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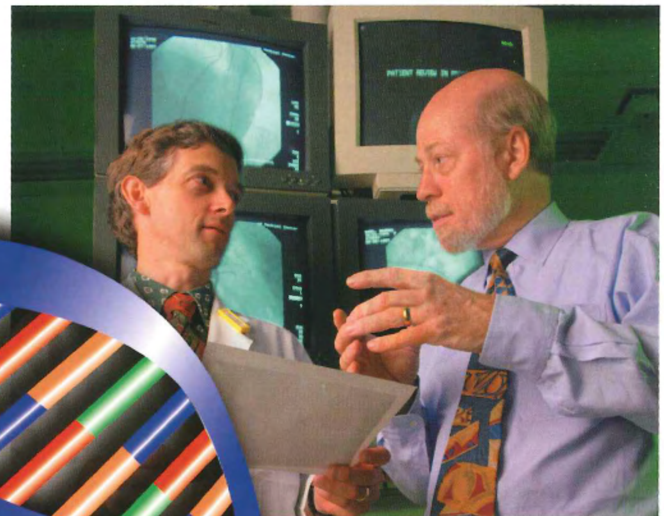
Oak Ridge National Laboratory REVIEW

Vol. 32, No. 2, 1999

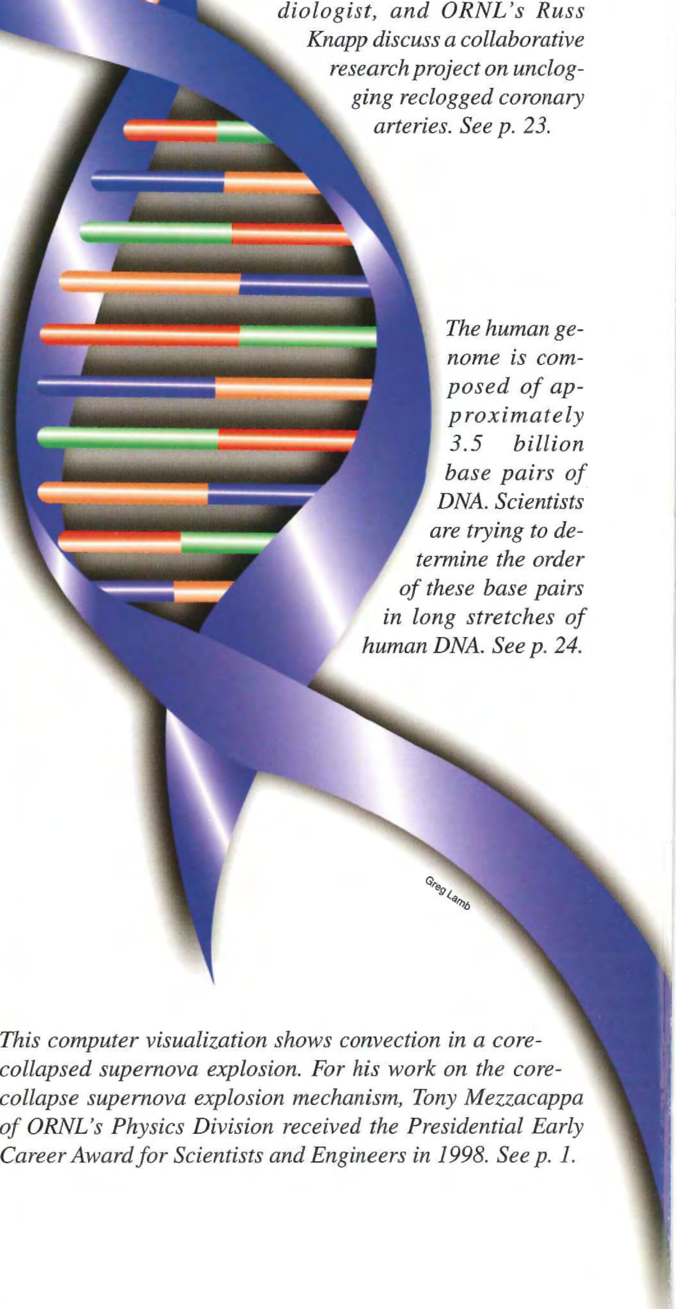
New Light on Exploding Stars...

Also in this Issue... Ways to Reduce Greenhouse Gases

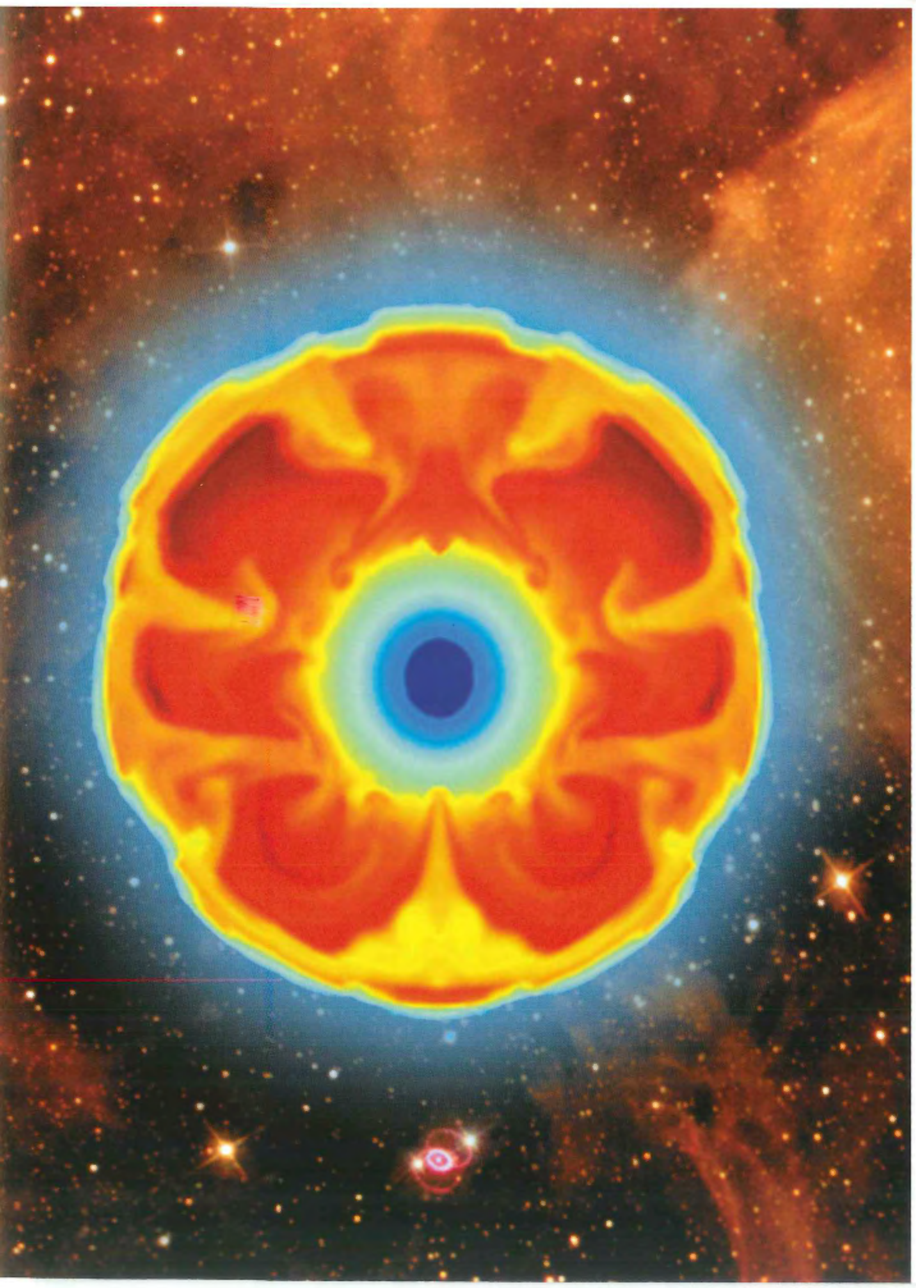
Features



Robert Spencer (left), a Knoxville cardiologist, and ORNL's Russ Knapp discuss a collaborative research project on unclogging reclogged coronary arteries. *See p. 23.*



The human genome is composed of approximately 3.5 billion base pairs of DNA. Scientists are trying to determine the order of these base pairs in long stretches of human DNA. *See p. 24.*



This computer visualization shows convection in a core-collapsed supernova explosion. For his work on the core-collapse supernova explosion mechanism, Tony Mezzacappa of ORNL's Physics Division received the Presidential Early Career Award for Scientists and Engineers in 1998. *See p. 1.*

ORNL Shines in the World's Astrophysics Community

One of the fastest-growing areas in ORNL's Physics Division is the nuclear astrophysics program, which has already become a shining star in the nation's astrophysics community. Five of its members have won major national awards. In 1998 Tony Mezzacappa learned that he had won the Presidential Early Career Award for Scientists and Engineers for his work on the core-collapse supernova explosion mechanism.[1] In 1996, this same award was presented to Michael Smith, who heads the Physics Division's Experimental Nuclear Astrophysics Program. In 1997, the award was won by David Dean of the Physics Division, who spends part of his time working on the nuclear theory aspect of the supernova problem. Earlier in 1998 two other Laboratory astrophysicists, Klaus Guber and Paul Koehler, received the Nova Award from Lockheed Martin Corporation for their outstanding research.

ORNL has become a magnet for outstanding theoretical and experimental astrophysicists for two reasons: The Laboratory has strong computational capabilities, and data of astrophysical significance are being obtained at our Holifield Radioactive Ion Beam Facility (HRIBF) and Oak Ridge Electron Linear Accelerator (ORELA).

Mezzacappa and the computational astrophysicists who work with him are among seven groups worldwide modeling core-collapse supernovas, spectacular stellar explosions that produce and disseminate elements such as carbon, nitrogen, and oxygen, which are responsible for life on the earth (see cover). In addition to Mezzacappa, the ORNL group includes Mike Strayer, head of the Physics Division's Theoretical and Computational Physics Section, part-time staff member and University of Tennessee (UT) professor Mike Guidry, postdoctoral scientist Raphael Hix, and UT graduate student Bronson Messer.

These groups are modeling stars greater than 10 times the mass of the sun to predict whether they will explode like Supernova 1987A. The problem is that the calculations of the various groups do not always agree that a star of a certain size with certain characteristics will explode, so efforts are under way to pin down the remaining details of the mechanism. A core-collapse supernova explosion is thought to be caused by a shock wave that results when the star's hot iron core shrinks, compressing its subatomic particles to the point where they repel each other and force the core to rebound.

Astrophysicists believe that the shock wave stalls while trying to propagate from the stellar core through the outer layers of the star and that the shock wave is reenergized by neutrino heating. Neutrinos are particles with no charge and infinitesimally small mass that interact very weakly with matter. Neutrinos of all "flavors," or types, emerge from the proto-neutron star that forms at the center of the explosion.

Mezzacappa says that this central object is like a neutrino "light bulb" radiating heat at the staggering rate of 10^{45} watts. It is believed, in fact, that these neutrinos power the supernova explosion. Current multidimensional supernova modeling has also uncovered the potential role played by convection—transfer of heat by the circulation of the core's proton-neutron fluid—in aiding this shock revival process.

The ORNL supernova effort leads the field of neutrino transport modeling in both one-dimensional and multidimensional supernova simulations. The most recent ORNL work has underscored the need for more realistic multidimensional simulations of neutrino transport using massively parallel computers.

The ORNL Physics Division also carries out a vigorous program of experimental research in nuclear astrophysics at the HRIBF and ORELA. Part of this work is described in this issue in the next article, "Facilitating Science: ORNL Research at User Facilities."

Al Trivelpiece

Al Trivelpiece
Director of Oak Ridge National Laboratory

[1] The other ORNL winner of this award for 1998 was James Lee of ORNL's Chemical Technology Division. He was cited for his "seminal contributions to photosynthesis research and its application to nanofabrication."

REVIEW

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Oak Ridge National Laboratory is a multiprogram, multipurpose laboratory that conducts research in energy production and end-use technologies; biological and environmental science and technology; advanced materials synthesis, processing, and characterization; and the physical sciences, including neutron-based science and technology.

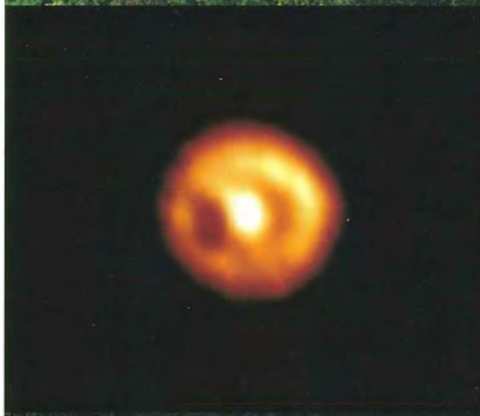
Facilitating Science:

ORNL Research at User Facilities

ORNL researchers are probing the nature of matter at DOE's scientific user facilities.

The Department of Energy's scientific user facilities are national treasures. They provide a gathering place for world-renowned scientists and engineers, and they house unique resources and state-of-the-art equipment for research. Without these large facilities, researchers throughout the world would be denied access to precious information about a material's smallest features.

ORNL researchers use protons, photons, neutrons, electrons, and ions to probe the nature of matter and recreate conditions that may at one time have existed in the universe. Among the sources of these probes are cyclotrons, electrostatic accelerators, reactors, synchrotrons, and now electron microscopes that can be controlled remotely over the Internet. In addition to facilities at ORNL, DOE facilities used by ORNL scientists include those at Argonne and Brookhaven national laboratories. DOE has also funded international experiments involving ORNL scientists at the European Laboratory for Particle Physics (CERN) near Geneva, Switzerland, and Oak Ridge researchers are involved in DOE's five-laboratory effort to design and build the Spallation Neutron Source user facility at ORNL (see sidebar on p. 7).

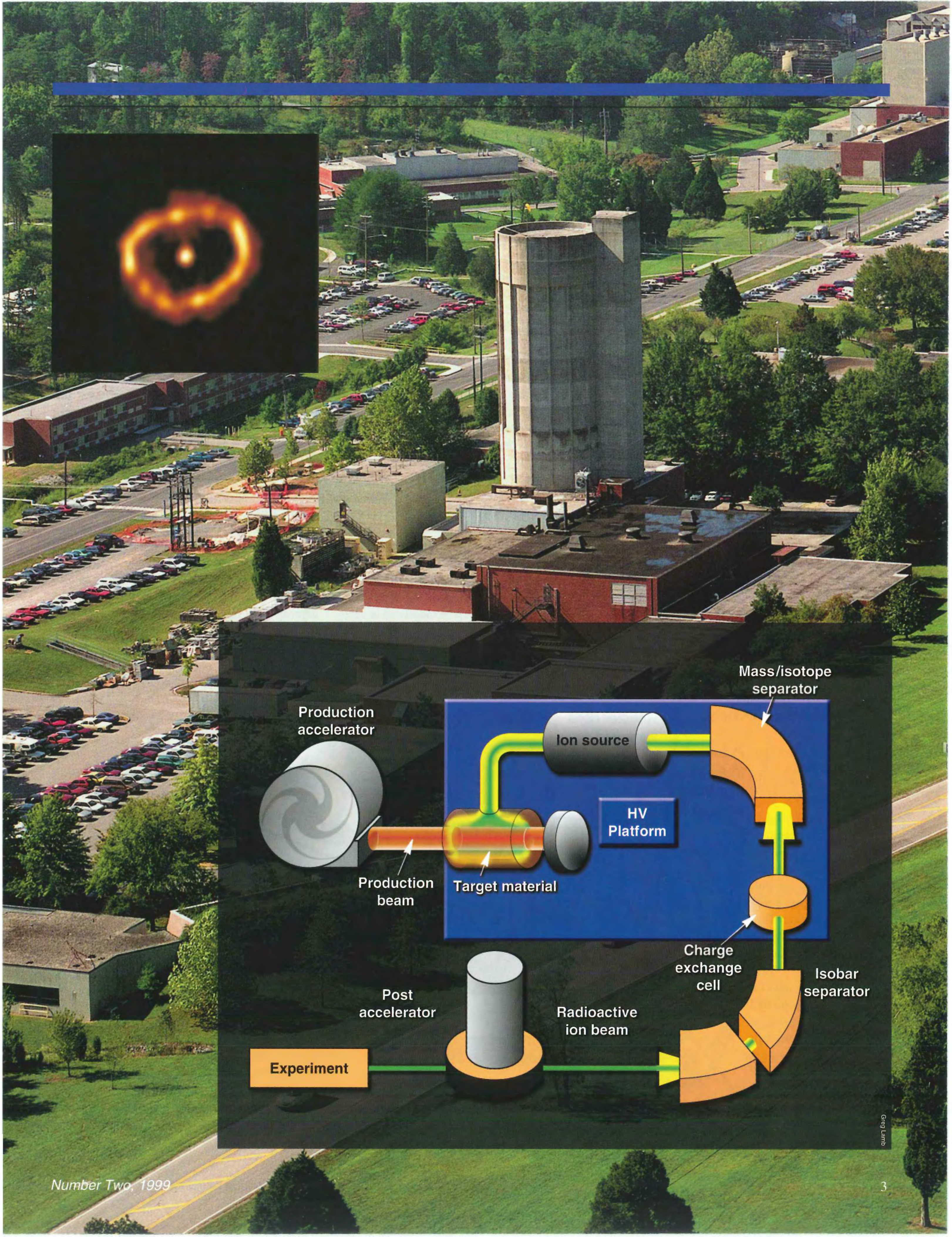


This Hubble Space Telescope image of Nova Cygni 1992 was taken about three-and-a-half years after this exploding new star was discovered in February 1992. The atomic spectra of the ring of debris surrounding such stars indicate that novae are sources for the synthesis of heavy elements. The nuclear state discovered in ORNL experiments using beams of radioactive fluorine-17 is crucial for determining the rate at which nuclear reactions that power such stellar explosions occur.

Nuclear Astrophysics: The Impossible Beam

The founders of radioactive ion beam physics said it couldn't be done, but ORNL proved it could. Conventional wisdom held that a beam of radioactive fluorine ions (fluorine-17) that would be sufficiently intense for research could not be formed because fluorine is too reactive. But, in 1998, beams of short-lived fluorine-17 were generated, accelerated, and used for research at ORNL's Holifield Radioactive Ion Beam Facility (HRIBF), a DOE user facility dedicated to the production of beams of short-lived radioactive nuclei that do not exist naturally on the earth. The experiment paves the way for nuclear astrophysics studies of how elements heavier than oxygen were formed in exploding celestial bodies by proton collisions with radioactive nuclei like fluorine-17, found only in the debris of stellar explosions.

The experiment—which served as the Ph.D. thesis work for Dan Bardayan, a doctoral student from Yale University—was led by Michael S. Smith, group leader for astrophysics research in the Physics Division. Smith established a program at ORNL to use radioactive ion beams from the HRIBF to measure reaction rates critical to our understanding of the production of the heavy elements in stellar explosions such as novae.


Mass/isotope separator
Production accelerator
Ion source
HV Platform
Production beam
Target material
Charge exchange cell
Isobar separator
Post accelerator
Radioactive ion beam
Experiment
Greg Lamb

"Michael Smith and the large group of outside and in-house collaborators he organized have developed the unique experimental apparatus needed to carry out the experiments," says Fred Bertrand, director of the Physics Division. "The development of the very difficult-to-produce fluorine-17 beam was made a top priority of the scientists and engineers working at the Holifield facility. Their success has allowed the work of Smith and collaborators to proceed."

The half-life of fluorine-17 is only 64 seconds, so the HRIBF operations staff had to devise a clever way to produce, extract, and prepare a beam of negative ions for acceleration before running out of material. This was complicated because fluorine is one of the most reactive of all the elements.

The beam of radioactive fluorine-17 was formed by a series of events, beginning with a beam of deuterons that was accelerated using the Oak Ridge Isochronous Cyclotron at HRIBF. A deuteron consists of one proton and one neutron.

After experiments with different targets, ORNL scientists learned to produce a beam of fluorine-17 ions of acceptable intensity by slamming the deuterons into a target of hafnium oxide, a material that functions at higher temperatures than any material tried previously. The deuterons transmute the oxygen-16 atoms in the target to fluorine-17 atoms. Aluminum vapor from an oven is then pumped through fibers of the thumb-size target. At a high temperature the vapor reacts with the fluorine-17 formed in the target and makes aluminum fluoride. This gas diffuses quickly out of the target and into a positive ion source, and the extracted beam is then passed through a chamber containing vapors of cesium, whose atoms' loosely bound electrons are easily snatched by fluorine ions. The positively charged aluminum fluoride is turned into negatively charged fluorine-17 ions that, after being selected by a magnetic field, can be accelerated in the HRIBF's 25-megavolt tandem electrostatic accelerator for use in the experiment.

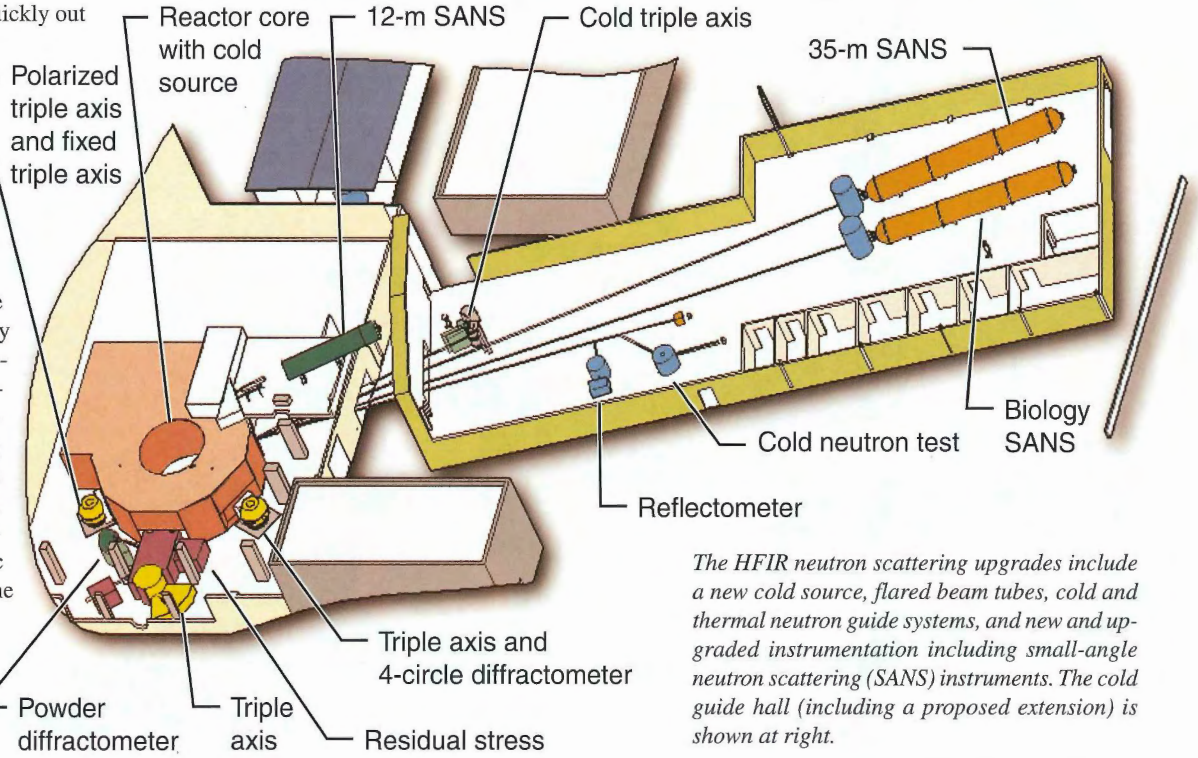
Once the "impossible" beam of fluorine ions was produced, it was accelerated by the tandem accelerator and directed at a target of polypropylene, which consists of carbon and hydrogen atoms. The scientists measured the number and energies of fluorine-17 ions that scattered from the hydrogen in the target at different angles. When they studied the neon-18 nuclei produced when fluorine-17 fused with hydrogen, they found a new quantum state, which is at the correct energy—and possibly has the correct properties—to significantly enhance the rate at which fluorine-17 fuses with hydrogen in a hot stellar environment. "Such an enhancement," Smith says, "may have significant implications for the particular isotopes that are synthesized in a stellar explosion and ejected into space, as well as for the rate at which energy is prodigiously generated in the explosion."

An additional experiment is needed to determine if the properties of this new nuclear state in neon-18 will enhance the fusion rate of the fluorine-17 and hydrogen. In this experiment, a fluorine-17 beam from the HRIBF will be directed onto a polypropylene target at the proper energy to form the neon-18 nucleus in this special quantum state, and a sophisticated research device—the Daresbury Recoil Separator—will be used to count the number of such nuclei formed. In this way, the nuclear reaction that helps power the stellar explosion will be measured in a laboratory here on the earth.

HRIBF's electrostatic accelerator enclosed in its landmark tower will provide the energy needed to overcome the natural repulsion between the positively charged fluorine-17 and hydrogen nuclei, allowing the "stellar reaction" to occur. In a star the fusion of these nuclei is made possible by the extreme heat produced in the stellar explosion. The number of the outgoing neon-18 nuclei detected in the experiment will indicate the rate at which this reaction occurs in space. Such nuclear reactions occurring in stellar explosions synthesize the heavier elements that are then dispersed into space, including those that make life on the earth possible.

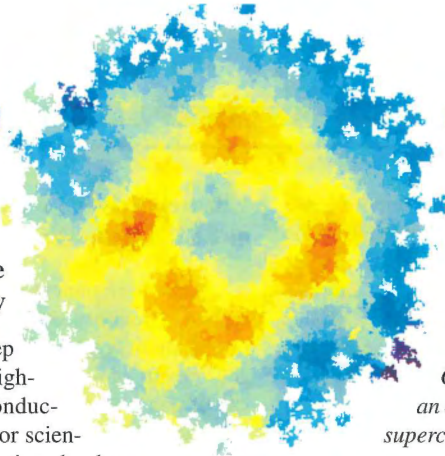
Neutron Scattering Upgrades for HFIR

When the planned neutron scattering upgrades are completed, ORNL's High Flux Isotope Reactor (HFIR) will exploit the world's highest thermal neutron intensities, and it will provide cold neutron intensities comparable to the world's best (and significantly higher than those currently available in the United States). ORNL will then have 14 of the most competitive steady-state neutron scattering instruments anywhere. Currently, two buildings are being constructed at HFIR to house the cold-source refrigeration equipment and the cold neutron guides and instruments. The ORNL team leading the neutron scattering upgrades includes Jim Roberto, Herb Mook, Colin West, Doug Selby, and Mike Farrar. The upgrades will be implemented in FY 2001 after completion of the scheduled HFIR outage to replace the beryllium reflector.



The HFIR neutron scattering upgrades include a new cold source, flared beam tubes, cold and thermal neutron guide systems, and new and upgraded instrumentation including small-angle neutron scattering (SANS) instruments. The cold guide hall (including a proposed extension) is shown at right.

Progress in Explaining High-temperature Superconductivity



Images of the magnetic excitations near the (1/2, 1/2) reciprocal lattice position in the high-temperature superconducting material yttrium-barium-copper oxide ($YBa_2Cu_3O_{6.6}$), where T_c = 62.7K, for an energy transfer of 24 MeV in the superconducting state.

An important step toward explaining high-temperature superconductivity, one of the major scientific challenges of our time, has been taken as a result of the neutron scattering research performed by ORNL scientists at HFIR and the ISIS spallation source in the United Kingdom. The work demonstrated similar magnetic behavior in two principal families of high-temperature superconductors, suggesting that a single mechanism is responsible for high-temperature superconductivity.

The new result obtained by Herb Mook and Pengcheng Dai, both of the Solid State Division, corrects previous misconceptions about disparate behavior of magnetic fluctuations in the different families and greatly simplifies the theoretical quest to explain high-temperature superconductivity. The research was published in 1998 in *Nature* and *Physical Review Letters*.

Polymer Alloys: Plastics of the Future

Developing completely new polymers to meet U.S. needs for plastic products has become an expensive business. Over the past 50 years industrial companies have spent billions of dollars inventing today's polymers, so they are naturally reluctant to invest billions more inventing new ones that must compete with existing materials produced in large volumes at competitive prices using current technologies. Thus, researchers have begun blending known polymers to obtain "polymer alloys" that possess new, desired properties. Currently, a time-consuming trial-and-error process is used to find compatible polymers and predict the properties of the resulting polymer alloys. However, a more direct approach may be possible, thanks to an integrated research effort that combines new theories of polymer mixing with experimental findings about polymers obtained using scattering methods.

Neutron scattering experiments at HFIR reveal the structure of various polymer alloys and the ability of different polymers to mix with each other to form alloys with desired properties. These experiments are being performed by Brian Annis and Tony Habenschuss, both of ORNL's Chemical and Analytical Sciences Division (CASD), and George Wignall of ORNL's Solid State Division, in collaboration with researchers at Sandia National Laboratories, the University of Illinois-Urbana, and the University of Minnesota.

"The refined understanding that we gained should lead to a cost-effective, efficient engineering approach to polymer blending that is guided by sound scientific principles," Wignall says. "The long-term result for consumers may be higher-quality but lower-cost plastic products."

Tony Habenschuss (left), George Wignall, postdoctoral researcher Man-Ho Kim, and Brian Annis examine a cell near a polymer alloy target at the Small-Angle Neutron Scattering facility at HFIR.

Curtis Boles

X-ray Microbeams Commissioned at Advanced Photon Source

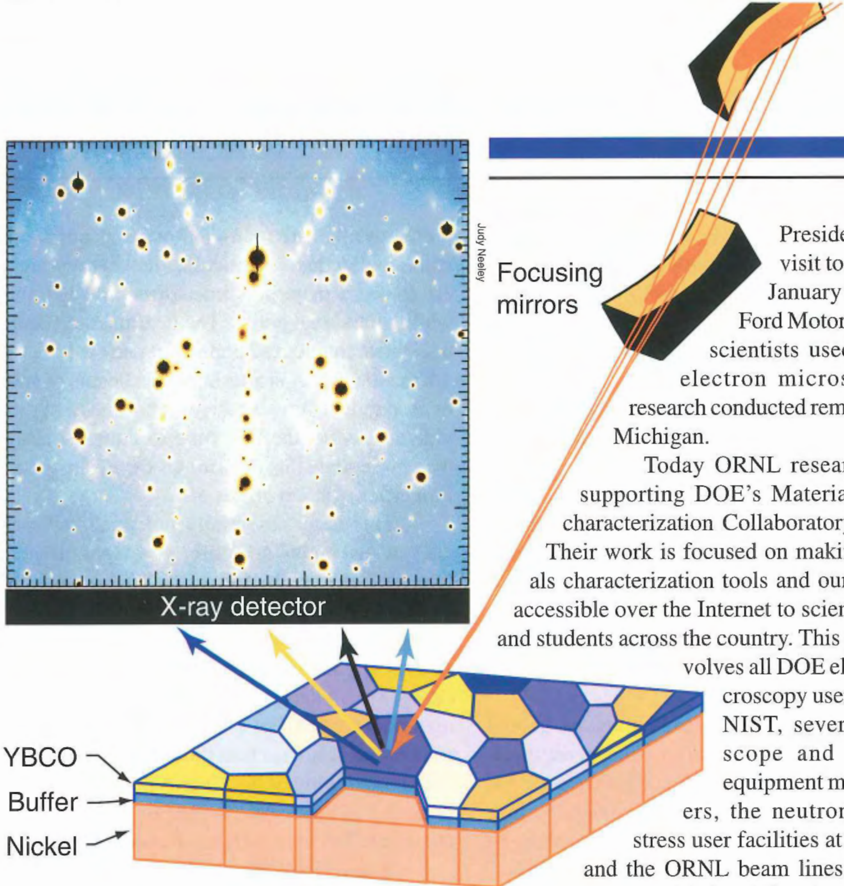
Materials ranging from massive steel girders to the microscopic aluminum wires in computer chips are made of grains—tiny crystals with diameters measured in millionths of a meter (microns). If scientists could "see" these individual grains, they could determine their orientation, as well as the effects of stress and chemical activity on them. They might also be able to determine how best to jam more circuits together in microelectronic components, making them smaller and faster, so computers can perform complex functions—such as speech recognition—more quickly. They could also find out to what extent grains of a superconducting material mimic the alignment of the substrate on which the material is grown; discovery of such orientation replication involving deposited thin films is essential to the design of effective high-temperature superconductors.

Scientists are now able to study the fine details of grain behavior in materials, thanks to new X-ray beam lines at the Advanced Photon Source (APS), an intense synchrotron X-ray source at DOE's Argonne National Laboratory. ORNL is a leader in efforts to develop microbeams at the APS. Microbeams are X rays that are focused down to beam diameters smaller than one micron, allowing researchers to see a material's microstructural features within individual grains. The instrumented beam lines now enable researchers to perform microdiffraction, X-ray scattering using beams of submicron dimensions. These microbeams will provide access for the first time to the mesoscale, the length scale that determines the macroscopic properties of many materials.

"This is an essentially untapped research area of enormous scientific and technological interest," says Gene Ice of the Metals and Ceramics Division. "Understanding mesoscale dynamics will revolutionize our understanding of several key materials problems for the next decade—stress-driven grain growth, aging, and materials failure. For example, important materials properties—such as the brittle fracture that led to the sinking of the *Titanic* and the magnetic response allowing VCR tapes to be watched—are controlled by mesoscale features."

Ice and Solid State's Ben Larson are leading ORNL's efforts to develop these new microbeam capabilities. Other ORNL scientists, including John Budai, Jon Tischler, Eliot Specht, Jin-Seok Chung, Nobumichi Tamura, and Mirang Yoon, have performed experiments using microbeam analysis with a resolution of <1 μm. They are studying strain in integrated circuit wires, a major source of electrical problems in developing smaller, denser microelectronic components for the next generation of computers. They are also studying the epitaxy of oxide films on nickel foils and the defects introduced by ion-implantation processing in silicon to help them understand and improve properties of materials.

The initial design, microbeam optics, and associated techniques for materials analysis are being developed by ORNL and Howard University at the APS on the MHATT-CAT beam line constructed by the University of Michigan, Howard University (a historically black university), and Lucent Technologies Collaborative Access Team. To exploit microbeam capabilities fully, ORNL is developing a dedicated microbeam facility directed toward 0.1 μm resolution on the recently commissioned UNICAT synchrotron beam line. (UNICAT stands for University National Laboratory Industry Collaborative Access Team.) UNICAT is a $10-million beam line collaboration involving ORNL, the University of Illinois, the National Institute of Standards and Technology (NIST), and UOP Research Inc. UNICAT provides access to the nation's most intense X-ray beams for a wide range of studies of the structure and properties of materials. ORNL has received funding through the new-initiative competition of the Division of Materials Science in DOE's Office of Basic Energy



Schematic drawing of an X-ray microbeam experiment. Curved mirrors focus the synchrotron X rays down to a diameter of less than one micron on the sample. The microbeam penetrates each layer of the sample, and an area detector measures the directions of the scattered X rays. Here, the sample consists of a roll-textured nickel substrate covered with two epitaxial films: a buffer layer and a superconductor (YBCO). The detector image provides a grain-by-grain description of the atomic structure, orientation, and strain of each layer.

Sciences to develop a mesoscale materials program at the APS using microbeams. It's a big project, and the reward will be insights into structures of materials that are very small.

Materials Microcharacterization Collaboratory: ORNL's Role

Can scientific research at DOE national laboratories be made friendlier and more accessible? Can science students in college classrooms watch the progress of a national laboratory experiment? Can a scientist working at home run an experiment at a DOE facility? The answer is yes, thanks to the Internet.

Several years ago, students at Lehigh University remotely operated an electron microscope at ORNL. By tapping on a computer keyboard, they moved the subject specimen and changed the microscope's focus and image magnification. They studied the various images on the monitor screen. Using teleconferencing tools, they had live video and audio contact with their ORNL collaborator.

Remote operation of the electron microscopes has been successfully demonstrated in a number of other venues (e.g., for Vice President Gore's visit to ORNL on January 21, 1998). Ford Motor Company scientists used ORNL's electron microscopes in research conducted remotely from Michigan.

Today ORNL researchers are supporting DOE's Materials Microcharacterization Collaboratory (MMC). Their work is focused on making materials characterization tools and our expertise accessible over the Internet to scientific users and students across the country. This project involves all DOE electron microscopy user facilities, NIST, several microscope and ancillary equipment manufacturers, the neutron residual stress user facilities at the HFIR, and the ORNL beam lines at DOE's National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory (BNL). The goal of the multipartner collaboration is to promote the development of common technologies for the remote operation of research equipment.

Remote operation of scattering instruments for experiments at HFIR and the NSLS is under way. Lessons learned from these operations should affect plans for enabling researchers to remotely operate neutron scattering instruments at DOE's proposed Spallation Neutron Source, which may be ready for experiments in 2006.

Participants in the research at ORNL are Michael Wright of the Instrumentation and Controls Division; Edgar Voelkl, Ed Kenik, Cam Hubbard, and Larry Allard, all of the M&C Division; and Jim Rome of the Computing, Information and Networking Division. The MMC is jointly funded by DOE's Mathematical, Information and Computational Sciences Division and the Division of Materials Sciences, both in DOE's Office of Science, and the Office of Heavy Vehicle Technologies in DOE's Office of Energy Efficiency and Renewable Energy.

For DOE, one of the appeals of remote access to and remote operation of research facilities is the reduced need for travel and energy for transportation. Instead of traveling to the scientific user facility, the facility can be brought to the home or office through the Internet. It is hoped that more and more researchers will be doing science from a distance.

Ultrarelativistic Collision Results at CERN Bode Well for DOE Collider

Like two remotely controlled cars careening around a circular racetrack in opposite directions, two beams of gold ions will smash into each other at a velocity of over 99% the speed of light. The site of this subatomic "demolition derby" is the Relativistic Heavy Ion Collider (RHIC), now being completed and tested at BNL.

The trick is to magnetically confine those positively charged ions traveling at ultrarelativistic velocities to the appropriate orbit for a long enough "storage time" to make use of the machine for experiments economical. If some ions in one beam collide with each other and change their nuclear mass or if some lose or gain an electron and change their charge, they may be lost from the orbit at too great a rate for supercollider operations to continue effectively.

Recent atomic physics data obtained through an international collaboration at the Super Proton Synchrotron at the European Laboratory for Particle Physics (CERN) near Geneva, Switzerland, suggest that it is feasible for BNL to attain hoped-for storage times at RHIC. Key contributors to this collaboration were Sheldon Datz, Herb Krause, and Randy Vane, all of ORNL's Atomic and Molecular Physics Section in the Physics Division.

In the CERN experiments, solid and gaseous targets were bombarded with an ultrarelativistic beam of "bare" lead ions that were completely stripped of their electrons before being accelerated at 33 trillion electron volts. The solid targets used were gold, copper, tin, aluminum, carbon, and beryllium films of different thicknesses. In some experiments using a thin gold target, up to 0.1% of the bare lead ions in the projectile beam each picked up an electron, changing their positive charge from 82+ to 81+.

The explanation? When a lead projectile ion comes close to a target nucleus, the electromagnetic field of the two nuclei is so strong that a virtual photon arises, generating at least one electron-positron pair. Because the lead ion has a strong positive charge, the pair's negatively charged electron may be captured into the lead electron shell and its positively charged mate, the positron, repelled. The probability of electron capture was determined by measuring the fraction of lead ions emerging from the target that changed their charge.

The researchers also participated in experiments that revealed the results of nuclear collisions between bare ions traveling at ultrarelativistic energies in the same beam. Normally, nuclei of like charge repel each other, but at these high energies, they get close enough together to allow exchanges of protons and neutrons that can alter some ions' nuclear mass.

In other experiments, many of the accelerated bare ions captured single electrons as they traveled through air to the beam tube leading to the target. The researchers found that the probability that a one-electron lead ion projectile would lose its electron in collisions with target atoms is lower at ultrarelativistic energies than once believed. As a result of these measurements, a Danish theorist has proposed a new theory that explains observed experimental results and predicts the outcome of new experiments.

In their 1998 experiments with targets of noble gases (argon, krypton, xenon) at various pressures (which mimic different thicknesses for solid targets), the ORNL physicists and their colleagues were surprised to find that the probability that the projectile ion would lose an electron was lower for collisions in gases than solids. It had been thought that the probability was the same for both types of matter. The physicists determined this probability by measuring the fraction of projectile ions that pass through the target with their single electrons intact. They found the probability for capturing an electron in dilute gas targets is lower than expected.

The small probabilities observed suggest that beam orbit losses at RHIC should be acceptably low. The ORNL researchers' atomic collision findings should also be of value to collider operations at CERN, which is building the Large Hadron Collider for international experiments.

Electronics for Nuclear Physics Detectors

Physicists have long desired to understand the environment that may have existed moments after the Big Bang. International experiments involving ORNL and other researchers were performed between 1992 and 1997 at CERN to gain this understanding. Physicists sought to verify the theory that, within the first 10 microseconds of the Big Bang, quarks existed in the free state, called the quark-gluon plasma. After that brief time, as the universe cooled, it is thought that the free quarks formed the protons and neutrons that 300,000 years later became the atomic nuclei of our universe.

Courtesy of Brookhaven National Laboratory

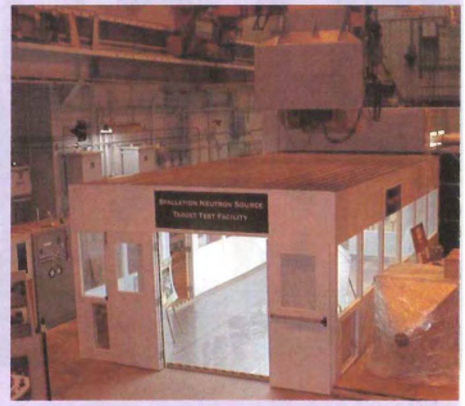
ORNL researchers are developing electronic components for the PHENIX detector, shown here under construction.

To do these experiments, special detectors were needed. A group led by Chuck Britton in ORNL's I&C Division supported the Physics Division group led by Frank Plasil and Glenn Young by developing detector electronics. The experiments produced questions as well as answers. Physicists still don't know exactly what happened during the first few moments of the early universe, and they are still wondering how the proton gets its spin. Now, ORNL physicists and their colleagues plan to bombard heavier ions together at almost the velocity of light to simulate more closely a quark-gluon plasma so they can find answers they couldn't get at CERN. The place to do that is RHIC. There the PHENIX detector is being built to collect particles spraying out from RHIC's high-energy collisions and measure their energies to answer the physicists' fundamental questions.

Data from all particle collisions at RHIC will enter some 350,000 detection channels in PHENIX. Some data will be more important to physicists than other data. ORNL researchers are developing the special electronics needed to sort through the data and select only the meaningful information the physicists want to see from every one of PHENIX's channels. Tune in next century for an update.

Target Test Facility: Replica of the SNS Mercury Target

To produce neutrons for scientific experiments, the proposed Spallation Neutron Source (SNS) must convert negative hydrogen ions into protons and slam them against a liquid metal target to knock loose (spall) and boil out the neutrons. That's how the largest neutron yield in the world will be produced for international research teams by 2006 at the SNS user facility at ORNL.



The technical components for the SNS project are being designed and will be built in Oak Ridge as a collaborative project among five DOE national laboratories—Argonne, Brookhaven, Lawrence Berkeley, Los Alamos, and ORNL. The facility will include an ion source, a linear accelerator to speed up the ions, a device to accelerate protons, a liquid-mercury target for the protons, and beam lines to carry neutrons produced in the target to experimental samples for measurements by scientific instruments.

The mercury target is being designed at ORNL under the leadership of Tony Gabriel. The SNS will be the first scientific facility to use pure mercury as a target for a proton beam. Research is being conducted at ORNL to determine which candidate materials for the target container are most compatible with mercury and how to design the target to shield workers from its radioactivity and to maximize the output of neutrons for research.

Because the SNS will be a DOE user facility, it must be available for experiments as often as possible. If a component in the mercury target wears out or fails, the component should be replaced rapidly to avoid a long shutdown. An ORNL team is developing methods to meet this need. The methods combine appropriate target-design features, remote-handling equipment, unique tools and fixtures, and operator training. To enable researchers to develop tools and procedures for the remote replacement of target system components, a full-scale replica of the SNS mercury target system called the Target Test Facility (TTF) is being assembled and installed at Building 7603 in the Robotics and Process Systems Division.

In 1998, the TTF components were purchased, and a contract was placed for fabrication and acceptance testing of the mercury system. An enclosure structure was built to contain the mercury system and protect operations personnel, and environmental, safety, and health issues of large-scale mercury handling were addressed.

The TTF will contain numerous sensors to measure the flow of mercury and variations in its temperature throughout the target module. These thermal-hydraulic measurements are needed to predict the locations of hot spots that must be eliminated to prevent overheating of either the mercury or its containment materials. The measurements will be compared with predictions of computer codes to help improve the codes.

The expected safe operation of this first, large-scale experimental system for handling mercury in the way envisioned for the SNS should increase the public's confidence that ORNL can safely manage large quantities of mercury at the SNS.

Driving the Transportation Revolution

ORNL is developing and evaluating technologies for producing highly energy-efficient, low-emission vehicles and for reducing traffic congestion.

Early next century, you buy your next car, a near-zero-emissions vehicle. The body of your car is made of a lightweight carbon-fiber composite, not heavy steel. It gets 70 miles per gallon, thanks to a hybrid-electric engine powered by diesel fuel combined with electricity from a battery or fuel cell. You are thrilled with your new car's awesome computing power and the information and control technologies that guide you around heavy traffic and help you avoid accidents. You watch the road ahead while looking through the head-up display (HUD), a virtual dashboard projected on the bottom of the windshield that stays in your peripheral vision. Clicking on the steering wheel control panel, you turn the HUD's speed and gas level readings into a color-coded map that shows you the fastest route to a new restaurant. That evening after dinner, you transform the HUD into a "night vision" thermal-imaging display so that the scenes on the way home look amazingly clear.

The internal-combustion automobile, called "the product of the century" by *Time* magazine, has driven the U.S. economy. Mass-produced, affordable cars, pioneered by Henry Ford, created the middle class. Cars and trucks spurred the growth of cities and suburbs and generally improved our quality of life. The automobile industry is having an important economic impact in Tennessee, which ranks fourth in the nation in automotive manufacturing.

Lean, Clean Cars Needed

Although clearly the automotive industry contributed greatly to an improved quality of life for many in this century, 20th-century vehicles may actually threaten our quality of life in the 21st century. Because of the travel boom, we face unwelcome increases in traffic congestion, dependence on foreign oil, fuel consumption, and emissions of pollutants (despite improvements in fuel economy). These rising emissions may threaten the health of both people and the environment. Additionally, the 26% of U.S. greenhouse gases emitted to the atmosphere as a result of transportation-related activities could ultimately influence the global climate's stability.

To help address these problems, the Department of Energy is sponsoring research for the U.S. Partnership for a New Generation of Vehicles (PNGV), whose chief goal is more-energy-efficient, emission-free transportation vehicles. With funding from DOE and other agencies, ORNL is playing a role in developing safe vehicles that will emit virtually no pollutants and that will travel three times as far as today's cars, buses, and trucks, using the same amount of fuel. These "smart" vehicles will offer advanced information technologies to make driving safer and more efficient. Below is a sampling of ORNL's research related to new information, materials, propulsion, and emissions-control technologies that may advance the transportation revolution.

These technologies will be further developed at the National Transportation Research Center (NTRC), a collaborative effort among DOE, ORNL, the University of Tennessee, and The Development Corporation of Knox County. The official groundbreaking for the NTRC building, to be completed by 2000 in the Pellissippi Corporate Center in Knox County, took place April 8, 1999. The center, whose director is ORNL's Bob Honea, will take advantage of local transportation research expertise to solve complex national problems and to attract transportation-related firms to the region.


Curtis Boles

Ron Harris, technician in ORNL's Instrumentation and Controls Division, has installed cameras, sensors, computers, and other equipment in this Dodge Intrepid, which is serving as the DOE Driver Research Vehicle.

Testing Driver Response to Information Systems

Drivers of future cars may be deluged with information from "intelligent transportation systems" (ITS). For example, they may see HUD displays of maps and verbal messages and hear computer voices telling them how to get around traffic to reach a destination faster or how to avoid a collision in time.

In 1999, ORNL is seeking to determine how 40 drivers respond to such automobile-based information technologies, using a DOE research vehicle and a driving simulator. The research vehicle, a 1999 Dodge Intrepid, has been outfitted with sensors, instruments, and computers integrated and installed by Ron Harris of ORNL's Instrumentation and Controls (I&C) Division. The reactions of the drivers will be studied by human-factors expert Dan Tufano of ORNL's Computer Science and Mathematics Division (CSMD). The research is supported by ORNL's Laboratory Directed Research and Development Program. "New information delivery systems are designed to make it easier for the driver to navigate through traffic to a final destination and to operate the car more safely to avoid accidents," Tufano says. "Ironically, some information systems may distract and startle drivers, making driving less safe. To evaluate the effectiveness and safety of these systems, we will be collecting data on the responses of drivers in various highway situations, using both the research vehicle and a driving simulator."


Curtis Boles

Here, Ron Harris connects the device controlling the lane tracker system with a computer.

Drivers of the research vehicle will wear physiological monitors linked wirelessly to the car's data acquisition system. The monitors will measure the driver's heartbeat rate, skin conductivity, and muscle tension, all of which signal the extent of a person's nervous reaction.

Wheel, steering wheel, and global positioning system sensors will indicate the speed, direction, and location of the vehicle on the road at any given time. Six miniature video cameras will allow the researchers to see the driver's hands and face and the forward and rear roadway scenes. An integrated data acquisition and storage system in the car's trunk will collect the vehicle, roadway, driver, and warning system data and "time stamp" it. Thus, the researchers will have information on events occurring inside and outside the car at any one point in time.

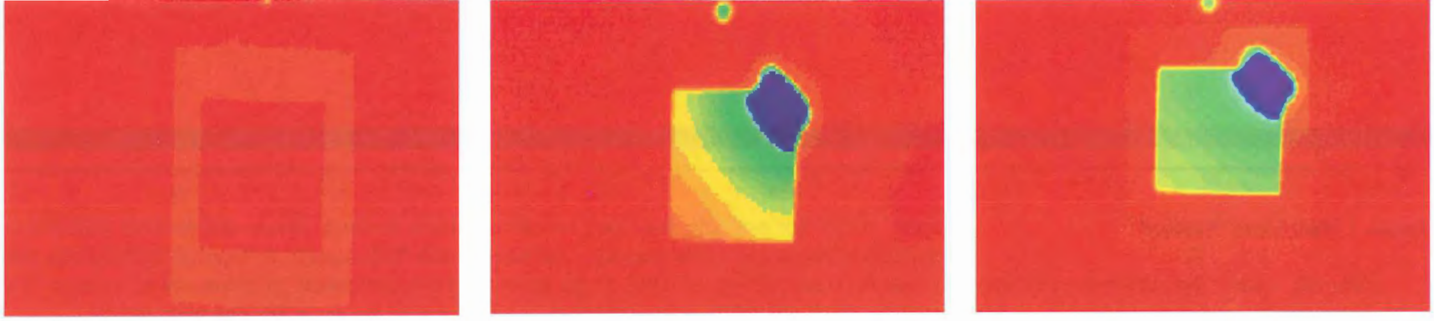
The test car has a radar headway collision warning system and adaptive cruise control, a left blind spot collision warning system, and a video-based lane tracker and roadway departure warning system. These systems collect data and, through beeping tones and flashing lights, warn the driver of an imminent collision that can be avoided by a quick response. They also can be hooked up to the car's throttle so they can automatically adjust the accelerator to help the driver avoid an accident.

The vehicle will also be equipped with an ITS data bus, a computer network that handles information from the engine, vehicle, navigation and collision avoidance warning systems, and communications devices, such as a cell phone or pager. A filter made possible by the bus prioritizes messages so that the driver receives the most urgently needed information first. For example, messages needed to help you avoid an accident and remind you to take the next exit precede the message about the cancellation of tomorrow's staff meeting.

Night Vision Seen for Drivers

ORNL researchers are working on technologies to help people see more clearly in the dark. Panos Datskos and Slo Rajic, both of the Engineering Technology Division (ETD), have developed the world's first uncooled infrared photon detector, which could help improve the vision of people driving at night. The researchers have solved the problem of detecting photons of infrared light by measuring the mechanical stresses these photons induce in the microstructure of semiconducting material. A micromechanical quantum detector bends in proportion to the stresses, and the amount of bending indicates the presence and intensity of the light.

Today's infrared photon devices must be chilled by liquid nitrogen, but the ORNL invention does not require cooling to cryogenic temperatures. Because the new device will not require cooling equipment, it will cost less, weigh less, and use less electricity than today's infrared photon detectors. The uncooled photon detector offers the sensitivity and speed of cooled infrared photon detectors but not the associated increase in cost, size, and complexity.



Infrared images of ice melting on carbon foam (Grafoam) developed at ORNL as a result of a discovery by James Klett.

Advanced Materials for Cars and Trucks

The next wave in carmaking? Steel is strong but it's also heavy. A car will go farther on less fuel if built using materials lighter than steel. Replacing steel body and chassis components with components made of the same carbon-fiber composite used in aircraft is expected to reduce vehicle weight by as much as 60%, significantly increasing vehicle fuel economy. Currently, production of carbon fibers is too expensive and slow for them to be used widely to replace steel as the primary material used in new cars and trucks. The problem: the high cost of the carbon-bearing starting material (precursor), the energy needed to heat it to make fibers, and the large ovens and other capital equipment used in its manufacture. Today pitch, or polyacrylonitrile (PAN) precursor, is converted to carbon fibers by thermal pyrolysis, a slow, energy-consuming process, combined with stressing to achieve the right properties.

In research for PNGV, Felix Paulauskas of ETD is working with industrial collaborators (AKZO, Amoco, Hexcel, Zoltek) to use microwave heating instead of less-energy-efficient thermal processing to increase the speed and reduce the cost of producing carbon fibers. They have already demonstrated that microwave-assisted processing of PAN precursors is a viable alternative to conventional thermal processing for manufacturing carbon fiber.

"Microwave technologies offer the potential to accelerate processing of precursors to produce carbon fibers with the appropriate properties," Paulauskas says. "Our early studies show that a properly designed and implemented microwave energy delivery system may enable a fourfold increase in the production speed, from 60 minutes to 15 minutes. Our economic studies show it has the potential to reduce fiber price by approximately 20% and the amount of energy required by approximately 15 to 20%."

Because the microwave units are smaller and cheaper and only several units are required to replace the massive single ovens now being used, maintenance downtime, capital equipment costs, and plant space requirements will be greatly reduced. Widespread implementation of this technology could replace about 50 to 70% of the conventional carbon-fiber processing line with very inexpensive equipment.

April McMillan and Felix Paulauskas examine the result of using microwave energy to bond two glass-fiber-reinforced composite parts.

Coming unglued. Adhesives will be used to join vehicle parts made of carbon-fiber composite materials. The problem is that components so bonded cannot be easily disassembled for repair without cutting or otherwise damaging the assembly. What's the solution? Microwave-reversible bonding can nondestructively take apart the adhesive bonds between components so they can be repaired or replaced.

"In our research," says Paulauskas, "we have identified suitable adhesives that can be taken apart by microwaves at low temperatures. We are developing adhesives that can be debonded at even higher temperatures."

Working with Barbara Frame of ETD and April McMillan of ORNL's Metals and Ceramics (M&C) Division, Paulauskas has shown that microwave-reversible bonding can facilitate the repair and maintenance of adhesive-bonded components made of plastic, carbon-fiber composites, and other nonmetallic materials. "By making repairs and upgrades more affordable," Paulauskas says, "microwave-reversible bonding could extend the life cycle of cars."

Curtis Boles

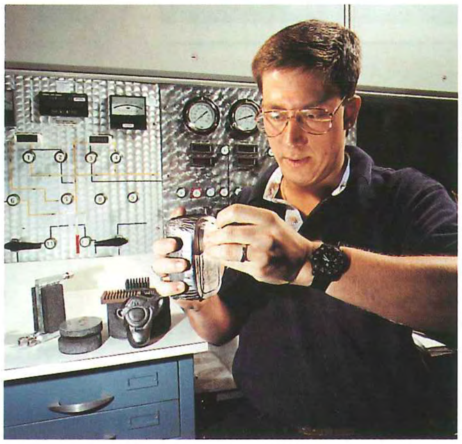
Tim Burchell shows carbon-fiber composite samples of various shapes produced and studied at ORNL.

Better brakes and radiators. Lightweight carbon composites could be even more valuable for components of automobiles and computers if they could be made so that more heat flows through them more quickly. For example, by increasing the thermal conductivity of carbon materials, they could be used to make safer automobile brakes. Today's brakes when applied may overheat or develop hot spots that can cause annoying vibrations.

In ORNL's M&C Division, Tim Burchell and James Klett have developed novel carbon-carbon composite preform materials with the increased thermal conductivity needed to make safer brakes. They have developed processing technologies that will reduce the time for and cost of fabricating these materials. They have developed novel carbon foams with improved heat-flow properties for automotive applications.

The brake products developed from carbon-carbon composite preform materials using the ORNL fabrication process have 3 to 5 times greater thermal conductivity than conventional brake materials. The ORNL technique cut processing time requirements almost in half.

Klett developed a new low-density carbon foam that has a very high thermal conductivity. It transfers heat so rapidly that if you hold the foam in your hand and press an ice cube on top of the foam, your hand feels cold almost immediately. "The key to the foam's conductivity is its unusual graphite crystal structure," Klett says. "Add foam to a bag of marbles and remove them, leaving air pockets, and you'd have a similar skeletal structure. This foam conducts heat almost as well as aluminum but at one-fifth the weight. Because our foam is only 25% dense, we hope to increase its thermal conductivity by finding a way to fill the air pockets with graphite." This foam, now called Grafoam, can be easily fabricated into complex shapes. The technology has been licensed to Poco Graphite in Decatur, Texas. It could be used to make a smaller, lighter car radiator that could be placed away from the car's front to allow an energy-saving and less-polluting aerodynamic design.



Curtis Boles

James Klett demonstrates the rapid melting of an ice cube applied to a carbon foam sample held in his hand. The sample transfers heat from his hand rapidly to the ice cube, causing the cube to melt quickly and his hand to feel suddenly cold. Such carbon foam could prove useful for making car radiators.

Lighter electrodes for fuel cells. One way to decrease emissions and increase fuel economy in cars is to power them with electricity from fuel cells (after gas stations start offering hydrogen or methanol for your fuel tank). Like an electric battery, a fuel cell has positive and negative electrodes (bipolar plates) with an electrolyte between. In a proton exchange membrane (PEM) fuel cell, hydrogen fuel is supplied to the negative electrode, and oxygen from the air is pulled into the positive electrode. During cell operation, the fuel is oxidized, and the hydrogen nuclei, or protons, produced in the reaction are transported through the polymer electrolyte to the negative electrode, while electrons freed by the reaction provide the current. A car operating on hydrogen and powered by a fuel cell would likely be considered an efficient, "zero emissions" vehicle.

The problem with using today's PEM fuel cells to power cars is that their bipolar plates, which are made of machined graphite, are too heavy, too brittle, and too costly for use in automobiles. The solution is to make bipolar plates from a carbon-fiber composite, which is lighter, tougher, and cheaper.

Ted Besmann, Klett, and Burchell, all of the M&C Division, have developed a method for making composite plates. "We mix chopped-up carbon fibers with a phenolic resin in a water solution and pour it into a mold having a screen on the bottom that is under a vacuum," Besmann says. "The water is pulled through the screen, leaving the fibers behind. The resulting shape is the bipolar plate. We call this slurry molding. We cure the plate to activate the resin, so all the fibers are glued together to give sufficient strength for handling. Then we stamp channels and holes into the plate to make it an electrode."

The next step is called chemical vapor infiltration. "In production we will be able to put thousands of plates into a furnace and flow methane over them at 1400°C," Besmann says. "Carbon from the methane will be deposited on the fibers, penetrating as much as half a millimeter below the surface of the fibrous material. That's why we call it chemical vapor infiltration rather than chemical vapor deposition. The deposited carbon will fill the pores, sealing the surface."

Why is this important? A fuel cell is really a series of cells, or a Dagwood-sandwich-like stack of bipolar plates with electrolytes between. The cells will not work if hydrogen and oxygen leak from one cell to another, so it is essential that the porous plate surfaces be sealed.

If carbon-fiber composite plates can be made to perform as well as graphite, they may make useful components for automotive fuel cells because, besides being tougher, they are only half as heavy and will cost perhaps one-fifth as much as machined graphite, meeting PNGV goals.

Increasing Efficiency of Electric Buses

To reduce air pollution, noise levels, and dependence on imported oil, Chattanooga, Tennessee, allows only electric shuttle buses on one downtown route. Electric buses are cleaner and quieter than their diesel counterparts. As a partner in Chattanooga's Clean Cities Initiative to improve the environment and as part of a PNGV project, ORNL researchers are demonstrating that new technology can increase the energy efficiency of electric buses manufactured by Advanced Vehicle Systems (AVS) of Chattanooga.

One of Chattanooga's electric buses has an ORNL soft-switching inverter that makes the vehicle lighter and more energy efficient.

The electrical energy for each AVS bus comes from a battery pack, which supplies 300 volts of direct current (dc). The dc must be converted by an inverter to alternating current (ac) to drive the vehicle's ac induction motor. The problem with conventional inverters is that they use a "hard-switching" technique—their solid-state transistor switches operate at full load voltages and currents as they open and close up to 20,000 times per second to create an alternating current. As a result, they waste electrical energy, generate heat, wear out components quickly, and produce high voltage spikes in the motor and significant electromagnetic interference (EMI) that can disrupt operations of other electronic devices.

One of the Chattanooga buses has a new generation of inverter technology developed at ORNL by Fang Peng, Gui Ja Su, Cliff White, George Ott, Matt Scudiere, and Laura Marino, all in ETD. This "soft-switching inverter" is more efficient, more compact, and more reliable than conventional inverters and eliminates the problems of voltage spikes and EMI.

ORNL's auxiliary resonance tank soft-switching inverter has small components that temporarily divert electrical current from the main switches so that no power is lost when they are turned on and off. The device also has light, inexpensive "sinks" to absorb operating heat so that components can be placed closer together safely. As a result, the device weighs only one third as much and occupies only one-tenth as much space as the newest conventional inverter. Thus, it is ideal for electric cars and buses because its lighter weight will increase vehicle energy efficiency.

Catalyst Candidates for Auto Emission Control

Smog and ground-level ozone could be reduced in large cities if nitrogen oxides could be removed from the exhaust from internal-combustion and diesel engines. Past research suggests that nitrogen oxide (NO) can be captured using an elemental metal and metal oxide if the surface interactions are right. The actual mechanism for NO removal remains unknown. Trying to understand this mechanism, ORNL researchers Steve H. Overbury and David R. Mullins have been studying a candidate catalyst for emission control, especially in future lean-burn engines. It contains a metal—rhodium (Rh)—and a metal oxide that has multiple oxidation states, cerium oxide (CeO_y; $y = 1.5\text{-}2$). They prepared Rh-CeO_y materials as thin films and found that this form is promising for laboratory study to determine how surface interactions actually capture NO from exhaust. Using surface-sensitive spectroscopic techniques to characterize the thin films, the researchers obtained unprecedented detail on interactions among NO, rhodium, and cerium oxide. Such insights should help researchers design improved catalysts for advanced automotive engines.

Technology Truck Travels around the Country

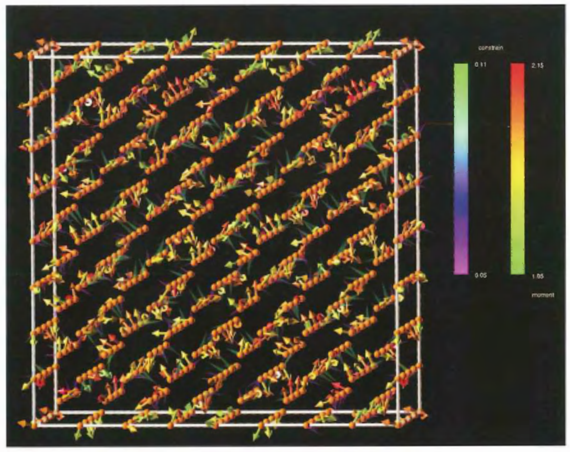
ORNL helped develop and operate the Federal Highway Administration Technology Truck (shown here in Long Beach, California) to showcase technologies that could help the commercial motor vehicle industry lower its costs and accident rate. The operators of this specially outfitted vehicle have traveled all around the nation to demonstrate new commercial software and hardware that will improve motor carrier safety and productivity, streamline administrative processes for both the commercial motor industry and state regulatory agencies, and minimize carrier delays.

The Technology Truck is an expandable 48-foot, 18-wheel tractor-trailer rig that houses portable intelligent transportation systems; informational, multimedia kiosks; in-cab simulator; hands-on demos; and classroom presentations. Policymakers, regulators, and members of the trucking industry and public visiting the Technology Truck are being shown "smart" hardware to allow trucks to bypass weigh stations and to prevent drivers with alcohol on their breath from starting their trucks. Other devices will help drivers detect obstacles ahead, avoid collisions in their blind spots, read license plates, and identify containers. Software being demonstrated to visitors will help drivers schedule their trips, select the best routes to a destination, keep track of miles traveled, and calculate fuel tax and the load on axles. Other programs will ensure drivers that they are complying with hazardous materials regulations and remind them to do preventive maintenance and checks on their vehicle systems.

Characterizing Diesel Particle Exhaust

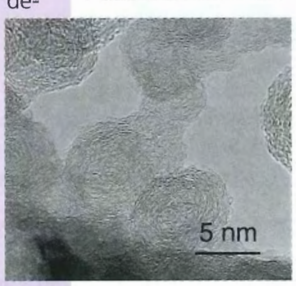
Besides their high emissions of nitrogen oxide, advanced diesel engines that are being developed to use 35% less fuel per mile than today's gasoline-burning, spark-ignition engines present another environmental problem—airborne particulates that are hazardous to humans inhaling them. Diesel exhaust particles are generally less than 2.5 micrometers (μm) in diameter—a potentially dangerous size range because the smaller they are, the easier it is for them to sneak past the body's filters and land in the lungs. They also reduce visibility in populated areas.

John Storey and others in ORNL's ETD have developed an electrostatic method for capturing diesel particulates from a test diesel engine's exhaust so that their structure and makeup can be analyzed. He has also developed ways to measure the varying sizes of agglomerates of particles for experiments that will determine the effect of changes in diesel fuel combustion and exhaust aftertreatment (using catalysts) on particle sizes.

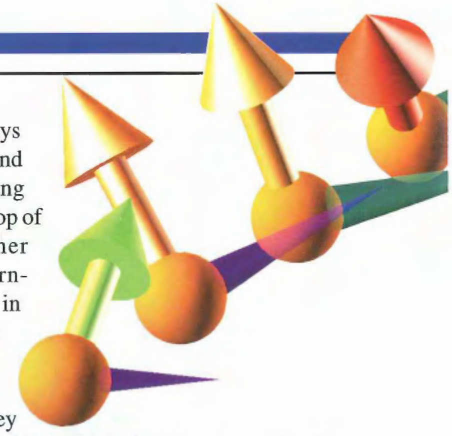


A computer code developed largely at ORNL that won the 1998 Gordon Bell Prize for the fastest application in high-performance computing was used to perform a first-principles simulation of the magnetic behavior of 1024 atoms of iron (shown here). This code will be used to simulate the electronic structure of materials to enable the design of better catalytic converters and lighter batteries for electric cars.

Ted Nolan, Karren More, and others in the M&C Division have used the Hitachi HF-2000 transmission electron microscope and other characterization tools to determine the structures of diesel particulates. They found that particles measuring 20 to 40 nanometers may range from a noncrystalline (amorphous) structure to a semicrystalline (turbostratic) structure in which atoms are lined up in sheets, but the sheets are not oriented the same as they are in graphite. "It's like tearing off all the sheets from a pad of paper," says Nolan, "and then laying them on top of each other while turning them in different directions."



Micrograph of diesel particulate showing the semicrystalline, "turbostratic" structure in which sheets of atoms in rows are turned in different directions.



Storey is also working with DOE's Lawrence Berkeley National Laboratory to build and calibrate real-time scatterometers for both labs. These instruments will be used to scatter light off particulates in diesel exhaust to measure their relative sizes. It is important to know the fractions of particulates of various sizes in the exhaust because new particulate standards will limit the total mass of particle sizes under 2.5 μm. In addition to monitoring emissions compliance, these rapid-response instruments could also provide information to engine manufacturers and service facilities to guide the development of cleaner diesel engines and the adjustment of current ones.

Computer Simulations: Designing Cleaner, More Efficient, Safer Cars

A prize-winning computer code written at ORNL for use on powerful supercomputers may advance transportation research. This code is being used to simulate the electronic structure and properties of materials to enable the design of better catalytic converters, lighter batteries for electric cars, and better coatings on aircraft turbine blades. The code, which ORNL Corporate Fellow Malcolm Stocks helped develop, won the 1998 Gordon Bell Prize for the fastest application in high-performance computing. It was the first code to run at greater than one teraflop, or more than one trillion calculations per second. Using the code, Stocks and his collaborators (including ORNL's Don Nicholson, Xaioguang Zhang, and Bill Shelton) performed a first-principles simulation of the magnetic behavior of 1024 atoms of iron, using increasingly powerful Cray T3E supercomputers.

By crunching numbers on ORNL's powerful parallel supercomputers, Laboratory researchers are reducing the need to crunch metal by crashing cars together to determine how well their materials hold up in a collision. By making billions of calculations per second and creating visualizations of mounds of data using these computers, they have developed a nonviolent method for designing the lightweight, fuel-efficient cars of tomorrow that are at least as safe as the heavier steel cars of today.

Researchers at ORNL, in collaboration with the National Highway Traffic Safety Administration and George Washington University, are developing detailed computer models of a variety of vehicles after disassembling them and scanning in the parts. In the past few years, they have completed models of the Ford Taurus and Explorer, both among the top-selling vehicles in the United States. Researchers are now modeling an Audi A8, an all-aluminum car that is one of the first to use a lightweight material that may be used extensively in future cars.

"We use a computer model of a car and its components combined with a model of the lightweight material used in the car to analyze how well the material will hold up in a wide variety of crashes," says model developer Srdan Simunovic of the Computer Science and Mathematics Division. "We can substitute different materials in individual parts in our model and compare the results to determine which material performs best during a collision between cars.

"Our development of the parametric finite-element model has enabled us to tune the grid—in which the vehicle is divided into hundreds of small sections—according to the kind of crash we're going to simulate and number of computer resources available. This innovative solution has made car crash simulation more manageable for the computer."

ORNL researchers will soon be using a recently acquired IBM RS/6000 SP supercomputer for PNGV studies to support development of advanced transportation vehicles and alternative fuel technologies. The initial IBM system is configured to perform 100 gigaflops (a billion calculations per second), or a tenth of a teraflop. It will be upgraded to 400 gigaflops later this year and to 1 teraflop in the middle of 2000. The new machine will be more than seven times faster than ORNL's Intel Paragon XP/S 150, which in 1995 was the world's fastest computer.

This warning device could help drivers avoid a truck rollover.

Reducing Congestion: Truck Rollover Warning System

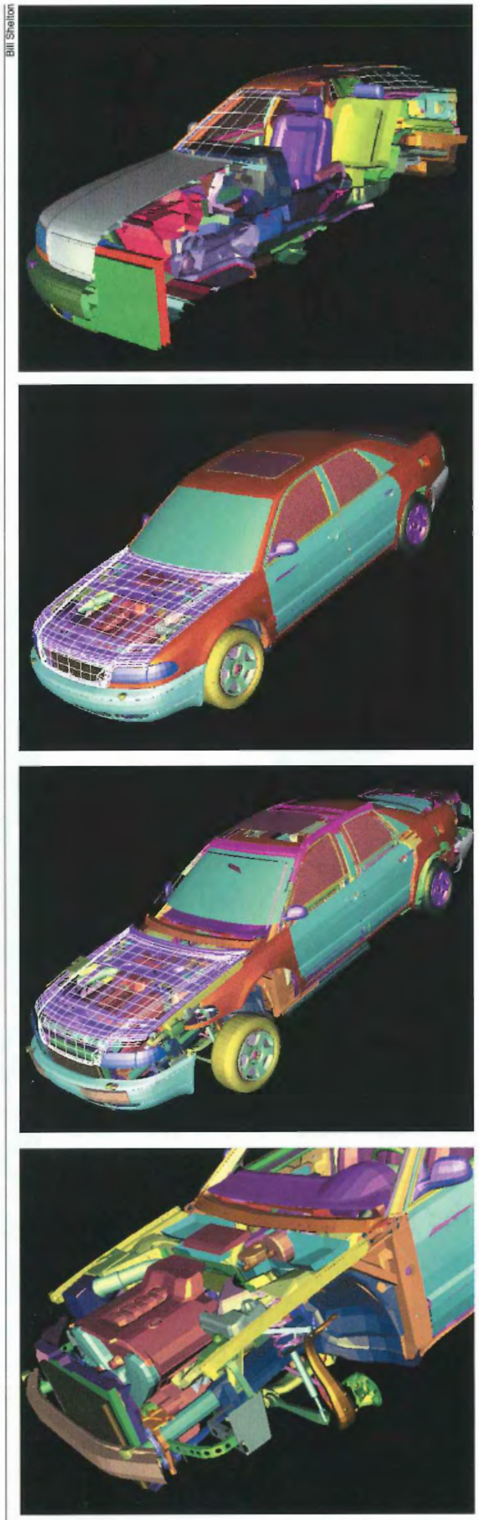
Most of us have at some time been delayed by a traffic jam caused by an overturned truck. Truck rollover crashes are responsible for at least $3 billion a year in losses associated with deaths and injuries, property damage, lost productivity, and lost time because of traffic backups.

To address this problem, an ORNL-led team has designed a system to warn truck drivers who are at risk of rollover in time for them to take corrective action. This prototype system will be implemented, tested, and evaluated by Scott Stevens of the Energy Division and Phil Spelt of CPMD, in collaboration with representatives of the Tennessee Department of Transportation, the Transportation Research Center at the University of Tennessee, and U.S. Xpress Enterprises, a Chattanooga trucking company.

"Our system of on-board sensors and a computer will collect data and determine the instantaneous roll stability of three tractor-trailer rigs," Stevens says. "We will deploy roadside beacons at selected sharp curves or ramps in Tennessee to broadcast curve characteristics to oncoming vehicles. Our smart test trucks will receive the broadcasts, estimate the risk of rollover, and warn the drivers if they are approaching the curve at a speed that is likely to cause rollover. An alarm will be sounded in time for the drivers to take corrective action. The on-board instruments will also collect data about the drivers' response to highway design features and various traffic situations." It is estimated that 4000 of the annual 15,000 truck rollovers could be prevented with a rollover alert system.

ORNL is helping to drive the transportation revolution by evaluating intelligent transportation systems, developing better ways to make lightweight materials for vehicles, improving efficiency in electric vehicles, developing and testing methods for reducing and characterizing emissions, evaluating the safety of lightweight vehicles in collisions, and developing information systems to reduce traffic congestion by lowering the risk of truck rollovers.

Bill Shelton

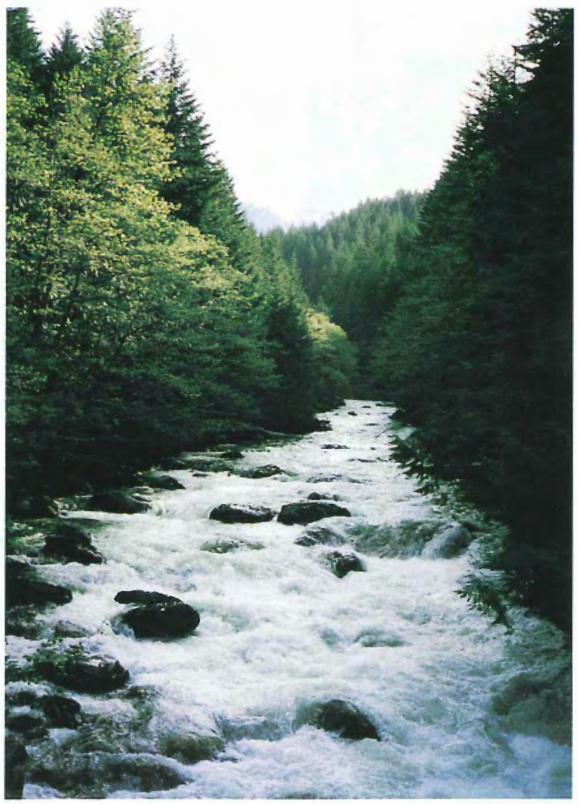


ORNL researchers are modeling an Audi A8, an all-aluminum car made of a lightweight material that may be used in future cars. A computer model of a car and its components, combined with a model of the lightweight material making up the car, help researchers analyze how well the material will hold up in a variety of collisions.

Clean Energy and Climate Effects

Developing clean energy sources, using energy more efficiently, and understanding the effects of increased energy-source emissions on regional climate and forest productivity are targets of ORNL research.

Satisfying the world's growing appetite for energy could set the stage for global climate change. Much of our electrical power and heat comes from the combustion of fossil fuels, which release carbon dioxide (CO_2) into the atmosphere. CO_2 is one of the primary gases that contribute to the "greenhouse effect"—the phenomenon in which certain trace gases in the atmosphere trap the earth's radiated energy, causing a gradual warming of its surface. Significant global warming might lead to regional shifts in agricultural and forest productivity and cause the spread of disease and the relocation of coastal populations.



Small mountain streams in northwestern Washington have been proposed as sites for hydroelectric projects.

To delay the onset of significant global warming, the developed nations may change their portfolio of energy sources. Some are considering replacing coal with natural gas because combustion of gas emits almost half as much CO_2 as the combustion of coal. Other options are to make greater use of renewable energy sources (including hydropower facilities) and nuclear power because they do not produce CO_2.

A second approach to cutting CO_2 emissions is to develop technologies, such as "smart" cars, buildings, and appliances, that use energy more efficiently (see the article, "Driving the Transportation Revolution," starting on p. 8). ORNL also has contributed in this area by developing more efficient refrigerators and heat pumps. A third approach is to focus on both understanding the effects of rising levels of atmospheric CO_2 and preventing it from building up to undesirable concentrations. Computer modeling experts are predicting the impacts of increasing emissions of CO_2 on climate, and ecologists are studying the effects of elevated atmospheric CO_2 concentrations on forest productivity. Other scientists are exploring the emerging science and technology of carbon sequestration—the capture and secure storage of CO_2 emitted from the combustion of fossil fuels. The U.S. Department of Energy supports all these approaches. In 1998 ORNL researchers had some outstanding achievements in these areas.

ORNL Recommends Building Three Hydro Projects

Small dams that generate electricity are needed to help meet growing power demands in the Pacific Northwest, but the benefits of proposed hydroelectric projects must outweigh their environmental costs. To balance power needs with potential environmental impacts, as required by the Federal Power Act and National Environmental Policy Act, the Federal Energy Regulatory Commission (FERC) conducts environmental assessments of new and existing projects proposed for licensing.

In April 1998, ORNL completed for FERC the final environmental impact statement for eight new hydroelectric projects proposed for the Skagit River Basin in Washington. The ORNL group—Bo Saulsbury, Rich McLean, and Bill Staub (Energy Division) and Warren Webb, Glenn Cada, and Mark Bevelhimer (Environmental Sciences Division)—recommended that three of the eight projects be licensed for construction and operation, provided that the applicants implement certain mitigation measures. If constructed, these three projects would generate about 72 gigawatt hours of electricity annually.

ORNL ecologist Warren Webb stands in an old-growth forest near a proposed hydroelectric project site.

Complex environmental issues arise around the plan to clear land and dam streams for hydroelectric projects in the Pacific Northwest. Will old-growth forest be cleared or protected? Will project construction or an accidental rupture of the project pipeline adversely affect slope stability and result in erosion that could affect water quality? Will water quality degradation or changes in stream flows further threaten Pacific salmon stocks? Can threatened and endangered species, such as the spotted owl and marbled murrelet, still be protected? Will Native American treaty rights and cultural practices be respected and preserved? What will be the socioeconomic effects of construction and operation, such as the impact on housing and schools of workers and their families moving into the community?

The ORNL team recommended these mitigation measures for the three projects: (1) prevent erosion and control sediment to protect water quality; (2) increase stream flows and restock resident fish populations in the projects' bypassed reaches; and (3) acquire and preserve between 7 and 10 acres of forest along other streams to replace the forest habitat cleared for the projects. These mitigation measures would be implemented along with other environmental measures proposed by the applicants.

"We did not recommend licensing the five other proposed projects," Saulsbury says, "because they would pose significant environmental impacts even with available mitigation measures."

Computational Tool Could Aid Search for Oil and Gas

The propagation of sound waves underground may contain relevant information about

To solve the problem of faulty seismic image focusing, which plagues the oil and gas exploration industry, (from left) Jacob Barhen, Edward Oblow, Vladimir Protopopescu, and David Reister developed TRUST, a computational method for global optimization. For their work on TRUST, they received an R&D 100 Award in 1998.

the presence of oil and gas. Therefore, many petroleum exploration companies use seismic analysis for hydrocarbon exploration. Seismic data are obtained by recording the energy returning to the earth's surface from an underground source of acoustic waves. These waves propagated into the earth are reflected back whenever they encounter a change in acoustic impedance (e.g., passing from a dense shale into a porous sandstone layer that may contain oil). An array of receivers on land or underwater picks up sound waves from each reflected signal. Petroleum industry researchers plug the recorded data into a computer code that provides an image of the subsurface geological structure.

Unfortunately, the reflected signals carrying useful information are often buried in the noise from the sensor electronics and from disturbances arising from the degradation and misalignment of some seismic signals. Misalignment is caused by unpredictable delays in the recorded travel time of the seismic waves (which pass more quickly through solid rock layers compressed deep underground than through less rigid rock layers near the surface). As a result, the image of subsurface structures is highly distorted. For large-scale seismic surveys, this problem typically had been considered intractable by industry experts, until ORNL came up with a mathematical and computational solution.

To address the challenge of faulty seismic image focusing, Jacob Barhen, David Reister, Vladimir Protopopescu, and Edward Oblow, all of ORNL's Computer Science and Mathematics Division, developed Terminal Repeller Unconstrained Subenergy Tunneling (TRUST), a computational method for global optimization. This fast, powerful, and robust tool could be used with a petroleum industry computer code to combine and correlate relevant data from all the receivers to get the sharpest possible image. By enabling a multisensor fusion algorithm to identify the meaningful reflections by separating them from the noise, the TRUST algorithm solves the seismic-image focusing problem plaguing the oil and gas industry, potentially reducing exploration costs.

"TRUST rapidly and reliably eliminates large, useless regions of the search space before they are actually searched," says Barhen, an ORNL corporate fellow. "Hence, it increases the overall efficiency up to 45 times higher than any competitive approach."

The development of TRUST was sponsored by the Engineering Research Program of DOE's Office of Science. Its application for geophysical imaging was funded by DOE's Office of Fossil Energy in conjunction with the DeepLock petroleum industry consortium. In 1998 the TRUST developers received an R&D 100 Award.

From left in front of the field test model of the triple-effect absorption chiller at the Clark County Government Center in Nevada are Ronald Fiskum, DOE program manager and, from ORNL, Bob DeVault, Patti Garland, Abdi Zaltash, and Tony Schaffhauser. The five were celebrating an agreement signed by various partners October 27, 1998, to proceed with the test deployment of the world's first triple-effect absorption chiller at the center.

A More Efficient Gas-Fired Heat Pump

ORNL, in a cost-shared program with York International, has developed a triple-effect absorption chiller, an advanced natural-gas-fired heat pump that is 30 to 40% more energy efficient than other heat pumps. The device will be used to provide space cooling for large commercial buildings. In comparison with the double-effect chiller developed more than 40 years ago, the ORNL chiller's emissions of CO_2 are 99.9% lower. In addition, its emissions of sulfur dioxide and total particulate solids are reduced by 73% and 99% respectively.

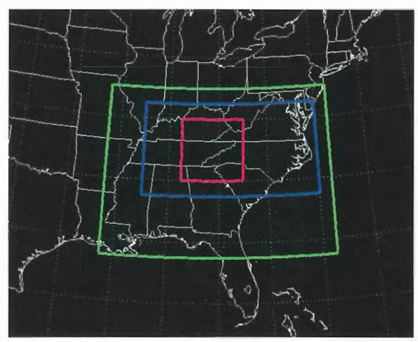
Bob DeVault of the Energy Division, a co-inventor of the triple-effect absorption chiller, says the "triple effect" comes from feeding a refrigerant-containing absorbent solution through high-, medium-, and low-temperature generators. "The high-temperature condenser receiving vaporous refrigerant from the high-temperature generator is coupled to both the medium-temperature and low-temperature generators," DeVault says. "As a result, the internal recovery of heat within the system is boosted, increasing its thermal efficiency, improving indoor comfort and indoor air quality, and greatly reducing CO_2 and other emissions."

In an October 1998 speech, Secretary of Energy Bill Richardson noted that laboratory testing of the triple-effect chiller prototype at York International showed that it uses 40% less energy than other types of heat pumps. He also announced that the first field test of a full-size triple-effect chiller will be conducted in Clark County, Nevada, in 1999 and 2000. Patti Garland of the Energy Division is leading ORNL's participation in the test.

ORNL's Role in Energy Savings Performance Contracting

By 2005, all U.S. federal agencies must use 30% less energy in their buildings than they consumed in 1985. That's the mandate of the Energy Policy Act of 1992 and Executive Order 12902. But energy efficiency improvements cost money, so how can federal government agencies reduce their energy use when their capital expenditures budgets are so tight? One solution is an alternative financing arrangement called energy savings performance contracting (ESPC).

Instead of relying on traditional congressional appropriations of capital funds to finance energy efficiency improvements in federal buildings, federal agencies sign contracts with private energy service companies that agree to pay up-front costs for identifying building energy cost-saving measures and acquiring, designing, installing, operating, and maintaining the energy-efficient equipment. In exchange, the contractor receives fixed payments from the cost savings resulting from these improvements until the contract period expires, up to 25 years later. At that time, the federal government retains all the savings and equipment.



This map shows the Super ESPC regions in the United States. ORNL has played a major role in energy savings performance contracts for the Southeast region.

ORNL and DOE's Oak Ridge Operations (ORO) are participating in the Super ESPC program for DOE's Federal Energy Management Program. Super ESPCs are regional "all-purpose" or national "technology-specific" contracts that allow agencies to negotiate ESPC delivery orders with an energy service company without having to start the contracting process from scratch.

The Oak Ridge team has awarded contracts potentially worth $750 million to six private companies for "all-purpose" ESPC in the Southeast. The team has also awarded contracts potentially worth $500 million to five private companies for geothermal heat pump "technology specific" ESPC nationwide. Key technical participants on the Oak Ridge team are Patrick Hughes and

George Courville, both of ORNL's Energy Division, and Angela Carroll and Wayne Lin, both of ORO.

Energy services companies are being contracted to help government agencies reduce their energy costs, meet federal energy savings requirements, and eliminate the maintenance and repair costs of aging or obsolete energy-consuming equipment. The contractors also are responsible for operating and maintaining the new energy-saving equipment during the contract term if the federal site so desires.

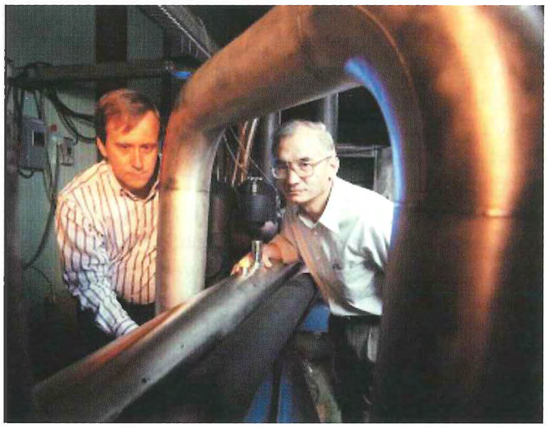
For example, under an ESPC agreement, energy-efficient lighting, variable-speed motor drives, and an energy management control system are being installed at the Statue of Liberty. For ORNL a contract has been signed with Duke Solutions, Inc., to work with Hicks & Ingle Corporation to quickly replace a failed water chiller with a more efficient one in an Environmental Sciences Division building. In other federal complexes, lighting retrofits, additional insulation, cogeneration systems, and geothermal heat pumps (to replace conventional heating and air conditioning units) are being installed.

Angela Carroll at DOE-ORO is the contracting officer for the six Southeast region and five geothermal heat pump contracts. The DOE contracting officer's representatives for all 11 contracts are Doug Culbreth and David Waldrop of the DOE Atlanta Regional Support Office. Patrick Hughes and a team of project facilitators from ORNL's Energy and Engineering divisions lead acquisition teams at federal agency sites through the delivery order process and provide technical assistance.

"Our team," says Hughes, "will verify that each project's annual cost savings from reduced need for energy and maintenance will exceed the agency's annual payments to the energy service company for providing the energy efficiency improvements and negotiated services." The ORNL-ORO team will also support an appropriate integration of advanced technologies sponsored by DOE's Office of Energy Efficiency and Renewable Energy into the Super ESPC program, such as was accomplished for the geothermal heat pump.

Superconducting Cable and Transformer

A newer way to use energy efficiently is to harness superconducting wire chilled by liquid nitrogen because the high-temperature superconductor offers no resistance to electrical flow. Researchers in ORNL's Fusion Energy Division have been involved in developments that would use this wire to transmit higher amounts of electrical current underground and to change voltage and current levels.



Jonathan Demko (left) and Winston Lue check out components of the superconducting cable at the test facility at the Southwire Company plant in Georgia.

ORNL has entered a partnership with Southwire Company to develop a 30-meter, high-temperature superconducting (HTS) cable at the company's Georgia headquarters. The cable will carry enough energy to power a small city. In 1998 ORNL staff researchers J. Winston Lue, Michael J. Gouge, and Jonathan A. Demko designed, completed, and operated a research facility to support the successful development and testing of the first U.S. system prototype of an HTS power transmission cable. The goal is to retrofit HTS cables in existing underground ducts with cables that can carry 3 to 5 times more current.

The Laboratory played a significant role in the fabrication and testing in 1998 of the first U.S. experimental electric transformer made from HTS wire. The team included ORNL, Waukesha Electric Systems, and Intermagnetics General Corporation. The ORNL team members were Bill Schwenterly, Jonathan Demko, Andy Fadnek, Randy James, Ben McConnell, and Isidor Sauers.

"We were responsible for the innovative cryogenic system that allowed the 1-million-volt-ampere (MVA)-rated transformer to be cooled to 20 Kelvin without liquid helium," Schwenterly says. "Our work set the standard for cryogenic cooling systems for emerging electrical applications based on HTS technology."

Compared with traditional paper-oil-insulated transformers wound with copper wire, HTS power transformers will increase efficiency of power delivery, eliminate the use of oil (a fire hazard and environmental contaminant), and upgrade the capability to handle power overloads. The team is now participating in the development of a 5-MVA transformer to be operated on the utility grid at Waukesha Electric's factory in Wisconsin.

Regional Climate Modeling and Assessment at ORNL

First, think globally. What are the effects on future climate of rising concentrations of CO_2 from increased fossil fuel combustion? No one knows for sure, but global climate models now being developed for parallel supercomputers may predict these effects accurately someday. Now, think locally, or at least, regionally. If significant global climate changes are expected, what are the implications for the southeastern United States? The answer depends on the ability of computer specialists to predict changes in regional climate based on results of global scenarios.

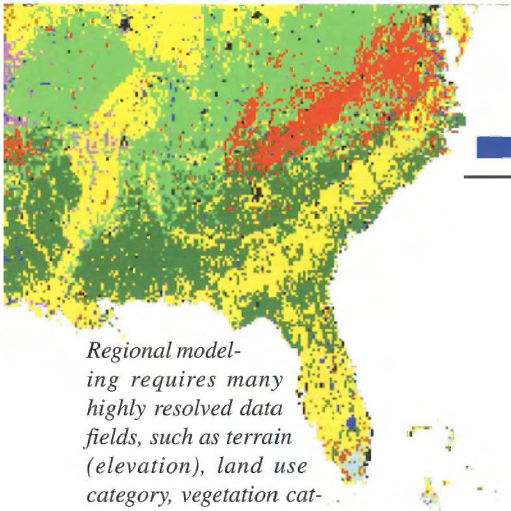
The challenge is to present these changes on a much finer spatial and temporal scale. If such "downscaling" could be done, it might be possible, for example, to predict accurately whether East Tennessee will have less precipitation and more tornadoes in the next decade. Or whether the Carolinas will endure more hurricanes in the first two decades of the next century than they did during the last two decades in this century. Or whether the sea will rise and inundate the coast of Florida in the middle of the next century.

John B. Drake of ORNL's Computer Science and Mathematics Division and three investigators in ORNL's Environmental Sciences Division—Mac Post, Tony King, and Mike Sale—recently received funding for a regional climate modeling and assessment project. The source was ORNL's internally funded Laboratory Directed Research and Development Program.

"We have developed a statistical conceptual framework for simulating regional climate," Drake says. "The framework will house a variety of models, compare models, and combine results of different models. It uses physically based weather models, results of ecological experiments, and historical climate observations. Eventually, we will be able to predict temperature and precipitation data for any 1-kilometer grid for a particular decade or longer.

"But, what our customers want is predictions of extreme events. Our goal is to be able to predict that a region in the Southeast during a certain decade will experience, for example, 30% more tornadoes, or 20% fewer hurricanes, or 25% more big storms that cause major floods than it did in the 1980s. Of course, we will also provide error bounds because we cannot make such predictions with 100% certainty."

The ORNL group has been studying the ability of today's global circulation models to predict the fate of rainfall in the Southeast and



Regional modeling requires many highly resolved data fields, such as terrain (elevation), land use category, vegetation categories, soil categories, and ground temperature. The color scheme for land use for the Southeast (shown here) is as follows: black—urban land; yellow—agriculture; purple—treeless grassland; green—deciduous forest; dark green—coniferous forest; red—mixed forest and wetland; blue—water; and light blue—marsh or wetland.

keep an accurate freshwater budget. "Our model tells us how much rain goes east of the continental divide to the Atlantic Ocean and how much goes west to the Mississippi River or to the Gulf of Mexico coast," Drake says. "But we want to improve the model's resolution by partitioning rainfall so we can predict how much actually goes into each of the major rivers, such as the Ohio and Tennessee rivers."

Making predictions for the Southeast will require scientific discovery of the relationship between local biogeochemical processes and large-scale weather and climate shifts. "If the climate becomes warmer and drier," says King, "the growth of smaller, shallow-rooted trees in a region's forests may be reduced, decreasing the region's uptake of carbon. The rise in temperature could increase the rates of tree respiration and decomposition of soil and litter, resulting in greater releases of carbon to the atmosphere that could bring increased climatic warming.

"In addition, w1e need to discover the effects on climate of changes in water availability to regional forests. These changes affect transpiration, the way in which trees transfer rainwater back to the atmosphere. We also must determine the effects on forests of seasonal changes such as early springs—which could result in early leaf production, increased growth, and greater carbon uptake—and early springs punctuated with later freezes that could hamper reproduction, reducing the long-term productivity of the forest.

"We will look at the impacts on forests of summer and winter droughts, which are expected to have different effects on forest growth," King adds. "Our models will run different climate scenarios to determine how they affect the ability of forests, crops, and other plants to take up carbon and influence future climate."

The purpose of the regional climate model is to provide scientifically grounded information for modelers in the assessment community. These researchers seek to predict the impacts of climate change on health, food production, the environment, and the economy.

"Suppose that our model predicts a slightly warmer and drier climate for the Southeast in the next few decades," Drake says. "These results could be plugged into models used to determine the effects of temperature and precipitation changes on mosquito proliferation and the spread of malaria."

Other modelers will look at climate impacts on agricultural production, growth of forest trees, and reproduction of wildlife species. Some modelers will try to determine if a climatic warming could have immediate economic impacts, such as severe coastal flooding from a rise in sea level and a higher frequency of hurricanes.

The ORNL modelers are expecting to examine the impact on regional climate of various CO_2 emission levels in the Southeast. They may be running different scenarios in which regional firms burning fossil fuels pay other nations for the right to exceed limits in emitting carbon. They will also look at the effects on climate of enhancing the natural sequestration of carbon by improved management of land, forests, and agriculture.

"By predicting future climate for the Southeast," Drake says, "our community of ORNL researchers could become an important link between the modeling community and the policy-oriented impact assessment communities who are devising strategies to deal with increasing atmospheric CO_2 and the predicted impacts of global and regional warming."

For that reason, as part of the U.S. Scientific Simulation Initiative, ORNL is proposing to serve as the regional climate prediction center for the Southeast. ORNL researchers use global circulation models, but for climate prediction, they are starting to think regionally.

High-Performance Storage System and Climate Data Archive

A scientist needs data about how different types of clouds reflect, absorb, and transmit the energy of sunlight. The data, based on measurements taken by instruments on the ground and aboard airplanes and satellites, will help the scientist improve the accuracy of a computer model in predicting the influence of human activities on climate.

The scientist accesses a web-based interface and requests 100 files of data from DOE's Atmospheric Radiation Measurement (ARM) data archive, located at ORNL. In this archive are more than three million files containing more than 15 terabytes of data. Three robots retrieve the tapes on which the requested files are stored and load them for copying on the disk drive of the ARM web-site server. Within an hour, the scientist can access the requested files.

For the past two years, the ARM data archive has been using the High-Performance Storage System (HPSS), storage-system software that leads the computer industry in capacity and transfer speeds. HPSS was developed by a consortium of DOE national laboratories and IBM. The DOE participants are ORNL, Sandia, Lawrence Berkeley, Los Alamos, and Lawrence Livermore national laboratories. HPSS, which received an R&D 100 Award in 1997, is marketed by IBM.

Deployed at about 20 sites and used productively for more than two years, HPSS is now the standard for storage systems in the high-per-

This ARM millimeter cloud radar instrument in Oklahoma cattle country enables scientists to determine whether a cloud contains mostly ice crystals or liquid water. Such measurements help scientists predict the degree to which the cloud reflects, absorbs, or transmits sunlight.

formance computing community. The HPSS community has been joined by two new industrial partners, Sun Microsystems and Storage Technology Corporation.

HPSS 3.2 has been the version in production use at most sites for more than a year. In December 1998, HPSS 4.1 was released by the collaboration and is expected soon to become the production storage system software at most sites. Version 4.1 provides significant improvements in scalability, performance, end-user access, small-file support, and input-output support for massively parallel supercomputers.

ORNL's primary customer for HPSS is the ARM project; the Laboratory's role is to provide and support the data archive. The ORNL HPSS system manages the hierarchy of devices storing more than 3.5 billion measurements. It can place 2000 new files a day into storage. It will eventually be able to routinely find and retrieve up to 5000 files an hour to meet the growing requests for information related to global change.

Facing a Future of More Carbon Dioxide for Forest Trees

Take an eastern deciduous forest—the type that displays brilliantly colored leaves in the fall. Expose it to air enriched in 50% more CO_2 than is present in the atmosphere. Reduce the amount of water normally available to this forest.

Is this a recipe for slower or faster forest growth? Because of the expected rise in the combustion of fossil fuels to satisfy the world's growing energy appetite, scientists want to know if additional emissions of CO_2 might significantly affect the growth of forest trees. What about feedbacks from the forest to the atmosphere? If a forest is affected by increases in CO_2 concentrations that can influence the climate, could the forest itself affect the climate?

To face these tough questions, ORNL has a world-class user facility in a forest that features free-air CO_2 enrichment (FACE) technology. The hardware for the selected hardwoods—a 10-year-old sweetgum plantation in the Oak Ridge National Environmental Research Park—elevates the air's CO_2 concentration across the plantation's 25-meter-diameter plots. Because the plantation has no walls, the effects of elevated CO_2 can be studied under natural field conditions. The facility is open not only to nature but also to researchers from universities and other laboratories across the nation who wish to study the response of forests to atmospheric CO_2 enrichment.

"Plant physiologists and ecologists have learned a great deal about how small trees and other plants will respond to increasing CO_2 concentrations in the atmosphere, but it is much harder to say how a whole forest will respond," says Richard J. Norby, leader of the collaboration at the FACE facility. "Understanding the response of forests is challenging because they are tall and biologically complex. Fortunately, next-generation technology in the FACE facility should help us better evaluate the sensitivity of forests to global change and, in turn, understand the dynamic role played by forested ecosystems in the earth's climate system."


Curtis Boles

Standing tall in a small sweetgum plantation are a tower and vent pipes that provide the trees with additional amounts of carbon dioxide. This hardware is part of ORNL's novel free-air CO_2 enrichment system. During the first year of exposure to the increased CO_2 concentrations, the trees grew faster and conserved water.

It is known that forests provide a critical "biotic" feedback between the earth's terrestrial vegetation and our ever-changing climatic system. Each is dependent on the other largely because forests and the atmosphere are sources of water and CO_2 to each other. Large-scale studies of these interdependencies are needed for accurate climate predictions and for understanding the structure and function of our future forest resources. These interdependencies were underscored by the first-year results at the FACE facility—forest growth was increased and the limited supply of water was conserved in the CO_2-enriched plots.

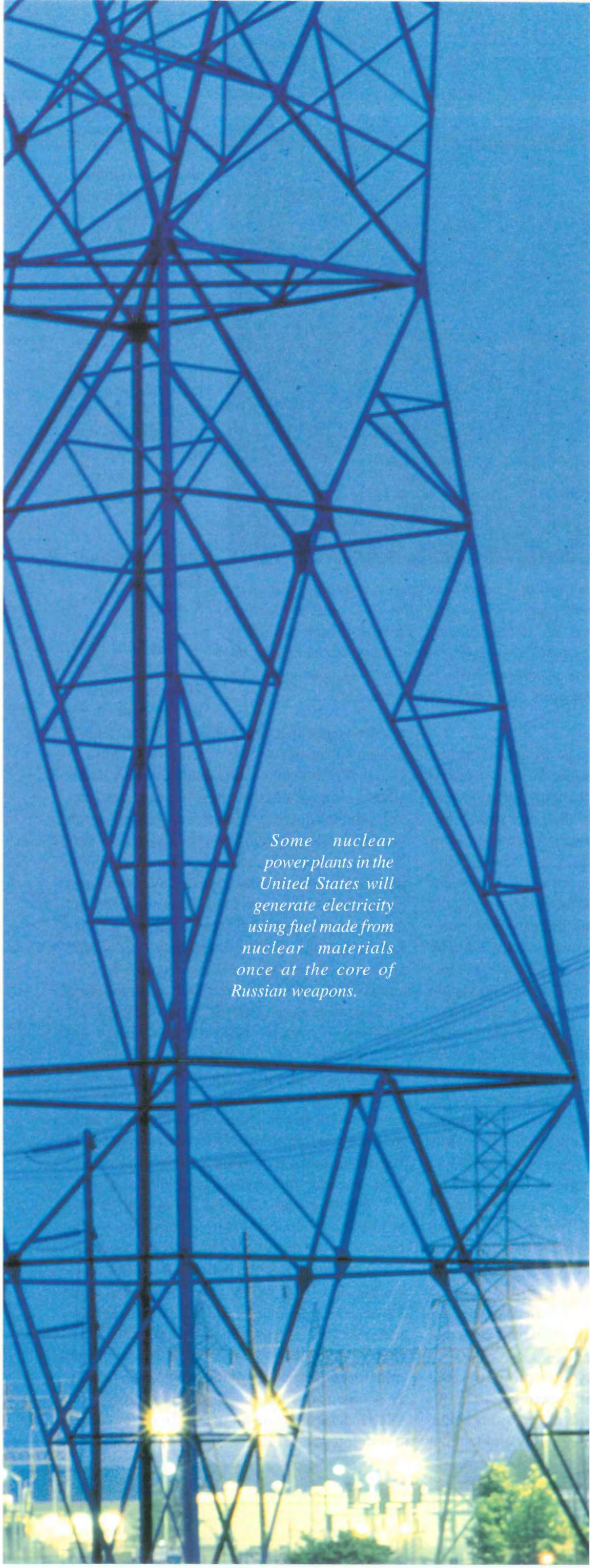
During the first year of the experiment, the ORNL scientists observed that the tree leaf pores (stomata) that allow CO_2 to enter and water vapor to escape were not open as wide in plots receiving the extra CO_2. As a result, trees in the CO_2-enriched atmosphere conserved water, while maintaining much higher rates of photosynthesis—the process by which plants use the energy from sunlight to convert CO_2 and water into the sugars needed for growth. The researchers also detected a significant increase in the production of wood in the tree trunks and very fine roots in the soil. Evaluation of changes in the nitrogen content in trees and soil will help scientists determine if these important growth responses will be sustained for many years.

The FACE facility complements the Throughfall Displacement Experiment in Walker Branch Watershed, which allows study of the responses of forest trees to not only ambient but also above ambient and below ambient levels of precipitation that may be typical of a changing climate. ORNL scientists are setting the standard for large-scale ecological research that could provide a recipe for success in predicting correctly the impact of future climate on forest productivity.

Capturing and Isolating Carbon

In April 1999, DOE released a 200-page "working draft" describing research paths that could lead to long-term technologies that might slow or stop the buildup of CO_2 in the atmosphere and delay possibly undesirable climatic effects. This "research and development roadmap" identifies key research needed to allow development of a variety of carbon sequestration technologies. These technologies might separate and capture CO_2 from energy systems, make products from some of the carbon, and sequester the rest in oceans, geological formations, and terrestrial ecosystems such as forests, vegetation, soils, and crops. Just recently DOE awarded a research contract for a collaborative team of ORNL, Pacific Northwest Laboratory, Argonne National Laboratory, and several universities to form a center to perform research on ways to enhance uptake and long-term sequestration of atmospheric CO_2 by terrestrial ecosystems. DOE also awarded a center to Lawrence Livermore National Laboratory and Lawrence Berkeley National Laboratory to perform research on ocean sequestration of carbon.

The draft was compiled, edited, and printed at ORNL. Its chapters were coauthored by experts from DOE national laboratories and universities throughout the nation. One of the leaders for this DOE effort was ORNL Associate Director David Reichle, and key chapter authors included ORNL researchers Rod Judkins, Gary Jacobs, Allen Croff, and others. The expected need for carbon sequestration technologies is likely to open up new research opportunities for ORNL scientists and engineers in clean energy technologies and climate effects research.



Photograph courtesy of the Tennessee Valley Authority

Some nuclear power plants in the United States will generate electricity using fuel made from nuclear materials once at the core of Russian weapons.

Dealing with Nuclear Materials

ORNL is developing methods to enhance national security and nuclear reactor safety, produce radioisotope forms to improve human health, and remove hazardous nuclear materials from the environment.

Originally, ORNL was considered a nuclear lab. Now, it's an energy and environmental research lab, but our missions include protecting nuclear materials, producing electricity from nuclear energy, isolating the hazardous nuclear materials from the environment, and making the beneficial ones available for medical purposes.

Our nuclear programs have changed over the past half century. At first we were dedicated to helping the nation build an atomic bomb to end a terrible war. Then our major goal was to develop nuclear energy as a safe and reliable source of part of the nation's electricity. Now, our most pressing goals are to support the conversion of bomb-grade uranium and plutonium from U.S. and Russian weapons into fuel suitable for power-generating reactors—and to confirm that the conversion occurred.

Converting Nuclear Weapons to Energy

At the end of the Cold War, the United States and the former Soviet Union agreed to dismantle a large number of nuclear weapons, creating a surplus of plutonium and highly enriched uranium. Such large inventories of nuclear material in both countries are potentially dangerous. Outlaw groups could divert this material for use in making nuclear weapons.

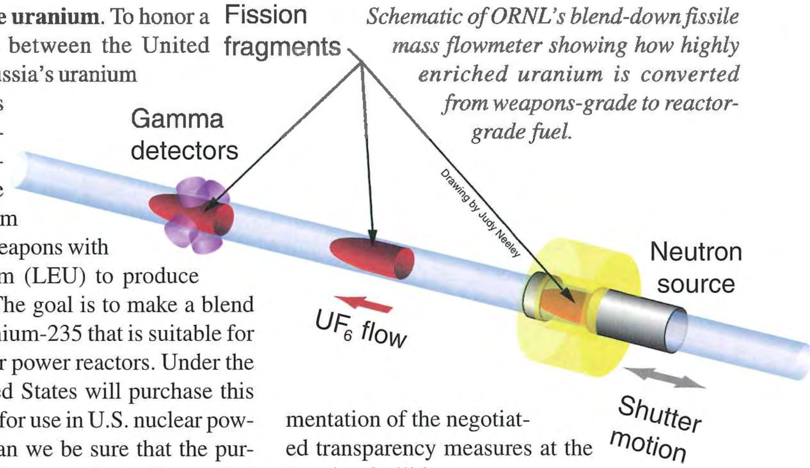
Weapons-grade plutonium. Last year, based on the results of ORNL studies, the Clinton administration decided to pursue a dual-track strategy for dealing with weapons-grade plutonium. One approach is to immobilize some of it in glass or ceramic logs. The second is to mix the rest with depleted uranium to form a mixed oxide (MOX) fuel for use in power reactors.

"ORNL is participating in experiments with several national laboratories to demonstrate technologies needed for such a plutonium disposition program," says Gordon Michaels of the Engineering Technology Division. "This past year we designed and managed a program to test nuclear fuel fabricated with plutonium extracted from nuclear weapons."

MOX fuel may harbor small amounts of gallium contained in the plutonium. Gallium may interact with the reactor fuel's zirconium cladding enough to damage it. Thus, tests must be conducted to determine if a gallium problem exists. In addition, the effects on fuel performance of other unique isotopes found in weapons-grade plutonium must be evaluated. Also, it must be determined whether it is safe to use MOX fuel containing plutonium oxide powder produced from a metal alloy using a "dry" conversion process. This process is being considered, if sufficient purity can be obtained, because it may produce less waste than the "wet" plutonium-production process used in commercial MOX fuel fabrication facilities in Europe.

This past year, under ORNL management, reactor fuel made from weapons-grade plutonium was tested for the first time. Eleven fuel capsules containing MOX pellets were fabricated at Los Alamos National Laboratory. The capsules, each slightly larger than a pencil, were then taken to Idaho National Engineering and Environmental Laboratory, where they are being irradiated with neutrons for different lengths of time at the Advanced Test Reactor. The first set of partially irradiated capsules was shipped here in November 1998. An ORNL group led by Steve Hodge, who designed the capsule irradiation hardware, is now examining the first set of irradiated fuel. "So far," Hodge says, "we have seen no sign of harmful effects caused by gallium. But the full story won't be known until the planned irradiation is completed in 2000."

Weapons-grade uranium. To honor a bilateral agreement between the United States and Russia, Russia's uranium processing facilities are blending (diluting) the highly enriched weapons-grade uranium (HEU) from dismantled nuclear weapons with low-enriched uranium (LEU) to produce reactor-grade fuel. The goal is to make a blend that is below 5% uranium-235 that is suitable for use as nuclear fuel for power reactors. Under the agreement, the United States will purchase this material from Russia for use in U.S. nuclear power plants. But how can we be sure that the purchased blend actually came from dismantled Russian weapons rather than from enrichment facilities? ORNL has the answer.



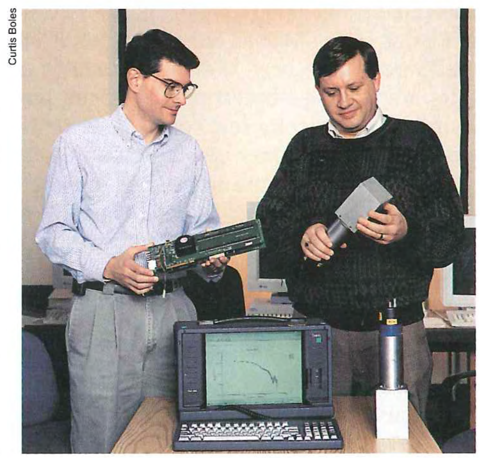
Schematic of ORNL's blend-down fissile mass flowmeter showing how highly enriched uranium is converted from weapons-grade to reactor-grade fuel.

Drawing upon our many years of experience in noise analysis, José March-Leuba, Jim A. Mullens, John T. Mihalczo, and others in the Instrumentations and Controls Division developed a technique using californium-252 neutron sources for activating the gaseous HEU streams as they flow through blending points in Russian facilities, thereby confirming that the blend-down is occurring. The technique measures the velocity and concentration of fissionable uranium-235 flowing into and out of the blending points, thus determining if the HEU gas mixture has been blended down to the desired LEU product level. ORNL engineers, under the leadership of Jim McEvers, designed and built these systems to not only accomplish the required measurements but also to comply with Russian facility safety and radiation regulations. The system was successfully demonstrated with flowing uranium hexafluoride gas in the uranium enrichment facility at Paducah, Kentucky. Under the continued leadership of Bill Sides, current plans are focused on installing and placing into operation three HEU flow monitor systems at Russian facilities at Novouralsk and Zelenogorsk. Two complete systems were installed at Novouralsk in January 1999. This work was performed in support of the U.S.-Russian Highly Enriched Uranium Purchase Agreement in which the Department of Energy's Office of International Nuclear Safety and Cooperation, HEU Transparency Implementation (NN-30), is responsible for implementation of the negotiated transparency measures at the Russian facilities.

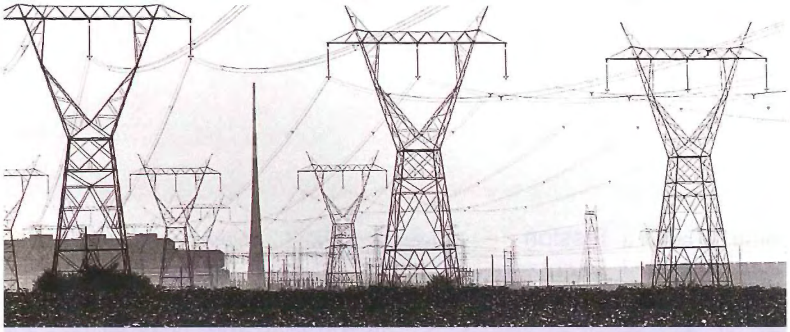
Identifying Nuclear Materials

When a nuclear weapon is dismantled, how do we know that all the fissile material has been removed? How can we be sure that the removed uranium-235 or plutonium-239 is present in the designated storage area? How can it be verified that a nation has no more nuclear weapons or nuclear material than it declares and that it is complying with bilateral treaties? How can a facility's managers be sure that a shipment contains the nuclear material ordered or that nuclear material is absent from a container? How can we be certain that highly enriched uranium is in a storage vault or that a train carload of spent nuclear fuel won't go critical, causing an inadvertent release of radiation?

To answer these questions reliably, a group of ORNL researchers including Mihalczo, T. E. Valentine, J. K. Mattingly, Jim McEvers, and others have developed a nonintrusive nuclear materials identification system. It uses neutrons from a fissioning californium-252 source to induce fission in fissile material present in a target container; two detectors on the opposite side of the container detect the emitted gamma rays and neutrons, which indicate the type and amount of nuclear material present, if any.



Eric Breeding holds the electronic board that is the heart of the more compact version of the nuclear materials identification system, while he and Jim Mullens examine its detector.



Helping NRC Advance Reactor Safety

Since its creation in 1974, the U.S. Nuclear Regulatory Commission (NRC) has been a principal sponsor of research to advance nuclear technologies. Because ORNL has been a leading participant in the performance of NRC research, we have been better able to maintain our role as a nuclear laboratory, especially over the past 15 years. "We are still doing important nuclear safety work for the NRC," says Claud Pugh, head of NRC programs at ORNL.

For example, in 1998 ORNL investigated whether electric utility industry restructuring would increase the risk of loss of off-site power (LOOP) to nuclear power plants. Risk analyses have shown that LOOP events lead to increased risk of reactor fuel core damage in the event of an accident. An ORNL team—B. J. Kirby of the Engineering Division and A. Bruce Poole and John D. Kueck, both of the Engineering Technology Division—found significant differences in the way restructuring is being carried out during their visits to 17 nuclear plants in 10 regions.

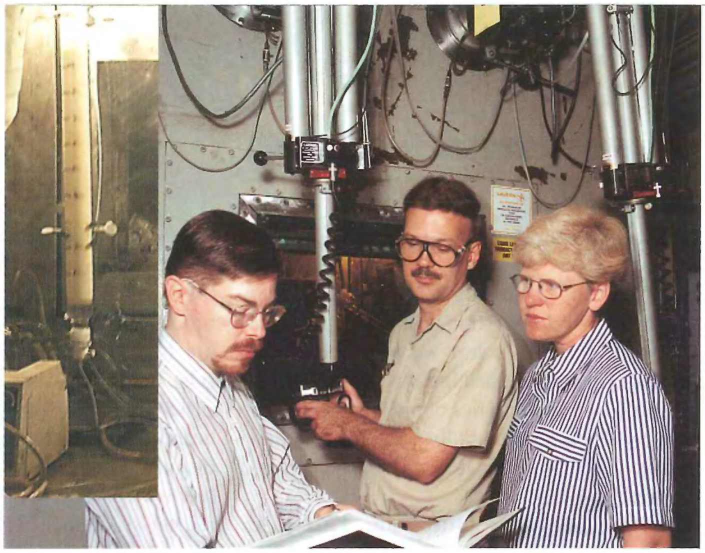
Historically, the electric power industry in the United States has been dominated by utilities that control the generation, transmission, and distribution of electricity in their service areas. With restructuring, power suppliers will compete for customers located anywhere on the national transmission grid, and regional grid control will be the responsibility of independent system operators (ISOs).

"It is uncertain how the ISOs will maintain reliability of the grid, and specifically, the reliability of the circuits that provide power to nuclear power plants," Kueck says. "The nuclear industry and NRC need to better understand the synergism among power plants within a given region." They also must understand how distribution of responsibilities and increased competition for the most economical power (often obtained from outside an ISO's geographic area) can affect the potential for LOOP events. To get better answers, probabilistic risk assessments may be performed.

In the Heavy-Section Steel Irradiation Program, Randy Nanstad, Shafik Iskander, Don McCabe, and Mikhail Sokolov, all of ORNL's Metals and Ceramics Division, have been developing data to account conservatively for irradiation embrittlement of reactor pressure vessel steels. Neutrons from reactor fuel cores cause the ferritic steels in reactor pressure vessels to become a little brittle, but they normally don't develop cracks from the high temperatures and water pressures typical of reactor operation. To determine how resistant these embrittled vessel steels are to fracture, the researchers, including ETD's John Merkle, have developed a new experimental fracture mechanics method that requires fewer experiments than were needed before for each steel examined.

"The method helps the reactor operator and the NRC determine whether the embrittled steel is sufficiently resistant to fracture to ensure that the continued operation of the vessel is safe," Nanstad says.

This "master curve" concept has been accepted as an American Society for Testing and Materials standard. Other countries are considering using the concept in their commercial nuclear power programs. This accomplishment is one of many reasons why ORNL has long been the NRC's lead laboratory for nuclear pressure vessel technology.



Jim Richmond.

Dairin Malkemus, Greg Groover, and Rose Boll discuss plans for extracting actinium-225 from the thorium column in a hot cell to meet a request of a research project sponsored by the National Institutes of Health. Inset: closeup of the thorium column (yellow tube) in the hot cell from which actinium-225 is produced for nuclear medicine research.

"Over the years," says Mihalczo, an ORNL Corporate Fellow, "we have made this system more sensitive, more portable, and easier to use. This technology has been transferred to the Russians so they can use it to verify that fissile material has been removed from their dismantled nuclear weapons."

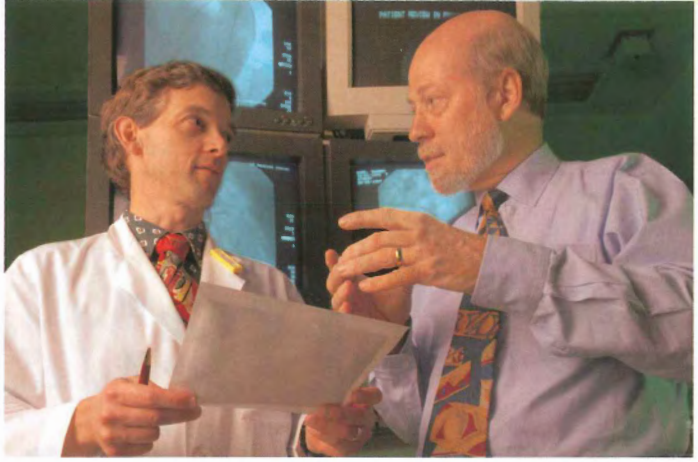
Therapeutic Isotope from ORNL Stockpile of Uranium-233

ORNL has its own stockpile of uranium, which is deemed a potential boon to health. We are storing more than 400 kilograms of uranium-233, which had been intended for use as fuel in our old molten salt breeder reactor program and for tests of other reactor concepts. Uranium-233 is valuable because it decays and forms thorium-229, which, in turn, decays and forms actinium-225. We have learned to recover thorium-229 chemically to meet the demand for actinium-225. When placed at the top of an ORNL-developed radioisotope generator, actinium-225 decays to form a continuing supply of bismuth-213, a rare emitter of high-energy alpha particles, which is being investigated as a radioimmunotherapy agent for treating cancer patients. "So far," says Jerry Klein, who leads ORNL's isotope program, "early results with leukemia patients in clinical trials at Sloan-Kettering Cancer Center have been promising." ORNL's Brad Patton notes that, as the demand for the radioisotope rises both for medical research on animals and for the treatment of patients, the only significant source of bismuth-213 in the western hemisphere is ORNL's uranium-233 stockpile.

Isotope Technique Helps Heart Patients

A heart attack may strike when a coronary artery has been narrowed by the accumulation of fatty deposits. Some heart patients are treated with balloon angioplasty to clear the blockage, widen the artery, and restore full blood flow to the heart muscle. But, six months later 30 to 40% of the 450,000 Americans who have the procedure each year face a different type of blockage. Their coronary arteries become reclogged by the buildup of smooth muscle cells in response to balloon-induced vessel damage, a condition known as restenosis. Thus, these patients must undergo additional angioplasty or heart bypass surgery to unclog their reclogged arteries. These second operations add $1 billion to the nation's health care bill.

One promising approach to preventing restenosis is to couple angioplasty with radiation from rhenium-188, which is expected to inhibit smooth muscle cell proliferation, based on animal studies. This isotope can be easily produced for hospital patients by a radiopharmacy-based tungsten-188/rhenium-188 generator system developed at ORNL under Russ Knapp,



Robert Spencer (left), a cardiologist in the Knoxville Cardiovascular Group, and Russ Knapp, head of the ORNL Nuclear Medicine Program, discuss their approach for a new collaborative project between the University of Tennessee Hospital and ORNL for inhibiting restenosis.

head of ORNL's Nuclear Medicine Group in the Life Sciences Division. The source of the tungsten-188 is ORNL's High Flux Isotope Reactor.

"The idea is to use a highly concentrated rhenium-188 solution to inflate the balloon at low pressure following high-pressure balloon inflation with saline to unclog the artery," Knapp says. "At ORNL we developed techniques for concentrating the rhenium-188. We provide generators that are being used for restenosis studies at various sites under physician-sponsored protocols approved by the Food and Drug Administration or similar regulatory agencies in other countries."

An initial six-month follow-up study of the results of this experimental treatment for 25 patients in Perth, Australia, found that only 4% of the patients developed restenosis, or about one-tenth of the expected rate. The Nuclear Medicine Group considers these results encouraging.

Conversion Process Designed for Cleanup of Molten Salt Reactor

In March 1994, analysis of two samples drawn from the off-gas piping at ORNL's long dormant Molten Salt Reactor Experiment (MSRE) yielded surprising results. The gas was saturated with radioactive uranium hexafluoride (~10% $^{233}UF_6$), and 50% of it was fluorine, a highly reactive gas. This gas was found to have migrated to an adjoining underground charcoal bed where it formed potentially explosive compounds (partially fluorinated carbon) and a uranium deposit that posed a significant nuclear criticality risk. Employees working in the reactor building were immediately evacuated and relocated because of fears of a criticality incident or chemical explosion that could release U-233 to the environment.

Since the discovery of this condition, a number of important steps have been taken by ORNL's Chemical Technology Division (CTD) to minimize the potential hazards posed by mobile uranium and fluorine. By the end of 1998 CTD had eliminated the possibility of a criticality accident or chemical explosion in the charcoal bed and had removed and trapped the volatile UF_6 and fluorine in forms suitable for interim storage. Almost all of the volatile UF_6 was removed and chemically sorbed on sodium fluoride (NaF) traps in secure containers. Configuration changes were made to eliminate the potential for nuclear criticality. A novel chemical treatment of the charcoal with ammonia (devised by CTD's Bill Del Cul, Mac Toth, Darrell Simmons, and Lee Trowbridge) removed the possibility of a chemical explosion.

A longer-term remediation activity is under way to address the causes of this unsafe condition so it won't appear again. Now that the uranium deposit has been stabilized, preparations are being made to remove it from the charcoal bed. Because of its exposure to radiation, the reactor fuel salt is still generating fluorine gas that could convert the uranium tetrafluoride (UF_4) in the fuel to additional UF_6. The reactive-gas-trapping technology used in the first remediation phase will support the eventual stripping of the remaining uranium from the fuel salt. In the final remediation phase, the fuel salt will be stripped of its uranium, removed from the reactor system, and packaged for final disposal.

The final technical challenge confronting ORNL is to make the U-233 packages generated by the remediation suitable for long-term storage. The UF_6 sorbed on NaF traps and the uranium deposit on the charcoal bed must be converted to a stable oxide prior to storage. Conventional aqueous processes for converting fluorides to oxides are not appropriate for highly radioactive MSRE uranium. To efficiently meet the need for a highly contained system that prevents uranium losses and produces little secondary waste, a CTD team (Del Cul, Alan Icenhour, Simmons, and Jeff Rudolph) developed an integrated conversion process that will begin operating in Building 4501's hot cells in August 2000.

In a closed system, the UF_6 will be recovered from either an NaF trap or a charcoal deposit batch and then converted to a stable uranium oxide (U_3O_8). The converted MSRE uranium will be stored at ORNL's U-233 repository.

Novel Ion Exchange Resin Removes Groundwater Contaminants

ORNL and UTK researchers have prepared a novel material to cleanse groundwater of two persistent pollutants, one of which comes from nuclear operations. They have developed the BiQuat bifunctional anion exchange resin, which effectively and selectively removes trace levels of two hazardous groundwater contaminants, pertechnetate (TcO_4^-) and perchlorate (ClO_4^-). The new resin can cleanse five times more groundwater than the best water-treatment resin on the market.

These groundwater contaminants are present at parts-per-billion concentrations and as negatively charged ions, or anions. Pertechnetate and perchlorate at trace levels are not efficiently removed by routine cleanup methods.

The leader of the resin development effort funded by DOE was Gilbert Brown, of ORNL's Chemical and Analytical Sciences Division (CASD). His collaborators are Baohua Gu at ESD, Spiro D. Alexandratos of the University of Tennessee at Knoxville, and Peter V. Bonnesen and Bruce Moyer, both of CASD.

Because the BiQuat resin is so selective, it removes both compounds, making the treatment process more efficient and cost effective. It does not alter the water quality by adding undesirable secondary by-products or removing desirable minerals. "The resin is bifunctional," Brown says, "because it has two different kinds of exchange sites. One site is highly selective for pertechnetate anions and the other swaps chlorine ions quickly with the anions the first site attracts."

Pertechnetate is the chemical form of radioactive technetium-99, a fission product of enriched uranium used to fuel research, production, and power reactors. This beta emitter, which has a half-life of 213,000 years, is present in groundwater at many DOE sites, including Paducah, Kentucky; Portsmouth, Ohio; and Hanford, Washington.

Perchlorate, which comes from solid rocket propellants, is present in many groundwater contaminant plumes and surface water in California, Nevada, and other parts of the United States. Perchlorate, which has a chemical structure and properties similar to those of pertechnetate, is just now being recognized as a groundwater contaminant of concern because potentially it poses a threat to living organisms. Lockheed Martin Corporation came to ORNL for help in solving the problem.

A recent field trial demonstrated that the BiQuat resin can remove 60 parts per trillion pertechnetate and 50 parts per billion perchlorate to below detection limits. Larger-scale field studies using resin are being conducted by Purolite International to gather data to aid the design of a longer-lasting resin.

ORNL has made progress in finding ways to identify and protect nuclear materials, remove them from the environment, and convert them to energy and medical treatments.

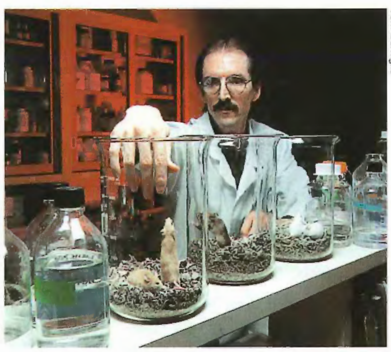
MYSTERIES of Life: From Molecules to Mice

Understanding how proteins work is a key to unlocking the secrets of life and health. Nothing happens in our bodies without them. As enzymes, proteins catalyze the living cell's chemistry. As hormones, these molecules regulate the body's development, direct our organs' activities, and organize our thoughts. As antibodies, they defend us against infection, but in their mutant forms or as coats on viruses, they help cause diseases such as sickle-cell anemia, cancer, or AIDS. What makes proteins so specific in observed functions are their unique shapes, which can range from ellipsoids to saucers to dumbbells.

Each type of protein has a highly specific, three-dimensional (3D) structure that determines its biological activity—that is, its function in each body cell. Each protein is a product of a specific gene, so to understand the function of each of the 80,000 to 100,000 genes in the human genome, it helps to know the shapes and activities of the proteins encoded by each gene. To understand how a cell works, it is crucial to know the 3D structures of its proteins.

A protein starts out as a string of amino acids (a combination of any of 20 different ones). The sequence of the amino acids is dictated by the order of the DNA bases in the gene that directs the protein's synthesis. The amino-acid string folds reproducibly to produce the protein's functional 3D shape. It's like bending a flexible wire connecting Ping-Pong balls of different colors to form a 3D complex shape that puts Ping-Pong balls of certain colors close together.

The protein's function depends largely on how it is folded to give it a specific 3D form. For example, folding brings together widely separated amino acids to form an active site—the catalytic region of an enzyme that binds with a biochemical substance to cause a specific activity in the body, such as digestion.



Tom Cerniglio

Ed Michaud watches the activity of normal and mutant mice in large beakers at the Mammalian Genetics Section research laboratory.

ORNL uses several technologies to determine the sequence of bases in genes and the structures of proteins, especially in the mouse (which is related genetically to humans). The ORNL-developed lab on a chip, mass spectrometry, and high-speed sequencing robots are being used to determine the order of bases in DNA sequences thought to contain genes. X-ray crystallography and mass

Greg Lamb

The human genome is composed of approximately 3.5 billion base pairs of DNA. Each base pair has the chemical letters A and T (for adenine and thymine), which are colored blue and orange; or it has the chemical letters C and G (for cytosine and guanine), which are colored red and green. Scientists are trying to determine the order of these base pairs in long stretches of human DNA.

spectrometry are used to decipher the structure of mouse proteins, including those involved in inflammation, a characteristic of diseases found in both mice and humans. Another approach at ORNL is to predict protein structure using computer modeling.

Predicting Protein Shapes

Although the amino-acid sequences of tens of thousands of proteins have been determined, the 3D structures of only about 1500 different proteins are known today. Amino-acid sequencing is a fairly rapid process, whereas determining the 3D structure of a protein is very time consuming and expensive. It can take a year for a crystallographer to determine the structure of a protein. Considerable time and money would be saved if the 3D structure of every protein could be predicted from its amino-acid sequence. Some researchers believe that, by 2005, computer modeling will accurately predict the structures of 75 to 100 unknown protein sequences a day. Then therapeutic drugs to block disease-causing proteins by matching their shapes might be developed more quickly.

The Computational Protein Structure Group in the Computational Biosciences Section of ORNL's Life Sciences Division has developed a suite of computational tools for predicting protein structure. The group, led by Ying Xu, includes Oakley Crawford, Ralph Einstein, Michael Unseren, Dong Xu, and Ge Zhang. Their computer package, called the Protein Structure Prediction and Evaluation Computer Toolkit (PROSPECT), allows a user to predict the detailed 3D structure of an unknown protein, including its shape and the location of each of its amino acids.

Using PROSPECT, the ORNL group has made predictions for all 43 target proteins in an international contest for protein structure predictions, called CASP-3. ORNL placed in the top 5% of about 100 groups worldwide.

One approach the group uses is "protein threading," a term suggested by embroidery in which a thread is pulled through a predetermined design. In this case, the thread is a string of amino acids. ORNL scientists computationally superimpose the same amino-acid sequence in 1000 different representative protein structures to determine the structure that is the best fit. They do calculations to determine which structure aligns the amino-acid atoms at their lowest energy level (where the atoms want to be) and in positions where they are compatible with their neighbors. The representative protein structure that best fits a target amino-acid sequence is predicted to be the target's approximate structure.

"We also use an approach called homology modeling to fine-tune the predicted structure," says Ying Xu. "We computationally 'tweak' the structure of the new protein by calculating the detailed forces between atoms and making adjustments in the final predicted structure to minimize the atoms' energies."

Research groups from the National Institutes of Health, the Department of Energy's Lawrence Berkeley Laboratory, Amgen, and Boston University have expressed interest in using PROSPECT in their research and in collaborations with ORNL to further develop the computer toolkit. By folding their ideas together, the collaborators may soon solve a classic problem.

Computing the Genome

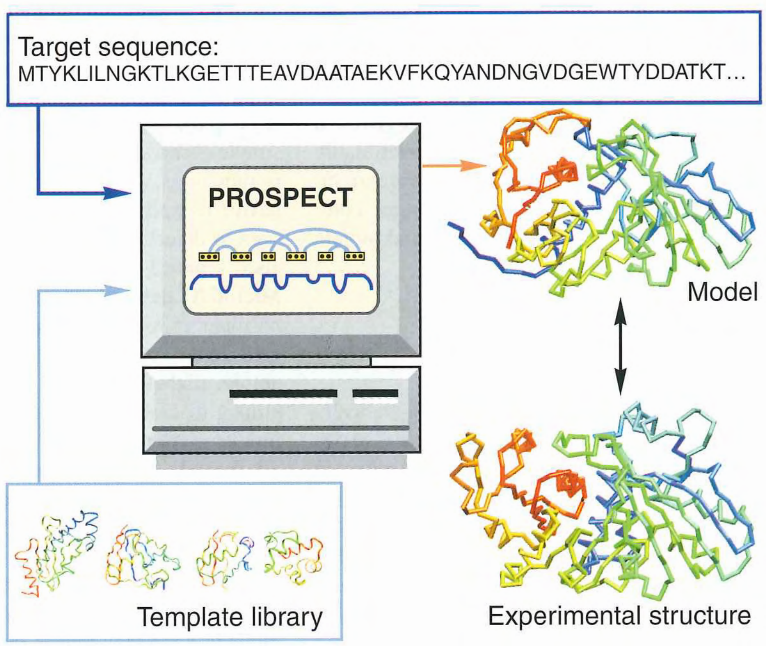
A team of researchers in Europe spent two years searching for the gene responsible for adrenoleukodystrophy, a disease described in the movie *Lorenzo's Oil*. The team tried the standard experimental techniques of mapping and sequencing. The researchers fragmented the chromosome believed to harbor the gene, producing ordered pieces of a manageable size. They placed these fragments into high-throughput sequencing machines. They obtained the order of the chemical bases in the entire chromosome. But they still couldn't find the gene. So in 1995 they e-mailed information on the sequence to the Oak Ridge computer containing the ORNL-developed computer program called Gene Recognition and Analysis Internet Link (GRAIL™). Within a couple of minutes, using statistical and pattern-recognition tools, GRAIL™ returned the location of the gene within the sequence.

The ability of computing to find patterns in a flood of data gathered through mapping and sequencing is being increasingly appreciated by biologists. In the next four years, a new sequence of approximately 2 million DNA bases will be produced every day. Each day's sequence will represent about 75 to 100 new genes and their respective proteins. This information will be made available immediately on the Internet and in central genome databases.

The DNA building blocks of several living organisms—a methane-producing microorganism from deep-sea volcanic vents, an influenza virus, yeast, and the round worm (*C. Elegans*)—have been completely sequenced. The sequencing of other organisms (e.g., the fruit fly) will be completed soon. The three million links in the human genome chain are expected to be completely sequenced by 2003, and 10,000 of our 80,000 to 100,000 genes will be identified then. Plans call for the order of DNA bases in the mouse genome to be determined by 2005.

But a complete set of sequence data for any organism may not be very useful to medical researchers, molecular biologists, and environmental scientists without organized and comprehensive computational analysis. Such comprehensive genome analysis is needed to help researchers understand the basic biology of humans, microbes, plants, and other living organisms.

To provide a comprehensive genome-wide analysis of genome sequence data from different organisms and help integrate biological data around a genome-sequence framework, ORNL and a team of researchers at the DOE Joint Genome Institute, Lawrence Berkeley National Laboratory, Baylor College of Medicine, Hospital for Sick Children (Toronto), Johns Hopkins University, Washington University, University of California at Santa Cruz, University of Pennsylvania, and the National Center for Genome



Using a computer program such as PROSPECT, ORNL researchers can predict the likely three-dimensional structure of a protein from the order of the amino acids in the "target sequence."

Resources have constructed a computational resource that uses GRAIL-EXP, GENSCAN, and a suite of other tools to annotate genome sequences. Annotation is the process of organizing biological information and predictions in a sequenced genome framework (e.g., linking what a gene does to its structure). (See http://compbio.ornl.gov/gac/index.shtml).

The team has developed a plan and has built a first prototype of the needed genome analysis framework and toolset. The prototype can do the following:

- Retrieve biological data and assemble genomes;
- Compute genes, proteins, and genome features from sequences and experimental data (e.g., the group that developed PROSPECT is predicting protein structure from amino-acid sequences available on ORNL computers);
- Compute homology and function among genomes, genes, and gene products (e.g., proteins);
- Model the three-dimensional structure of gene products; and
- Link genes and gene products to biological pathways and systems.

"We have made considerable progress in addressing some data management, data storage, and data access issues," says Ed Uberbacher, head of the Computational Biosciences Section in ORNL's Life Sciences Division. "For example, we developed a unique information resource and Web browser called the Genome Channel, which is available on the Internet. It gathers the results from sequencing centers around the world. It provides a fully assembled view of what is known about the human genome and its chromosomes, sequences, and experimentally cloned genes. It also provides information on computationally predicted genes. The Genome Channel is currently being used by the worldwide genome community to identify and predict gene and protein sequences of interest."

Producing and Screening for Mouse Mutations

Because mice and humans are genetically so similar, biologists can study genetic diseases in mice to better understand similar disorders in humans. DOE considers the mouse to be the most important mammalian model organism, and DOE's Human Genome Project has proposed to devote 10% of its efforts in DNA sequencing to the mouse genome. ORNL is playing a major role in determining the functions of mouse genes as a part of the Human Genome Project.

ORNL's Mammalian Genetics Section of the Life Sciences Division, with a large capacity for mouse production and a long history in mouse genetics and mutagenesis, has taken the lead in mouse functional genomics for DOE. The long-term goal of functional genomics at ORNL is to develop and employ the fastest, smartest, cheapest, and most efficient, high-throughput methods for generating and analyzing mouse mutations to help discover the functions of all 70,000 to 100,000 mouse genes.

Starting in the late 1940s, ORNL researchers led by Bill and Liane Russell developed mutant strains of mice as they studied the genetic effects of radiation and chemical exposures on the animals. Using these experimentally induced mutations as a starting point, current studies are designed to find not only obvious changes in characteristics (phenotypes), such as altered coat color, but also more subtle disease phenotypes caused by a change in or deletion of a gene (genotype). The mutant stocks generated in ORNL's historic program to assess the genetic risks of exposing mammals to radiation make ideal targets for current mutagenesis efforts. For example, some of these mutant stocks contain deletions of a known section of a chromosome, and when combined with a chemically induced single-gene mutation in the same section of the paired chromosome, results in a mouse lacking any normal copies of that single gene. Using this approach, the mouse lacking the normal gene will reveal the function of the gene based on the resulting disease phenotype, and the chromosome deletion serves to identify the approximate physical location of the gene.

Eugene Rinchik, one of the staff scientists leading research in this program, focuses on making mutations in mice and then using various techniques to discover the resulting phenotypes. Among the techniques employed, in addition to simple observation of the animals that could carry mutations, are tests for motor ability and behavior, as well as analysis of body fluids and tissues to detect subtle differences. The mice are also scanned in ORNL's newly developed MicroCAT device (see next section) to see internal changes such as fat deposits and enlarged organs. In these ways, mutations that cause, for example, diabetes, obesity, depression, anemia, kidney disease, nervous disorders, or stomach problems may be detected. Once a mutation is confirmed, various molecular mapping techniques are used to isolate the chromosome region and then the actual gene causing the disorder in the mouse. By linking the disorder to the mutated gene, the normal function of the gene can then be deduced. For example, by locating a mutated gene that causes cleft palate in mice, ORNL's Cymbeline Culiat was able to analyze the normal gene that assists the closing of the palate in the developing mouse.

One way to make mutations in single genes is to inject male mice with ethylnitrosourea (ENU), a powerful chemical mutagen discovered by ORNL's Bill Russell in 1979. ENU causes the substitution of one chemical base for another in the DNA of male spermatogonial stem cells, which continuously produce mature sperm. When the ENU-treated male mouse is mated with an untreated female mouse, some offspring may have new mutations. Over the past 10 years ORNL's Eugene Rinchik and Don Carpenter isolated 31 new mutations in more than 4500 pedigrees from one large ENU experiment. In a second ENU experiment focusing on a different section of the mouse genome, they have so far isolated 19 new mutations from 1250 pedigrees tested, have mapped their positions on the target mouse chromosome, and have begun cloning the genes responsible for four of the new mutations.

Mouse mutations, then, have historically been made by treating live mice with mutagens and breeding offspring to look for mutations. Now, mutations can also be made very efficiently in a culture dish using special cells from early mouse embryos; these embryonic stem cells have not yet differentiated into specific cell types but retain the potential to become any kind of cell in the mouse. After using molecular techniques to replace a particular normal gene with a mutant one, or to produce a deletion or rearrangement of a whole section of chromosome in the embryonic cell, ORNL's Ed Michaud and his colleagues can use the specifically altered cell to produce a live mouse carrying the desired genetic change. If the new mouse exhibits a mutation, such as epileptic seizures, then the engineered genetic change is assumed to have caused the seizures.

The ORNL researchers also have the capability to make different types of mutations in the same gene to see the whole spectrum of functions in which a gene might be involved. Different gene mutations may completely turn the gene off so it produces no protein, lower the quantity of protein the gene produces, or alter the normal structure of the protein, causing a disease or disorder. According to Rinchik, a slightly injured gene resulting in a slightly altered mutant protein may help us understand the origin of a disease, because most human genetic diseases can be tied to a subtle alteration in a gene rather than a complete loss of gene function.

ORNL researchers Dabney Johnson, Karen Goss, Jack Schryver, and Gary Sega have developed high-throughput biochemical and behavioral screening tests for the detection of subtle mutations in mice. These tests are routinely performed on 100 mice per week. For example, one test used in screening measures how long mice can maintain balance on a rotating dowel rod in a test for neuromuscular coordination,

Green Genes: Genetic Technologies for the Environment


Tom Cerniglio

This series of heat-pulse probes inserted at various depths in a cottonwood tree provide measurements to help ORNL scientists estimate whole-tree water use in an experiment examining the interactions between genetics and environment in determining plant growth and productivity. This research is part of a CRADA project with Union Camp Corporation.

Gene technologies are spreading at ORNL. They are being used to improve the usefulness of microorganisms and green plants.

Detecting land mines using microbes. Reengineered bacteria could save people from underground devices engineered to kill them. These devices are land mines, which kill or maim 25,000 people a year. They are extremely difficult to find once they are buried in the ground. Plastic mines are almost impossible to locate because they elude metal detectors. Fortunately, most land mines leak slightly and leave traces of explosive chemicals such as TNT shortly after they are installed. ORNL has developed a clever way of using bacteria to detect this faint explosive signature.

Bob Burlage, a microbiologist in ORNL's Environmental Sciences Division, has genetically engineered microorganisms to emit light in the presence of TNT. As they recognize and consume TNT, the engineered bacteria produce a fluorescent protein that appears as a green light when they are illuminated by ultraviolet (UV) light.

"When the bacteria of one of our strains of *Pseudomonas putida* encounter the TNT, they will scavenge the compound as a food source, activating the genes that produce proteins needed to digest the TNT," Burlage says. "We attached a green fluorescent protein gene obtained from jellyfish to these activated genes and included a regulatory gene that recognizes TNT. As a result, the attached gene will also be turned on. It will produce the green fluorescent protein, which emits extremely bright fluorescence when exposed to UV light."

In a field demonstration in October 1998 in South Carolina, Burlage and his ORNL colleagues Martin Hunt, Steve Hicks, Mike Maston, Mike Keleher, and Keith Williams (all of the Instrumentation and Controls Division) successfully used the microbial technique to detect five out of five simulated mine targets in a 300-square-meter field. "In less than a year," Burlage says, "we went from the lab bench to the field and got better results than we expected. Microbial mine detection is much closer to commercialization than we anticipated."

The technique offers several advantages. It is inexpensive. It poses no hazard to operators. And it is virtually the only mine detection technology that could be used in the near future to detect mines over a very wide area. Now that Burlage has shown a better way to find land mines, he is hoping for support to move the technology into the commercial sector to help save lives.

Genetics and biomass energy. Genetic research has played an important role in DOE's Bioenergy Feedstock Development Program since its inception 20 years ago at ORNL. The purpose of the program is to develop renewable, biomass resources (e.g., poplar trees and switchgrass) that can be converted to liquid transportation fuels and chemicals or burned to produce electricity.

Program researchers at ORNL and elsewhere have identified model energy crop species for major U.S. agricultural production regions. Using molecular genetics and other breeding techniques, they have developed highly productive poplar varieties now being used for paper production. They have produced the first genetic linkage map for a hardwood tree species. They are exploring genetic marker–aided selection to tailor energy crops to maximize the energy they will produce.

At ORNL the program is led by Janet Cushman and Lynn Wright. Participating ORNL researchers are Anne Ehrenshaft, Mark Downing, Sandy McLaughlin, Marie Walsh, Virginia Tolbert, and Jerry Tuskan. Tuskan recently helped identify the first genetic marker limited to sex determination in trees. He used hybrid willow trees, which grow fast and are a good fuel source. The marker is present in all female hybrid willow trees but absent in the male trees. Early gender identification is important because male hybrid willow trees are more resistant to drought than female willows. Thus, the male trees are potentially more desirable for bioenergy plantations during global warming.

The Bioenergy Feedstock Development Program, Cushman says, will continue to use genetic technologies to make bioenergy resources less expensive and more competitive with fossil fuels. The appeals of bioenergy resources are that they are produced domestically, they offer a potential new market for farmers, and their consumption will not boost carbon dioxide levels in the atmosphere, slowing the onset of potentially devastating climate change.

Mike Maston (left) and Billy Schaefer examine an area around a land mine, taking soil samples from a site that was identified as a mine using the ORNL Microbial Mine Detection System. The insets show a tube of the microorganism as it fluoresces and a typical antipersonnel mine.

while another instrument quantifies the startle response to a sudden sound.

To increase the breadth and accuracy of screening for mutant mouse phenotypes at what Johnson calls the Screenotype Center, ORNL has organized the Tennessee Mouse Genome Consortium (TMGC). The TMGC taps into the expertise of academic and clinical researchers across the state; membership consists of the University of Tennessee at Knoxville, UT-Memphis, St. Jude Children's Research Hospital, Vanderbilt University, and Meharry Medical College. The TMGC participates both in screening mice for new mutations and in more detailed analysis of confirmed mutations. If, for example, a mutant strain has epileptic seizures, ORNL sends mice or samples from mice to consortium members qualified to determine if the cause is neurochemical or neurophysical and if this mouse is a good model for some form of human epilepsy. Currently, consortium members are helping ORNL screen mice for vision and hearing problems, brain and other organ malfunctions, neurotransmitter content in the brains, and the normal production of sperm cells.

MicroCAT "Sees" Hidden Disorders in Research Mice

A mouse may be able to hide from a cat, but some types of genetic disorders hidden in mice can now be seen by the MicroCAT miniature X-ray computerized tomography (CT) system devised by Mike Paulus, Hamed Sari-Sarraf, and Shaun Gleason, all of the Instrumentation and Controls (I&C) Division. This high-resolution X-ray imaging system, a kind of CT scanner for mice, allows biologists to see a detailed, three-dimensional image of the internal structure of a mouse in just a few minutes. Traditionally, determining if mice carry subtle anatomical disorders has been a slow, labor-intensive, manual process. Now, this new tool greatly cuts the time needed to determine accurately if a mouse has internal malformations not visible upon external inspection. Thus, it may speed the process of finding cures for some human diseases. For example, imaging of specific fat deposits in an anesthetized mouse allows ORNL researchers to track both the accumulation of fat in a mouse that carries mutant genes involved in obesity and the result of dietary or other obesity treatments.

Bret Pate

Normal mice maintain their balance on the rapidly turning Rotor-Rod. Because mice having certain mutations lack the coordination and balance of normal mice, they can be identified in the Rotor-Rod test because they fall off the rotating rod more quickly.

The I&C group is writing software to allow the computer to inspect and analyze the images to alert researchers to possible abnormalities of interest. The MicroCAT tool has already attracted the attention of researchers around the country who would like to image their own research animals using the Oak Ridge prototype.

Mouse Gene for Stomach Cancer Identified at ORNL

In a search for a gene thought to cause some mice to be born deaf, an ORNL researcher determined that the same gene can cause stomach cancer in mice. The discovery could speed up understanding of how both mice and humans get stomach cancer.

The research was performed by Cymbeline (Bem) Culiat, a staff molecular biologist with the Mammalian Genetics Section in ORNL's Life Sciences Division, in collaboration with former ORNL researcher Lisa Stubbs, now with DOE's Lawrence Livermore National Laboratory (LLNL).


Bret Pate

Bem Culiat washes DNA samples of cloned mouse genes isolated and purified from bacterial cultures where multiple copies of the genes are made.

Former ORNL biologist Walderico Generoso had induced the deafness mutation, designated 14Gso, in mice by irradiating male mice with X rays and then mating them with untreated female mice. Unlike normal mice, 14Gso mouse pups were not startled by loud noises, their heads persistently bobbed, and they frequently ran in circles in their cage. These behaviors suggested defects in the inner ear, where hearing and balance are controlled. Studies of the inner ear structures showed they were too defective to allow sounds to be heard.

To locate the gene believed responsible for deafness in these mutant mice, Culiat focused on the tips of two of their chromosomes (7 and 10). Through microscope studies of stained chromosomes, ORNL's Nestor Cacheiro found evidence that genes on both tips had been disrupted and their parts exchanged. Culiat began hunting for the deafness gene in the tip of chromosome 7, which is mapped more extensively than chromosome 10 in the mouse.

Using various genetic and molecular mapping techniques, Culiat localized the mutated region in chromosome 7 to a DNA segment containing *muc2* (intestinal mucin 2), a gene coding for a major protein in the mucus lining of the intestine. A literature search indicated that one end of the protein produced by the human *MUC2* gene is very similar to another protein associated with deafness in humans, thereby making *muc2* a candidate gene for the inner ear defects observed in 14Gso mice.

"I checked the expression of this *muc2* gene in the deaf mice by measuring their levels of RNA, which carry the gene's instructions for synthesizing protein," she says. "The gene is normally expressed in the intestine and kidney, but I found it was overexpressed in the stomach and lungs and showed a loss of expression in kidneys of the mutant mice. In humans, the overexpression of *muc2* in the stomach is associated with chronic gastritis leading to gastric lymphomas and adenocarcinomas. Therefore, we predicted the same defects will occur in the mutant mice."

Stomach pathology studies and examination of the gastrointestinal systems of 14Gso mice by Xiaochen Lu, a researcher in Stubbs' LLNL laboratory, showed inflamed stomachs (gastritis), ulcers, and gastric cancer (lymphomas and adenocarcinomas), the same defects found in humans. "This mutant mouse," Culiat says, "is a good mouse model for studying how gastritis progresses to stomach cancer in both mice and humans."

So far examination of the mutant mice has revealed no abnormal expression of *muc2* in inner ears. More detailed analysis of this large gene and analysis of the mutated region of mouse chromosome 10 are both needed to confirm or rule out the involvement of *muc2* in the inner ear defect of 14Gso mice.

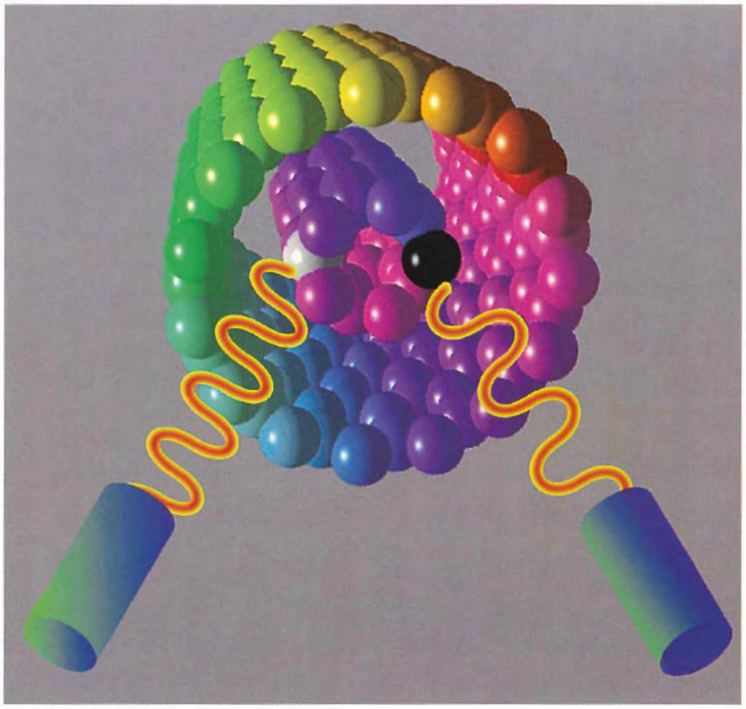
"If *muc2* turns out to be the deafness gene in our mutant mice," Culiat says, "then we may be able to determine if there are mutations in this gene in certain groups of deaf people."

Culiat performed most of this research at ORNL as a postdoctoral scientists working with Stubbs. She was supported by the Alexander Hollaender Postdoctoral Fellowship Program of the Oak Ridge Institute for Science and Education.

Certain segments of the gene *muc2* have been cloned and sequenced at ORNL. The sequencing and cloning of this very large gene will be completed at LLNL under Stubbs' direction. The cloning and characterization of the chromosome regions containing the 14Gso mutation are goals of a continuing collaboration between Stubbs and Culiat.

By identifying and characterizing genes and proteins using various technologies and mouse experiments, Oak Ridge researchers are finding clues that could lead to cures for human diseases.

Next Issue: Brave New Nanoworld



The next issue of the *ORNL Review* will explore the world of nanoscience and nanotechnology, where objects are as small as one-billionth of a meter (nanometer), or the size of a few atoms. Interest in nanoscience has been around since the 1980s when scientists learned how to assemble atoms and molecules into useful configurations such as nanocrystals. Today nanocrystals are used to make more protective sunscreens and better cosmetics. Interest in the field of nanoscience grew with the 1985 discovery of the buckyball—a cluster of 60 carbon atoms that resembled a soccer ball or one of Buckminster Fuller's geodesic domes. Since then researchers have been tinkering with a few atoms at a time, trying to coax them into assembling nanomotors (see ORNL-developed image at right), nanogears, nanopumps, nanowires, and nanorobots. Because of their small dimensions, nanomaterials can exhibit entirely new materials properties.

Using their world-class materials characterization expertise and equipment, ORNL researchers are making advances in nanoscience and nanotechnology that will be described in the next issue. The driving motivations for much of this research on making things very small using new materials include the semiconductor world's needs to (1) increase the speed and number of transistors on computer chips to maintain the current rate of improvement in computing power, and (2) reduce the cost of fabricating chips. In addition, ORNL researchers are developing ideas for new projects in nanoscience and nanotechnology because the Laboratory and federal government are supporting a new initiative in this area. The researchers who receive funding will assemble multidisciplinary teams to solve complex problems. Their mission? To learn how to exploit the strange quantum effects of the nanoworld for doing molecular manufacturing (sometimes called nanofacturing). The research could result in better and cheaper electronic equipment, including palm-size computers and flat panel displays, as well as more efficient solar electric cells.

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Visualizations by Don Spong Digital enhancements by Greg Lamb

ORNL continues to study fusion energy as a power source because it produces no greenhouse gases (see articles on other ways to reduce greenhouse gases, starting on pages 8 and 14 in this issue). ORNL theorists have invented a new fusion energy device (visualized here) that is smaller and less expensive than other fusion reactor concepts. Called the Quasi-Omnigeneous Stellarator (QOS), this magnetic configuration incorporates the best features of the tokamak and stellarator, the leading magnetic confinement concepts for fusion energy, and also eliminates the possibility of violent disruptions that plague conventional research tokamaks. The group proposes that a QOS experimental device be built at ORNL. If the proposal succeeds, ORNL will again have an experimental fusion facility for research on the energy source that powers the stars.