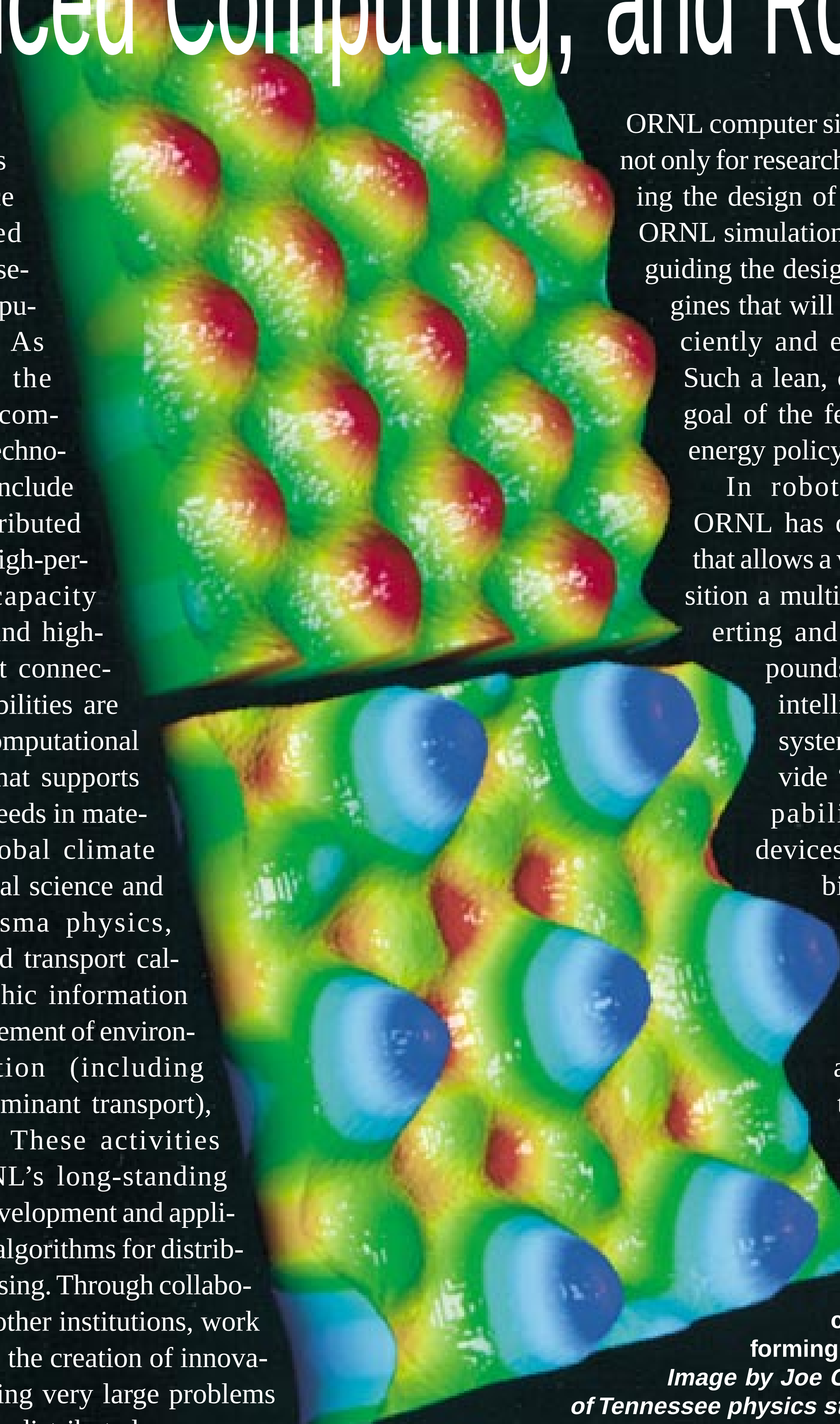
Computational Science, Advanced Computing, and Robotics

ORNL is one of the world's leaders in high-performance computing, related technologies, and selected areas of computational science. As home to one of the world's foremost computing centers, its technological resources include Intel Paragon distributed memory systems; high-performance, high-capacity storage systems; and high-bandwidth Internet connections. ORNL capabilities are integrated into a computational science program that supports national research needs in materials science, global climate simulation, chemical science and engineering, plasma physics, nuclear physics and transport calculations, geographic information systems, the management of environmental information (including groundwater contaminant transport), and informatics. These activities complement ORNL's long-standing leadership in the development and application of tools and algorithms for distributed parallel processing. Through collaborative efforts with other institutions, work in this area leads to the creation of innovative means of solving very large problems with geographically distributed resources.

ORNL computer simulations are useful not only for research but also for improving the design of industrial products. ORNL simulations of combustion are guiding the design of automotive engines that will burn fuel more efficiently and emit less pollution. Such a lean, clean car is a major goal of the federal government's energy policy.

In robotics development, ORNL has developed a device that allows a worker to lift and position a multi-ton payload by exerting and feeling just a few pounds of force. ORNL's intelligent transportation systems data bus will provide "plug and play" capability for electronic devices added to automobiles. The in-vehicle information system will manage "electronic traffic" within a car to avoid driver distraction.



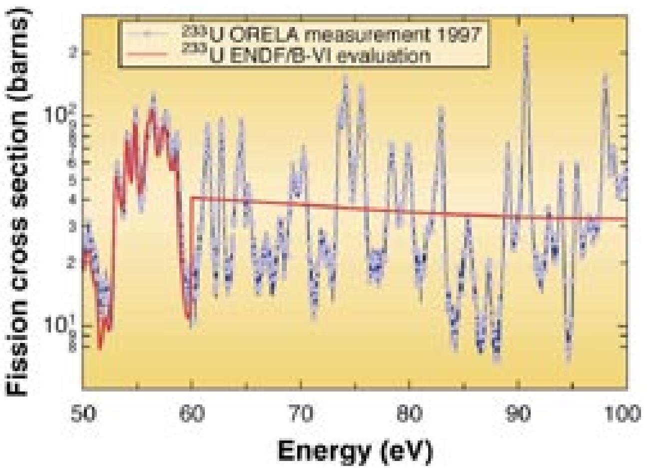
ORNL's computer visualization capabilities enhanced this image of a charge density wave forming on a crystal surface. ***Image by Joe Carpinelli (University of Tennessee physics student) enhanced by Dianne Wooten.***

Accelerator, Code Yield Needed Data for Nuclear Safety

The Oak Ridge Electron Linear Accelerator and the ORNL computer code SAMMY provide the nuclear data necessary for reliable nuclear criticality safety studies.

Across the DOE complex, tons of nuclear materials have been warehoused for decades. Sometimes they are moved either within or between facilities. When masses of nuclear materials are collected this way, there is a potential for criticality, a condition that could accelerate into a radiation-releasing nuclear chain reaction.

Nuclear materials in close proximity react under certain conditions to produce neutrons through fission. A neutron-absorbing substance is arranged among stored nuclear materials to control reactivity. However, if the materials are not stored in proper configurations, they may produce more neutrons than can be absorbed. If neutron production and absorption become equal, a critical mass is reached. If production exceeds absorption, an uncontrolled chain reaction can ensue. To avoid a critical mass, the people handling nuclear materials need precise information about how much neutron multiplication will occur if specific masses are placed at particular distances from each other in a certain pattern. Nuclear engineers who address these issues must analyze all possible scenarios that might lead to criticality safety concerns, and nuclear data play a crucial role in their analyses.



The impact of ORELA's capability to produce high-resolution neutron cross-section data can be seen in these fission cross-section measurements for uranium-233 (^{233}U), shown as circles. The heavy line shows the current ^{233}U representation in the Evaluated Nuclear Data File. Above 60 electron volts (eV), the detail in the cross-section data is clearly missing in existing files.

Because of deficiencies in the data available for criticality safety studies, the Defense Nuclear Facilities Safety Board (DNFSB) asked ORNL for help. The DNFSB seeks to maintain U.S. capability for ensuring that nuclear materials being stored and transported are kept economically in subcritical arrangements. ORNL researchers, led by Bob Roussin and Luiz Leal, are using the Laboratory's Oak Ridge Electron Linear Accelerator (ORELA) and the ORNL computer code SAMMY to generate the needed data.

DOE installations store nuclear materials in configurations such that the neutrons produced cover the energy spectrum from slow to fast. In the past, nuclear data measurement and evaluation placed little emphasis on the intermediate energy range, which can be extremely important in nuclear criticality safety calculations. Consequently, existing data in the intermediate energy range are likely to be inadequate to provide results within the desired criticality safety margin. This lack of adequate data results in overly conservative and expensive shielding, transportation, and storage systems.

ORELA is an intense neutron source for measuring the probability (cross section) that any neutron will interact with or be absorbed by a particular atomic nucleus. ORELA is a unique tool for cross-section measurements. It produces neutrons in nanosecond-wide bursts, each of which contains neutrons with energies ranging from 10^{-3} to 10^8 electron volts. Precise measurements can be made because of ORELA's long flight path—up to 200 meters; the longer the neutron flight path, the greater the spread between the peaks and valleys of the cross sections and thus in the detail that can be gleaned. ORELA is the best U.S. source of high-resolution data in every neutron energy range, including the one of importance to the criticality safety program.

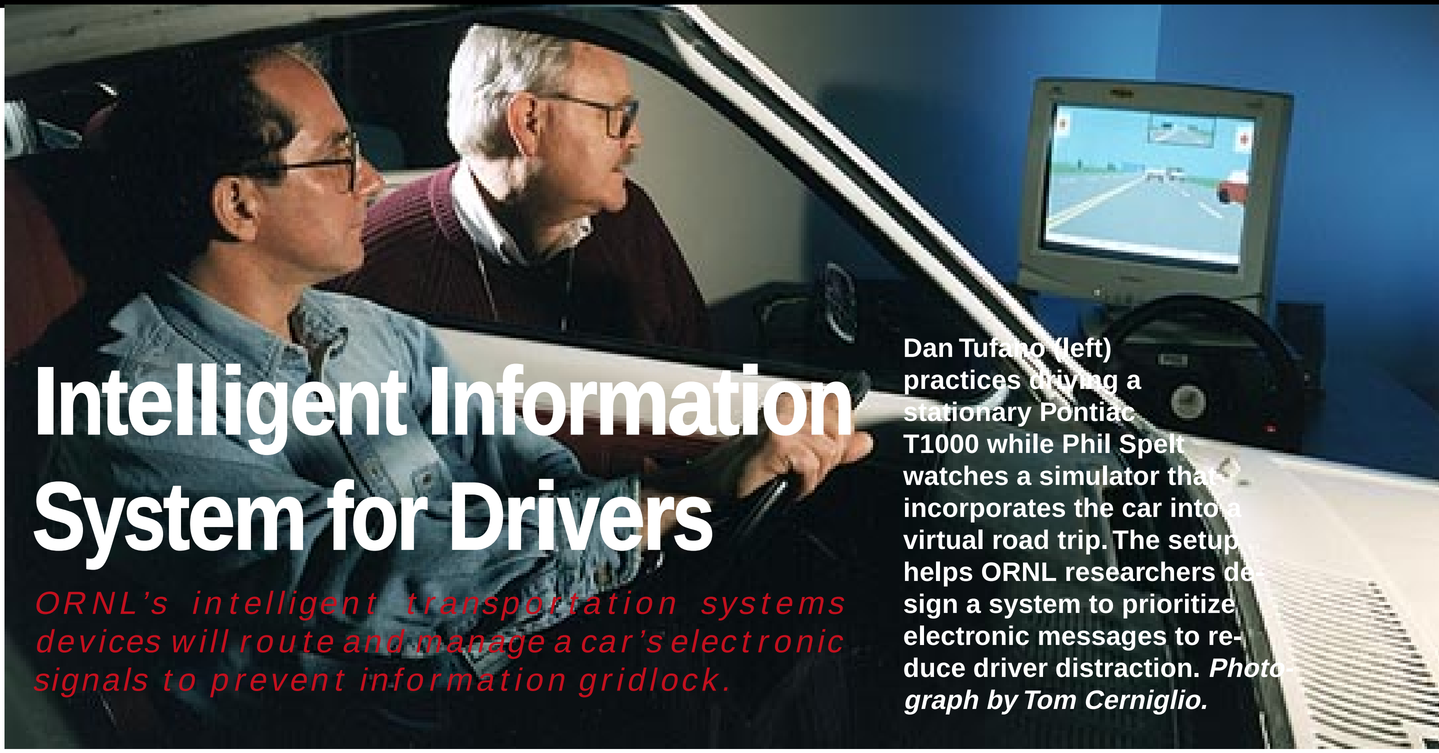
Because a vast amount of data is produced during an experiment, it is impossible to use the data directly to analyze and design a nuclear system. To make the measured data available in a form suitable for applications in nuclear technology, a procedure called nuclear data evaluation is used.

ORNL's computer code SAMMY, developed by Nancy Larson, is the best tool for evaluating neutron cross-section resonance data in the intermediate energy range. SAMMY provides uncertainties and correlations among data points (parameters) as a by-product of the evaluation process. These features play an important role in establishing uncertainty limits in analyses of nuclear criticality safety.

Evaluations using SAMMY are included in the national Evaluated Nuclear Data File and made available to the scientific community. The data are further processed into forms suitable for input to modeling codes such as KENO, MCNP, and VIM, which perform the actual criticality safety calculations for a given configuration of nuclear materials. The results allow nuclear engineers to infer how much absorber is needed in a given storage situation, how close the nuclear materials can be to each other, and how they can be arranged most economically to prevent criticality.

Using the unique capabilities of ORELA and SAMMY, nuclear analysts can ensure that cold war legacy materials are managed so that they remain a subcritical matter.

The project is funded by DOE's Environmental Management Program.



Intelligent Information System for Drivers

ORNL's intelligent transportation systems devices will route and manage a car's electronic signals to prevent information gridlock.

Dan Tufano (left) practices driving a stationary Pontiac T1000 while Phil Spelt watches a simulator that incorporates the car into a virtual road trip. The setup helps ORNL researchers design a system to prioritize electronic messages to reduce driver distraction. *Photograph by Tom Cerniglio.*

As you drive up I-75 to a meeting, several electronic signals bombard your car's computer network simultaneously: the navigation system reminds you to get off at the next exit, the collision avoidance system warns you about the car in your right-hand blind spot, your pager gets a message that the meeting room has been changed, and your cellular phone receives a call from home.

Now, which one of those signals would you like to receive first? If you get the exit notice before the collision-avoidance warning, or if you have to sort out all those messages at once, your automatic security system might soon be dialing 911 for you.

Every modern automobile relies on an onboard computer network. Considering the increasing numbers of devices that feed into the network, accommodating the electronic traffic and managing it to avoid signal gridlock are major concerns of automobile safety experts. To address these concerns, ORNL is helping to develop the intelligent transportation system (ITS) data bus (IDB), a data-routing system, and the in-vehicle information system (IVIS), an onboard information manager.

Automakers do not use a single standard for automobile data buses, channels along which data travel electronically. Because any electronic device added to a vehicle must be compatible with the data bus, the lack of a standard bus makes it necessary to build different versions of a product for various makes of cars. The IDB will provide "plug and play" capability for such devices, says ORNL developer Phil Spelt. Built according to a Society of Automotive Engineers standard, the IDB will plug into any vehicle's main data bus through a "gateway controller" that controls the data flow between the two buses. Add-on devices will then plug into the IDB. Having a single standard interface will allow device makers to design products that can plug into the data bus in any vehicle. In addition, many essential vehicle systems use the main bus to send data that must be shielded from interference from add-on devices; the IDB, by regulating data flow between the main bus and add-ons, will provide that protection.

The IVIS will function as an information manager to filter and prioritize information from the multiple devices that use the IDB. As experience with car phones has shown, drivers distracted by electronic gadgets are more likely to have accidents. As the number and variety of these products grow, so will the distraction, unless they can be prevented from competing for the driver's attention. The IVIS will monitor incoming signals to electronic devices, set priorities, and queue them for the driver's attention: this message about an accident is more important than the radio; this page can wait until you've seen the warning from the oil pump.

ORNL's IVIS project researchers have been asked by the ITS Data Bus Committee, which oversees IDB development, to help design testing protocols for electronic devices and conduct bench-level tests of the prototype IDB. In addition, several private companies have asked ORNL to help implement a prototype IDB within a vehicle. Chrysler and General Motors will donate a new vehicle for the project, and the prototype will be tested in the IVIS laboratory. ORNL is developing software to test the interfaces between the prototype IDB and devices plugged into it. Companies manufacturing electronic devices for autos will use the test results to improve the products.

ORNL also is developing the underlying logic for the software that will control the IVIS. To provide data for programming the IVIS, Spelt's team will place subjects inside a vehicle to "drive" in a simulated driving environment with projected scenes and sounds. Their responses to the driving environment, including signals from electronic devices, will be monitored and the data will be used in establishing the prioritization scheme.

The prototype in-vehicle IDB (which probably will include a rudimentary IVIS) is expected to be tested at automobile and trade shows around the country during 1998 and 1999. The IDB and the IVIS may be available commercially by 2005 to help drivers avert information gridlock.

Development of the IVIS was supported by the Federal Highway Administration, Information and Behavioral Systems Division. Funding for the IDB came from the Society of Automotive Engineers.

Computer Models Aim for Lean, Clean Engine Combustion

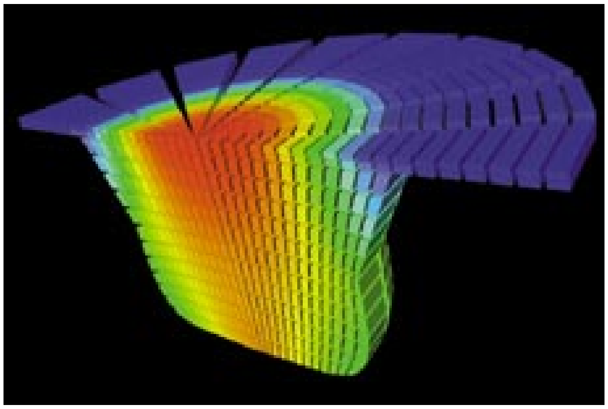
ORNL's model of spark energies is guiding the design of gas engines that will use less fuel and emit less pollution.

Many lean, clean cars of the future will have spark-ignited engines like the gasoline engines of today, but they may run on other fuels, such as natural gas. The reasons: Natural gas burns cleaner than gasoline and the United States has an abundant supply of natural gas. Lean-burn engines offer higher efficiency than conventional engines. Lean-burn natural gas engines would run more efficiently, reduce U.S. dependence on foreign oil, and emit less carbon dioxide, slowing the buildup of greenhouse gases in the atmosphere.

In such an engine, as each piston glides toward the top of a cylinder, it compresses the mixture of air and natural gas. Then a spark plug ignites the fuel-air mixture. An electrical current crossing the gap between the plug's electrodes at a voltage of 10 to 20 kilovolts ignites the gas in the gap. The combustion of the fuel-air mixture drives the piston, creating useful work at the flywheel.

The trick is to design natural gas engines and spark plugs to walk a fine line. If the deposited spark energy causes too hot a blast (2600 K), the engine will make the most efficient use of the fuel, but it will produce more nitrogen oxides—pollutants that contribute to the formation of acid rain and smog. Also, if the heat is too intense, it will rapidly erode the spark plugs, widening the gap between the electrodes and requiring a larger voltage to produce the needed ignition energy (some spark plugs last only about 200 hours because of erosion). If the spark plug voltage is too low, misfires result and the amounts of deposited energy are so low that much of the fuel remains unburned. The challenge is to design engine spark plugs to deposit energy in an amount high enough to achieve uniform combustion yet low enough to reduce emissions and spark-plug erosion.

Engine manufacturers such as Cummins Engine and General Motors are working to improve the designs of advanced engines, and ORNL is collaborating with them through cooperative research and development agreements by applying its expertise in computer simulation, spark stabilization, and engine diagnostics techniques. Using a suite of computational analysis tools, ORNL researchers led by Osman Yaşar, Jeff Armfield, and Isidors Sauers have developed a new spark ignition model and integrated it into the KIVA-3 engine combustion model. The model is being applied to newly designed Cummins Engine natural-gas (NG) and General Motors spark-ignited direct-injection engines that are being developed. This new spark ignition model provides the most detailed computation yet of the spark ignition process. When combined with ORNL's massively parallel version of the KIVA-3 engine combustion model, this new capability puts ORNL in a unique position in industry's eyes because of the ability to perform simulations of nanosecond-timescale physics and many-million-mesh-points spatial refinement of mathematical accuracy.



Temperature profile of combustion (the red part is the hottest) seen in a cross section of a spark-ignited internal combustion engine cylinder whose piston is near the top. ***Digital image enhanced by Allison Baldwin.***

Conventional models assume a constant, uniform deposition of spark energy, but the ORNL model shows that energy deposition is nonuniform and that temperatures throughout the spark gap area vary with location and time after ignition. The model correlates spark input parameters (e.g., discharge current, breakdown voltage values, spark duration) with engine output (i.e., efficiency of energy use and emission levels). The ORNL simulation results are expected to have an impact on the design of combustion engines by defining lean fuel limits and optimum spark energies that will result in lower fuel consumption, more efficient burning of the fuel, and reduced emissions.

ORNL's scalable combustion model is also being improved with the addition of a new radiation transport submodel that will be used to analyze coal combustion for utility boilers. ORNL and McDermott Technologies, Inc. (formerly known as Babcock & Wilcox) have an active collaboration to improve boiler designs through simulations on ORNL's massively parallel computers. In this type of combustion, 80% of the heat from the coal is transferred by radiation. Because the radiation changes much faster than the background flow motion (nanoseconds vs microseconds), it is fortunate that the ORNL model can simulate these changing dynamics by showing in detail the different length scales and time scales involved in physical phenomena.

ORNL's developments in spark ignition and radiation transport simulations not only open opportunities for the design of improved engines and boilers but also open avenues for basic research in plasma physics, computational science, and mathematics. The ORNL models may help engine designers think lean while providing meat for physicists, mathematicians, and computational scientists.

The research is sponsored by DOE's Office of Computational and Technology Research, Division of Mathematical, Information, and Computational Sciences; by DOE's Office of Energy Efficiency and Renewable Energy; and by matching funds from Cummins Engine, General Motors, and McDermott Technologies.

ORNL Device Gives Big Lift to Operators with Heavy Loads

ORNL has developed a "human amplification" device that allows a worker to lift and position a multi-ton payload by exerting and feeling just a few pounds of force.

When Sigourney Weaver straps on a robot suit that turns her into a gigantic kickboxer in the movie *Alien II*, it's all make-believe. But an ORNL-developed system based on the same concept works in the real world.

The concept is the engineers' dream of human amplification. A machine gives you the power to lift and handle multi-ton objects using only your hand's force. Because you can feel the forces operating on the payload, you can precisely and safely control and manipulate the load.

In a demonstration of the Advanced Telerobotics Technology Demonstrator (ATTD), an implementation of ORNL's human amplification technology, a single person deftly picked up a 2500-lb weapon and hooked it onto small holding brackets under the wing of a plane. The task usually requires several people; a crane and rigging equipment; and quite a bit of time to rig the weapons, position them without swinging them into the personnel or the plane, and maneuver them into the brackets. Military sponsors expect that replacing current munitions-handling methods with ATTD-like systems will enable them to reduce staff and costs and increase efficiency by 200 to 500%.

The ATTD grasps a load with a control arm rather than pushing, pulling, or suspending it. The operator lifts and controls the load with a small joystick-type handle on the machine. The ATTD senses the motion and forces exerted by the operator's hand and duplicates the motion while amplifying the forces. Essentially, the machine follows every move of the operator's hand, but provides power that multiplies (by a preselected amplification ratio) the operator's strength. Many types of end-effector tools can be mounted on the end of the control arm—a gripper, a power tool holder, jaws, large parts, stretchers. The apparatus sits on an omnidirectional platform that also can follow the operator's movements, allowing easy transportation of the payload

François Pin, ORNL's principal researcher on the ATTD, notes that human amplification systems are usually envisioned (e.g., as in *Alien II*) as wrapping around the human operator. In an accident, however, the human strapped inside could be crushed. The ORNL machine is operated by a person standing beside it, delivering the benefits of amplification while avoiding the potential safety problems.

The striking difference between the ATTD and other materials-handling technologies is not the load it can lift, but rather the stability and control it provides: submillimeter-level precision with payloads of several tons. Cranes, for example, can handle huge payloads but cannot hold them stable, so accidents from hoisting with cranes are common.

The ATTD is a first demonstration system of controls technologies that balance the real forces on the payload and the virtual forces on the human operator. The operator needs to feel what is happening to the payload to sense inertia and know when the load has made contact; otherwise, the load could be dropped or crushed. However, the force the operator feels is greatly deamplified. The ATTD was tested at a 500 amplification level: The operator exerts 10 lb of force to move a 5000-lb payload. Machines could be designed to lift 50,000 lb with 10 lb of human force. The methodology lends itself to amplification ratios ranging from 1 to virtually infinity.

The ATTD relies on several ORNL-developed technologies, including new controls for hydraulic systems, human amplification, the omnidirectional holonomic platform, and high-precision control of large payloads. The existing system is hydraulic, but pneumatic or electrical systems also could be developed.

Although funding for the ATTD research has come from the armed forces, ORNL is discussing agreements with private companies that want their own systems. The technology is expected to have applications in fields such as manufacturing, construction, mining, emergency response, and other areas in which precise handling of large payloads is important. In an automobile plant, for example, one person using an ATTD-like machine could position engines in chassis. In a disaster such as the Oklahoma City bombing, clearing rubble using human amplification would be less dangerous to rescuers and survivors than clearing it with bulldozers.

Although its usefulness for boxing aliens has yet to be tested, enough is known about this new technology to lift the spirits of operators who move heavy payloads.

Development of the ATTD was supported by the U. S. Air Force, U. S. Navy, and U.S. Marine Corps.

François Pin uses ORNL's ATTD to hook a 500-lb unarmed bomb into the holding apparatus under an F-15 wing pylon. This prototype machine can lift and control a 5000-lb payload with 10 lb of human force, but the technology could be used to lift 50,000 lb with the same human force. *Photograph by Tom Cerniglio.*

Radioactive Tank Cleaning System Working at ORNL

The robotic system being used to clean out ORNL's gunite and associated tanks may help remediate DOE's other tank wastes.

Historical photograph of gunite tanks at ORNL (1943).

Imagine removing thousands of gallons of radioactive waste from an underground tank. Some of it is hard sludge, and some is contaminated scale stuck to the walls. You can't go inside the tank, and the only access is a few 2-ft-diameter openings in the top.

That's the situation the Department of Energy faces in trying to clean up cold war legacy wastes across its weapons complex. Hundreds of waste tanks containing millions of gallons of waste, some of it highly radioactive, must be emptied and scoured to eliminate the potential for leakage of contaminants into groundwater systems. The gunite and associated tanks (GAAT) project demonstrated the first successful cleanup of two underground tanks at ORNL in 1997–98 using the radioactive tank cleaning system (RTCS) developed and integrated at ORNL.

About 98% of the contamination from tanks W-3 and W-4 in the tank farm at ORNL was removed with the RTCS, says project manager Dirk Van Hoesen. The successful demonstration of the RTCS will reduce the original tank remediation schedule by 13 years and reduce the estimated cost by $120 million.

The GAAT project focuses on remediating eight tanks at ORNL, each 25 or 50 ft in diameter, built in the 1940s to store liquid radioactive wastes from the Graphite Reactor and radiochemical processing plant. The tanks were constructed with gunite (a concrete-like material) sprayed over a reinforcing grid.

The RTCS can characterize waste, dislodge it, pump it out, and then decontaminate the tank walls and floor once the waste is removed, all without the need for a person to enter the tank. It is the result of collaboration among several DOE laboratories, universities, and private companies. ORNL served as the design and development lead, coordinating efforts of all the participants.

The RTCS integrates several remotely operated tools. The waste dislodging and conveyance system uses an end-effector with rotating water-cutting jets to dislodge waste from the tank's interior. A jet pump removes the waste slurry from the tank through hoses. A modified light-duty utility arm (MLDUA) with 7 degrees of freedom, a 16-ft horizontal reach, and a 200-lb payload capacity can descend 50 ft vertically into a tank. The MLDUA can position the retrieval end-effector to clean the tank walls and floor. A remotely operated vehicle called Houdini has a 4 × 4-ft chassis that folds up to fit through a 2-ft-diameter tank entrance. Houdini has a bulldozer blade to break up debris and push sludge toward the retrieval end-effector, on-board cameras, and an articulated arm to pick up debris and manipulate other tools.

The Houdini (left) and MLDUA (center) are among the components of the RTCS that work together to effectively clean a tank's interior. ***Image provided by the Gunite Tanks Remediation Project.***

The RTCS also includes tools to sample and characterize wastes and monitor radiation levels. Once the waste is dislodged and removed, the tank walls and floor are characterized to evaluate the depth to which contaminated materials have been absorbed. A scarifying end-effector is used to remove the layer of contaminated concrete. Remote cameras monitor tank cleanup, and the RTCS is controlled from a control trailer located near the tanks. The MLDUA can be controlled either manually or by preprogrammed sequences, and operators can switch back and forth seamlessly between the two modes.

ORNL's gunite tanks contain about 88,000 gallons of sludge. Tanks at other DOE sites have larger capacities and hold more sludge waste. The process at ORNL, part of the Oak Ridge tank remediation effort, serves as a pilot operation for the rest of the DOE complex; solutions can be worked out here on a smaller scale and tailored to fit specific needs at other sites. All sludge removed from the gunite tanks will be consolidated in one tank and then transferred by pipeline to the Melton Valley Storage Tanks (MVST).

Waste processing at the MVST is scheduled to begin in 2002. It takes 3 to 6 months to clean a tank and move the equipment to another tank. Finishing the GAAT project will take another three and a half years, Van Hoesen says. Just as the Graphite Reactor was a pilot for the nation's weapons program, the gunite tanks cleanup is a pilot for remedying its legacy of environmental contamination.

The project is funded by DOE's Office of Environmental Management.