processes, which require a thorough understanding of how molecules move and interact.

"Many important things in science depend on atoms and molecules moving," Smith says. "We want to create movies of molecules in motion and check experimentally if these motions are actually happening."

The collaborative work included researchers from L'Aquila, Italy; Wuerzburg and Bielefeld, Germany; and the University of California at Berkeley. The research was funded in part by a Scientific Discovery through Advanced Computing grant from the DOE Office of Science.

"The aim is to seamlessly integrate supercomputing with the Spallation Neutron Source so as to make full use of the major facilities we have here at ORNL for bioenergy and materials science development," Smith says.—*Morgan McCorkle*

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Sharon Rucker's gospel music website grows in popularity

Retiree Sharon Rucker's web-based broadcast, "The Gospel Train" enjoys a steadily growing listenership.

Sharon Rucker began singing and playing piano at age nine. At age 13, she was already directing an adult choir at Rogers Memorial Baptist Church in Knoxville.

She developed a love for music – particularly urban contemporary gospel music – at a very young age. That love is as strong now, at age 56, as it ever was.

After retiring in December 2003 from the former Computer Division, Sharon was offered a position as a radio personality at Knoxville radio station WNPZ, 1580 AM, where she hosted a call-in show for 19 months. This experience gave her the background she needed to start her online gospel show. Now, seven years after retiring, Sharon has launched an Internet gospel music site, "The Gospel Train," that received 30,000 hits from around the world the first year.

"I can't tell you how blessed I feel," Sharon said recently while sitting in the kitchen of her East Knoxville home with her husband, David "I was able to retire at age 49, come home, and do something that I love with music, right in my own studio."

Sharon initiated the 24-7 website January 1, 2010, with the assistance of LifestreamTV, which connected the Internet broadcast system for her. From there, she began programming gospel music into the system, and now, some 14 months later, she has uploaded more than 1,200 pieces of music from record companies and various artists, and that number is still growing.

"As more and more people learn about The Gospel Train, they send me more and more music," Sharon said. Since starting The Gospel Train 14 months ago, her listenership has risen to over 2000 hits per month and continues to rise exponentially. In addition, plans are currently under way for advertising the station on TV and through other media.

Sharon finds it particiuarly rewarding that not only is the Gospel Train providing good music, it is also having a positive impact on people's lives. "A listener contacted me from Cincinnati the other day and said she was listening to my site on her Android/cell phone while her granddaughter was undergoing a 5-hour surgery. She told me the music gave her peace and helped her through a very hard day."

Sharon's musical activities continue outside the home, as well.

"I direct several church choirs; perform at weddings, funerals, and on special programs; and have served as mistress of ceremonies for a number of nationally known gospel artists' concerts and have produced a CD titled *Thank You*."

Sharon has also been involved in a community-wide effort encouraging children to read.

While she feels blessed to be able to provide gospel music to listeners worldwide through The Gospel Train, she would still love to return to local radio. "It would mean so much to me if I could do this type of programming on a local radio station in this area," she said.

Looking ahead, Sharon hopes to add some new features to the web site.

"I would like to make the call-in show more interactive, she said. "I'd also like to get many more churches involved in our programming."

Retired almost eight years from ORNL, Sharon may be working harder than ever. "I'll be 57 in July, but with the success of The Gospel Train and all of the joy it has brought me and everyone who listens, I can say I'm doing something right and enjoying every minute of it."

The Gospel Train can be accessed on the web at www.sharonrucker.com. I-phones, I-Pads, Androids and Blackberries can access the show at www.thegospeltrainonline.com

More information about The Gospel Train is available by contacting Sharon at 865-332-3244 (srucker@comcast.net).—*Fred Strohl*

> "I can't tell you how blessed I feel that I was able to retire at age 49, come home, and do something that I love with music, right in my own studio."

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

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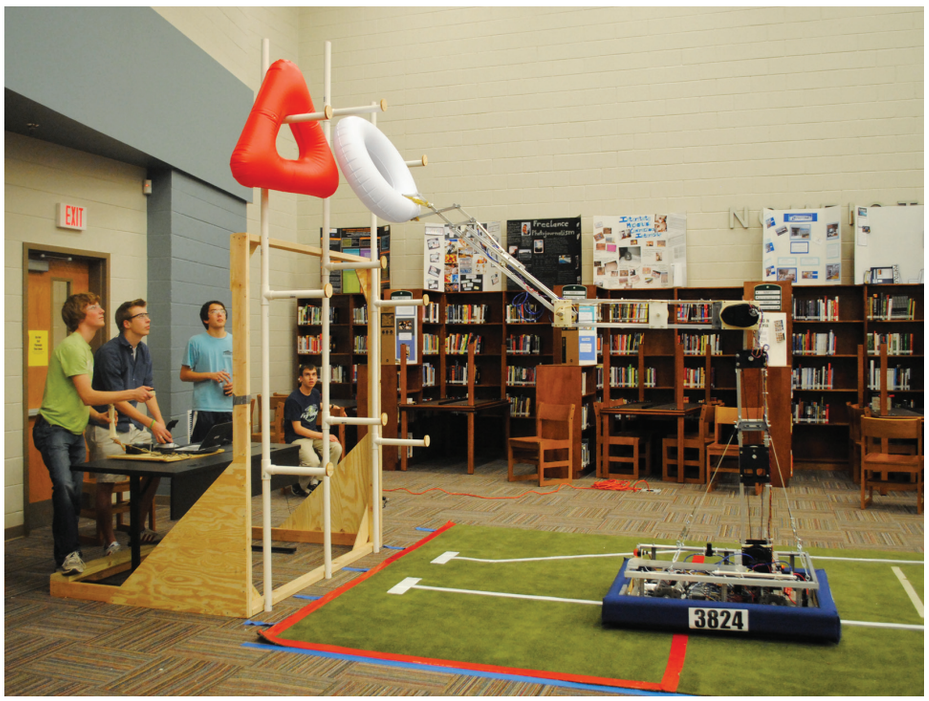
Robotics competition connects students with ORNL scientists

Sounds of whizzing and whirring robots echo through Hardin Valley Academy's library long after the school day has ended. The hubbub stems from 23 students and their mentors, including four of ORNL's top scientists, who are racing to design and build a set of robots that will compete in a regional tournament in Knoxville.

This year marks the first time Hardin Valley Academy students will compete in the FIRST robotics competition, a nationwide event that promotes science and engineering for high school students. Students are eligible for college scholarship opportunities that total more than $14 million.

For ORNL mentors Martin Keller, Lonnie Love, Craig Blue and Tommy Phelps, the competition is a chance to reach out to the next generation of scientists and engineers. Keller, whose son Philip helped launch the robotics club, said the program is a unique opportunity to encourage students in science at a critical age.



Students from Hardin Valley Academy test their robot, "Hawktimus Prime," in preparation for the regional FIRST robotics competition in April.

"What can we teach the kids to prepare them for their jobs in five to ten years?" said Keller, who serves as ORNL's associate lab director for energy and environment.

One skill ORNL mentors hope to impart is next-generation manufacturing, including new techniques that use digital design and powder materials to manufacture complex components. The students' main robot features customized parts made with a titanium powder manufacturing process pioneered at ORNL. The kids also have access to a 3-D printer, which was sitting unused in a classroom until Love stumbled upon it and realized its potential.

Love, along with his fellow mentors and HVA teacher Mary Lin, are helping the kids master the tough engineering and scientific elements of the robotics challenge by giving them crash courses in areas like computer-aided design.

> "What they're doing here is very similar to a work environment in the real world."

"For them, it's an immersion in problem solving as an engineer," Love said. "We were given this box of stuff, and there was a lot of scratching our heads and wondering what to do with it."

The FIRST competition gives teams a standard kit of parts and six weeks to complete a main robot that can be remotely controlled to pick up inner tubes and place them on pegs up to 10 feet high. Students must also construct a second mini-robot that can scale a pole. The final project element involves developing a website and essay to document the progress of the entire team.

"What they're doing here is very similar to a work environment in the real world," Keller said. "The kids have to learn things like project management and how to be on time. It requires their dedication and commitment."—*Morgan McCorkle*

Club ORNL events

Get the details and latest news online via https://info.ornl.gov/sites/clubornl. Request an XCAMS account, which will allow you to participate in these events or contact Lara James at 576-3753 or jamesla@ornl.gov.

April 29	Alive After Five
April 30	Smokies Baseball Game & Picnic
May 5	The 39 Steps
May 7-8	Townsend Overnight
May 13-15	Atlanta Overnight
May 21	Spamalot

DOE Advisory Board provides a vehicle for Lab employee to serve the community

Lance Mezga is the program manager of the Excess Facilities D&D Program and for Environmental Integration for New Facilities Development at ORNL and is in his sixth year as a member of the Oak Ridge Site Specific Advisory Board.

Lance Mezga has served on the Oak Ridge Site Specific Advisory Board since 2005, and in recent months, his position at the Lab and his passion for volunteer work have dovetailed nicely.

American Recovery and Reinvestment Act work at ORNL over the past year and a half has provided Lance with an opportunity to serve a valuable role on the board by allowing him to offer insights into environmental cleanup efforts at the Lab. Lance is responsible for the decontamination and decommissioning of Office of Science buildings, ensuring environmental integration across all construction projects.

"When I took on my current position, I felt like I could provide a level of expertise to the SSAB in understanding the functions and workings of the construction and technical scope," he says. "It was an opportunity to provide something to the community which fit perfectly with my technical background.

"Since I've been on the board, I think we've improved the technical knowledge of the members by instituting a number of training programs to get everyone on a common level of understanding. We've worked very hard to engage all of the members. Everyone needs to participate, and everyone's opinion is important and valid.

"With the economic stimulus package that's been implemented, the board has had an opportunity to provide comment and input to planning and how dollars are used."

"With the economic stimulus package that's been implemented, the board has had an opportunity to provide comment and input to planning and how dollars are used."

The SSAB is an independent, federally appointed citizens' panel that provides advice and recommendations to the U.S. Department of Energy on its Oak Ridge Environmental Management Program.

Lance stepped into a leadership position on the board within weeks of his appointment in June 2005 when he was elected chair of the board's Environmental Management Committee, following the board's August planning retreat. After just one year he was elected chair of the board.

Lance came to ORNL in 1979 to head the Geothermal and Biomass Energy Environmental Impact Assessment Program. He went on to head DOE's Low-Level Waste Technology Development Program and set up Martin Marietta's radiologic waste management organization to standardize procedures in Oak Ridge, Portsmouth, and Paducah.

In the late 1990s, he moved over to the K-25 site to run Lockheed Martin's central waste management organization and later the mixed- and low-level waste programs. He also worked to develop the first integrated burn plan for the Toxic Substances Control Act Incinerator, coordinating shipments from other DOE sites.

When Bechtel Jacobs Company became DOE's prime contractor for environmental cleanup of the Oak Ridge Reservation, Lance returned to the Lab to work with the Office of Science waste management program.

In addition to his work on the board, Lance is also active as a member of the board of directors of the Waste Management Symposium. He's been a member of the symposium's Program Advisory Committee for 20 years and has been chair of the Low-Level/Mixed Low-Level Waste Treatment Committee for the last 10 years.

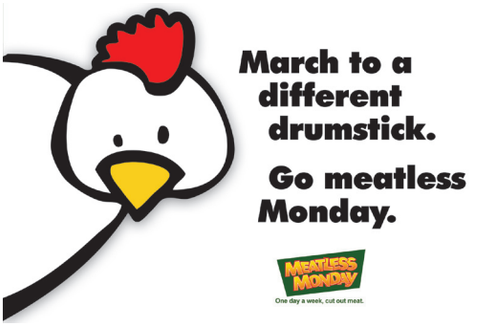
Lance also served as Vice Chair and Secretary of the Decontamination and Decommissioning Working Group for the Energy Facility Contractors Operating Group, which is composed of all the contractors at DOE facilities.

He has served as a technical expert of the International Atomic Energy Agency, the Organization for Economic and Community Development, and the Nuclear Energy Agency on low-level waste issues.

The Oak Ridge Site Specific Advisory Board meets the second Wednesday of each month at 6 p.m. at the DOE Information Center in Oak Ridge. For information see www.oakridge.doe.gov/em/ssab.

—Pete Osborne, Administrator, Oak Ridge Site Specific Advisory Board

Meatless Mondays: One day a week, cut out the meat



Oprah and Simon Cowell have signed the pledge. No longer just a trend, the Meatless Monday movement is taking the country by storm, challenging foodies to find healthy, plant-based alternatives to the all-American diet staple of red meat.

Why Monday? We all need to start somewhere. That's where Monday comes in; it's the January of every week—a "fresh start" built into every calendar. When asked what day they were most likely to begin healthy behaviors, half of a national sample of 1,500 adults over age 25 viewed Monday as a day to get their act together or make a change. People hope that a healthy start on Monday means they might just have a healthier week.

Move over, meat. The average American consumes 45 percent more meat than the recommended daily allowance, increasing possible health risks. Animal proteins are higher in saturated fat and can lead to a plethora of problems, including heart disease, diabetes and hypertension. With national obesity numbers skyrocketing at alarming rates, health experts strongly recommend a plate with less meat and more fish, fruits and vegetables. Doing this can create a diet with less saturated fat, more fiber, omega 3 fatty acids, antioxidants, minerals and other essential nutrients. In general, less meat means more room on the plate for healthier foods.

Beef up your diet with the right vitamins and nutrients. To meet recommended amounts of fiber, the average adult should consume at least two cups of fruit and three cups of vegetables a day. Choose a variety of high-fiber foods like berries, citrus fruits, oatmeal, beans, dark green leafy vegetables and 100 percent whole grain breads. Contrary to popular belief, fat is an essential nutrient; however, it doesn't have to come from animal proteins. By choosing more fruits and vegetables, you will also increase your intake of antioxidants, shown to decrease the risks for many diseases including heart disease, cancer, macular degeneration, diabetes and Alzheimer's dementia.

Diseases "meat" their match. Numerous studies suggest that diets high in both red and processed meat are associated with colon cancer. Recent data from a Harvard University study found that replacing saturated fat-rich foods (for example, meat and full-fat dairy) with foods rich in polyunsaturated fat (vegetable oils, nuts and seeds) reduces the risk of heart disease by 19 percent. A recent study from Imperial College London also found that reducing overall meat consumption can prevent long-term weight gain and can lower body weight and body mass.

Making the move. To plan a menu, research vegetarian cookbooks for animal protein substitutes. Soy beans, tofu, cheese, eggs and milk are complete proteins, while fish is high in protein and low in fat. If you dine out often, most restaurants now offer at least one vegetarian entrée. Indian, Asian and Mexican restaurants usually have several meatless dishes. For more recipes, tips and information, visit www.meatlessmonday.com.

—Stephanie Ritchie

Black Bean Tostadas

1 15 oz. can black beans
½ teaspoon garlic salt
1 teaspoon chili powder
6 whole-wheat tortillas
1 tablespoon olive oil
2 oz. Monterey Jack cheese, grated
4 cups frozen corn, thawed
1 cup grape tomatoes, quartered
1 avocado, diced
1 bunch scallions, chopped
1 lime

Preheat oven to 475 degrees.

In a small bowl, combine black beans, garlic salt and chili powder. Divide the bean mixture into two parts.

Brush both sides of tortillas with olive oil and place on a baking sheet. Top three of the tortillas with cheese and half the seasoned beans and leave the other three tortillas with just olive oil. Set the other half of the beans aside. Heat tortillas in the oven for about 10 minutes.

While the tostadas are heating, in a large mixing bowl, combine the corn, tomatoes, avocados, scallions and lime juice. Divide the corn relish into two parts. Combine one part of the corn relish with the reserved beans.

When tortillas and beans are thoroughly heated, remove them from the oven. Cut the plain tortillas into bite sized strips to eat dipped in the seasoned bean corn relish. Finish the bean and cheese topped tortillas with the reserved corn relish and enjoy!

Nutrition Information:

Servings per Recipe: 6	Sodium: 71mg
Amount per Serving	Potassium: 739mg
Calories: 274	Total
Calories from Fat: 83	Carbohydrates: 42.6g
Total Fat: 9.3g	Dietary Fiber: 10.8g
Saturated Fat: 2.9g	Protein: 11.9g
Cholesterol: 8mg	Sugars: 1.2g

Know your vitamins

Vitamin A – carrots, squash, broccoli, sweet potatoes, tomatoes, kale, collards, cantaloupe, peaches and apricots

Vitamin C – oranges, limes, green peppers, broccoli, green leafy vegetables, strawberries and tomatoes

Vitamin E – nuts, seeds, whole grains, green leafy vegetables, vegetable oil and liver oil

Selenium – grains and garlic

ORNL Wellness Program

THE NEWS
OAK RIDGE NATIONAL LABORATORY

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

Vol. 3—No. 40 OAK RIDGE, TENNESSEE Friday, April 20, 1951

THE FOURTH ANNUAL BIOLOGY CONFERENCE IN SESSION AT RIDGE HALL—Sponsored by the Biology Division of the Oak Ridge National Laboratory and the Atomic Energy Commission, the Conference attracted more than 100 scientists from wide-spread parts of the United States and Canada as well as many from the University of Tennessee and Oak Ridge.

P. R. Bell's On The Spot Pocket Radiation Meter Now Marketed

A pocket radiation meter that reads on the spot radiation and is slightly larger than a photographic exposure meter, but lighter in weight, is for the first time being commercially produced by the Raytheon Manufacturing Company of Waltham, Mass. But its history comes right back to P. R. Bell of the Physics Division of the Oak Ridge National Laboratory.

P. R. Bell

Designed for use in actual war operations, the meter detects gamma rays, soft beta rays and alpha particles and indicates radiation levels safe to stay in to those lethal in less than an hour.

Bell says it's not exactly new, a model having been around the Laboratory for about four years. The first approved one was made under his direction by Senior Technician Walter Jones, but today marks the first time the meters have been made in mass production on a commercial basis. The design was submitted to the Raytheon company under contract last fall and in a month or so the meters should be ready for the open market at about $40 apiece. The Laboratory has contracted for about 20.

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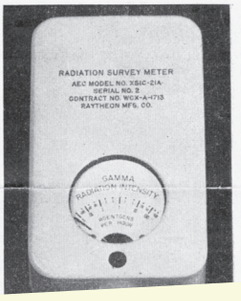

About a half inch longer and half again as thick as an ordinary photographic meter, the pocket instrument, which may also be worn around the neck by a strap, weighs but eight ounces. Actual measurements are 4 1-8 inches long, 2 1-2 inches deep and 1 1-2 inches thick.

The meter scale reads from five milliroentgens to 500 roentgens per hour on the same logarithmic scale

Coordinator Reports Indicate 'All Out' Effort For Success Of Clean-Up Drive

Judging by the enthusiastic tone of early reports rounded up from divisional coordinators by Fire Department Capt. B. M. Beeler, cooperation on an area-wide basis has been assured in making the 1951 Spring Clean-Up Week campaign the most successful hitherto undertaken at the Laboratory. All reports indicate that attention all this week of the clean-up campaign will be devoted to removing fire hazards, cleaning up and rearranging labs and shops for better housekeeping as well as lending particular emphasis to the salvaging of materials for restoration to stockpiles. The latter phase is of

Continued on Page 3

New Appointments

Recent appointments to technical staffs of the Oak Ridge National Laboratory include the following: **David Billen**, to the Biology Division, Ph.D. degree in bacteriology in 1951 from the University of Tennessee, member Society of American Bacteriologists, and American Association for the Advancement of Science; **Tom M. Gayne**, to the Instrument Department, formerly division service manager for Fischer & Porter Co., Hatsboro, Pa., B.S. degree in mechanical engineering in 1946 from the University of Oklahoma, member of American Society of Mechanical Engineers, Institute of Aeronautical Sciences, and Instrument Society of America; **Cleland H. Johnson**, to the Physics Division, Ph.D. degree in physics in 1951 from from the University of Wisconsin, member of American Physical Society; **William McSwain Breazeale**, to the Reactor Technology Division, formerly professor at the Georgia Institute of Technology and associated with ORNL, Ph.D. in physics in 1935 from the University of Virginia; **Byron J. Massey**, to Radioisotope Development, formerly at K-25, B.S. degree in chemical engineering in 1944 from the Georgia Institute of Technology; **Drew Schwartz**, to the Biology Division, formerly research associate at the University of Illinois, Ph.D. degree in biology in 1948 from Columbia University; **William K. Ergen**, to the Physics Division, formerly with NEPA, Ph.D. degree in physics from the University of Vienna (Austria) in 1934, member American Physical Society and American Chemical Society.

New View Points Expressed At 4th Biology Meeting

More than 100 representatives from the United States and Canada—many from Southern universities—and 30 from the University of Tennessee attended the fourth annual Biology Research Conference sponsored jointly by the Biology Division of the Oak Ridge National Laboratory and the Atomic Energy Commission in Oak Ridge April 12-13.

With "Physiological Effects of Radiation at the Cellular Level" as the subject, new views on radiation damage were given and

Proud Of Expanded Glass-Blowing Shop

By R. J. Steere

Those who haven't recently visited the newly remodeled glass-blowing shops should do so. These shops, which come under the supervision of the Research Shop Department, have been undergoing a complete remodeling operation for the

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

- ORNL Biology Division sponsors its fourth annual research conference. Papers were presented on enzymatic functions, metabolism and osmotic relations, mammalian problems, erythrocyte problems and neurophysiology.
- Since the initial shipment of one millicurie of carbon-14 to the Barnard Free Skin and Cancer Hospital in St. Louis on August 2, 1946, ORNL has completed 22,263 shipments of radioactive materials.
- Dr. Alex Zucker spoke at the Oak Ridge Physics Seminar on the "Separation and Bombardment of Neon and Argon."
- P.R. Bell of the Physics Division is credited with a pocket radiation meter that reads on-the-spot radiation, which differs from the current pencil-like minometers and film badges that tell only the total radiation received to date. The meter will be produced commercially by Raytheon Company.
- The ORNL glass-blowing shop has been expanded to twice its former size and now includes a facility for flame operations, as well as additional space for the assembly of special glass apparatuses.
- ORNL has introduced a new method of decontaminating concrete and stainless steel. The Vacu-Blaster machine uses a dry method that removes contamination almost completely.—*prepared by ORNL History Room volunteers*

From the Lab Director

All of us were saddened by the recent events in Japan. The damage to their nuclear facilities, caused by the double natural disasters of a massive earthquake and resulting tsunami, have underscored the importance of factoring extreme scenarios into reactor facility designs. ORNL, by virtue of our historic strengths in nuclear research and new initiatives such as the Consortium for Advanced Simulation of Light Water Reactors innovation hub, is positioned to work with all DOE labs to enhance the safety of nuclear power.

UT-Battelle has joined with the city of Oak Ridge, DOE, and Oak Ridge contractors to assist Naka, Oak Ridge's Japanese Sister City, which was directly affected by the quake. Donations to the Sister City effort may be made at the ORNL Federal Credit Union.

Thom Mason thanks the ORNL partners at the unveiling of the Lab's new solar-assisted charging stations on March 31st. Thom announced that his new red Leaf made it on the boat from Japan before the earthquake, and he will soon be driving his Leaf to the Lab and using one of the stations. The Nissan Leaf in the foreground is connected to a charging station.

I have recently made several trips to Capitol Hill for budget discussions that included a meeting with Secretary Chu and other laboratory directors. ORNL continues to seek ways to reduce costs and apply more resources to the science mission. The departure of 161 valued staff members under our Voluntary Separation Program, including two Leadership Team positions, will save us several million dollars.

Recent activities included participation in the ribbon cutting and celebration of the Oak Ridge Playhouse renovation, which UT-Battelle supported with a $175,000 gift. Here on campus, I hosted a service award breakfast for employees who have worked 30, 35, 40, and 45 years at the Laboratory.

Recent visitors include Tennessee Commissioner of Environment and Conservation Robert Martineau and Assistant to the Governor Mark Cate, who discussed environmental management projects. Congressmen Chuck Fleischmann (Tenn.) and Heath Shuler (N.C.) were guests at our annual Small Business Award Ceremony. Physical Sciences' AD Michelle Buchanan welcomed two distinguished visitors: Professor Victor Ustinov, Deputy Director of the St. Petersburg Ioffe Physical-Technical Institute, and Corresponding Member of the Russian Academy of Sciences Dr. Nikita Gordeev, Group Leader and Advisor to the Director of the Ioffe Institute.

Rep. Chuck Fleischmann, Thom Mason and Rep. Heath Shuler talk at the Small Business Subcontractor Awards breakfast.

Two ORNL research projects were acknowledged by Secretary Chu as examples of how DOE science is answering the energy challenge. The BioEnergy Science Center, including partners at the University of California at Los Angeles, produced isobutanol directly from cellulose through a genetically engineered microbe, a potentially major step toward economically viable production of cellulosic biofuels. He also praised the application of ORNL's supercomputing resources to the development of South Carolina-based BMI Corp.'s Smart Truck UnderTray System, a fuel-saving fairing that may become a common sight on semi trucks.

Finally, congratulations to the Laboratory staff for working five million hours without a day lost to injury.

Thomas Mason

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That's no UFO!

These 1948 gems from Lab archives document meteorological studies under way next to the now-demolished Building 1000. When Union Carbide took over the management of X-10, they launched efforts to understand the environmental system of Bethel Valley, including geological and meteorological surveys.

Studies were conducted across the Lab site to measure wind speeds and directions throughout the year at different altitudes and create a more accurate model of various forms of contaminants. The balloons served dual roles: for sampling and for modeling wind conditions throughout the year.