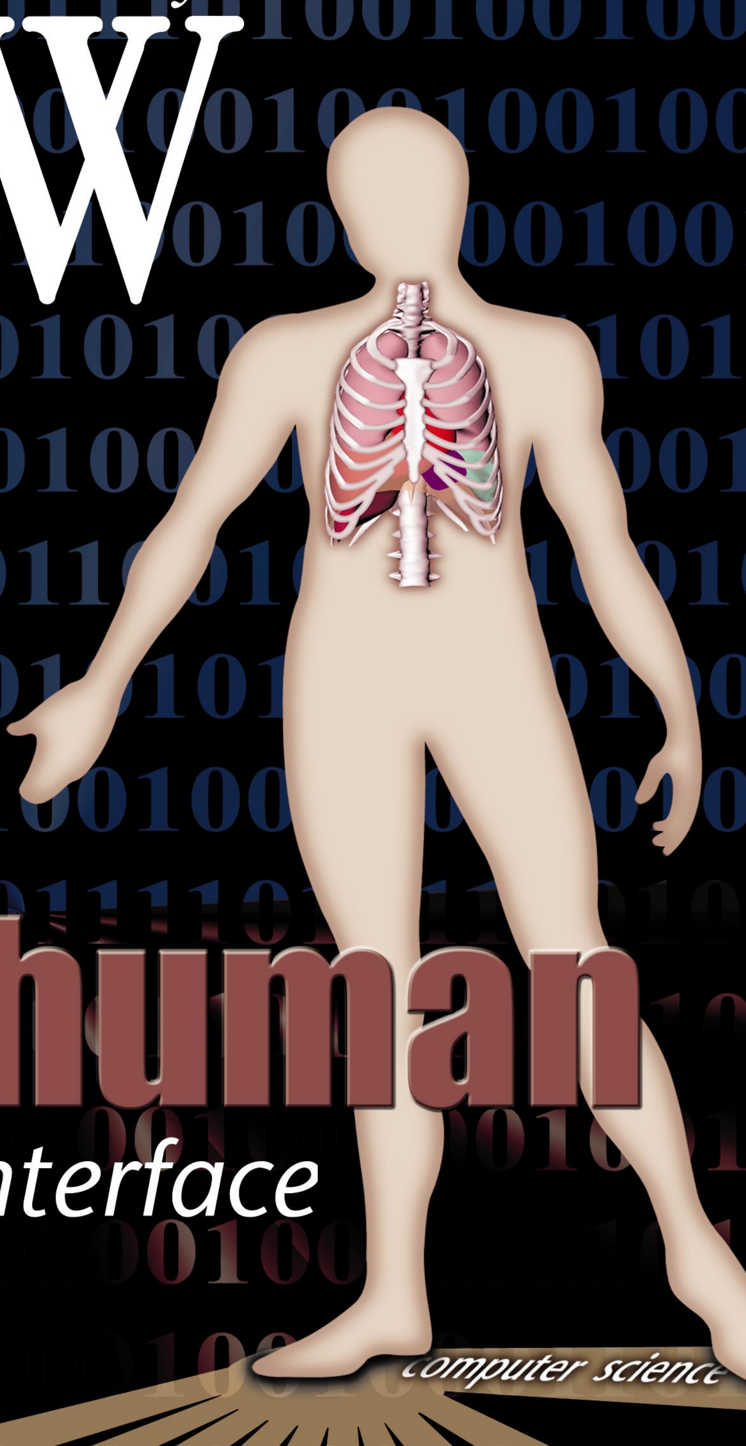
U.S. Department of Energy
Oak Ridge National Laboratory

REVIEW

Vol. 33, No. 1, 2000



virtual human

Science at the Interface

computer science
biomedical engineering
electrical engineering
systems engineering
information technology
medical technologies
anatomy
physiology
biophysics
physics

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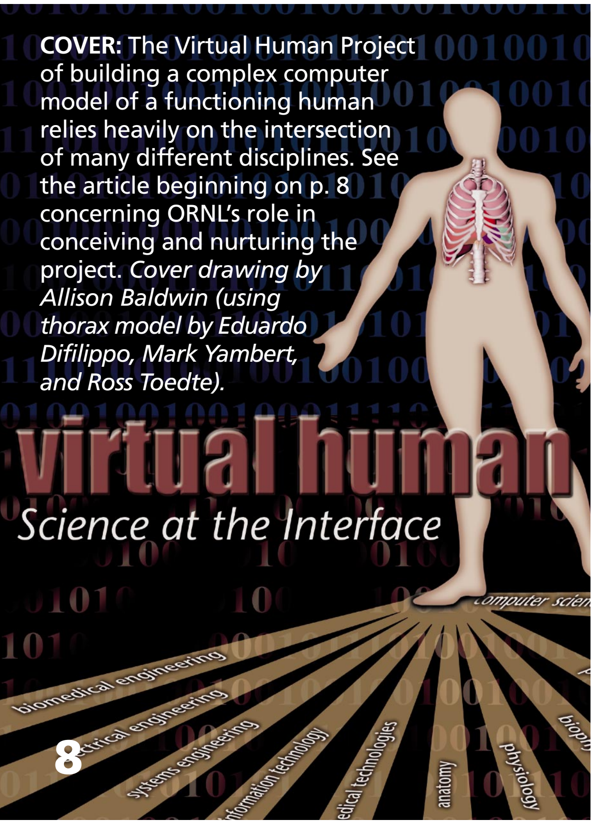
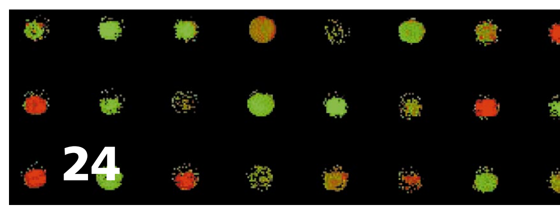
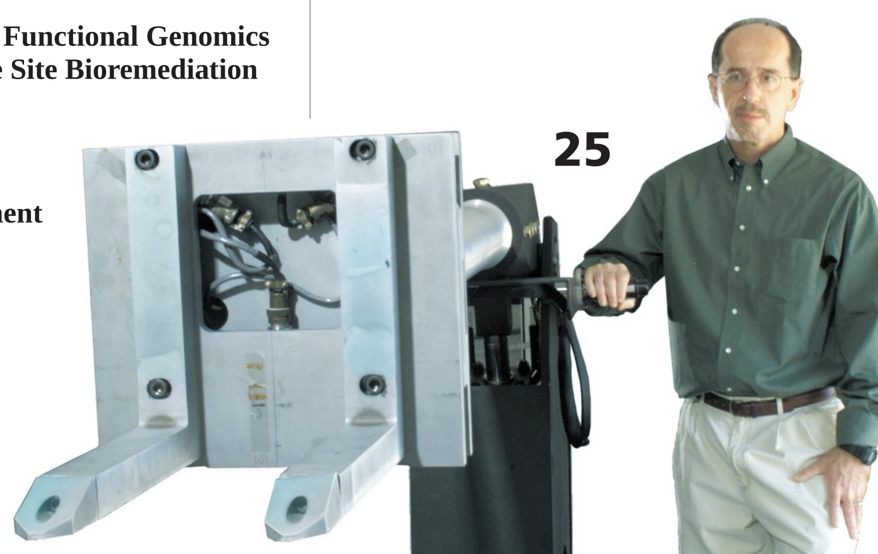
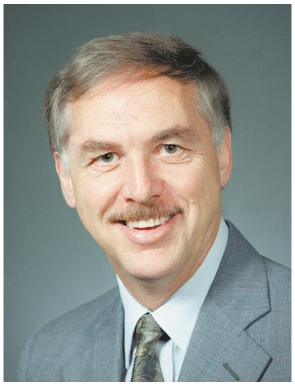


COVER: The Virtual Human Project of building a complex computer model of a functioning human relies heavily on the intersection of many different disciplines. See the article beginning on p. 8 concerning ORNL's role in conceiving and nurturing the project. *Cover drawing by Allison Baldwin (using thorax model by Eduardo Difilippo, Mark Yambert, and Ross Toedte).*







Editorial: Science at the Interface

The first article in this issue of the *Oak Ridge National Laboratory Review* is titled "Science at the Interface: A Roundtable Discussion." The idea for this roundtable discussion came out of a meeting of the *ORNL Review* Editorial Board. We were looking for interesting ideas for future articles for the *Review*. We concluded that gathering a group of senior scientists in a lively discussion could accomplish this goal and also uncover some interesting opportunities in science and future directions for ORNL.

We chose "science at the interface" as a theme for the discussion because Oak Ridge National Laboratory has long recognized the importance of working across traditional boundaries. The vision in the current *ORNL Strategic Plan* acknowledges the advantages of the expanding opportunities in "science at the boundaries." Major ORNL initiatives such as nanoscale science, engineering, and technology and complex biological systems, as well as Laboratory Directed Research and Development projects in these areas, have purposefully engaged all scientific competencies. We believe that ORNL should continue this commitment to ensure that it remains a center for scientific excellence in the new century.

Another article in this issue concerns a project that would not be possible without multidisciplinary research and collaboration among various institutions. Its focus is the ORNL-conceived Virtual Human Project, whose goal is to develop a highly sophisticated computer model of the structure and functions of the human body and all its organs. New information is expected to arise from the intersection of various disciplines, which occurs, for example, when computer scientists interact with biomedical engineers, chemists chat with biologists, and physicists talk to physiologists.

This issue also provides an update on the U.S. government's largest civil construction project, the Spallation Neutron Source (SNS), which will be built at ORNL by 2006. Its design and construction will be the product of multidisciplinary research and a partnership of six Department of Energy laboratories. In addition to providing neutrons for studies of the structure and atomic interactions of physical and biological materials, the SNS also will be a source of neutrinos, which ORNL proposes to use for neutrino detection research of astrophysical interest.

Other examples of ORNL's multidisciplinary research and collaborations involving laboratory, academic, and industrial partners are also reported in this issue. Here's a sampling of the topics: Natural gas turbine power plants that have higher efficiency and lower emissions partly as a result of ORNL's materials research. More efficient energy technologies, such as a gas-fired heat pump air conditioner, a heat pump water heater, and a method of using sunlight to both produce electricity and directly illuminate building interiors. The opening of DOE's Center for Structural and Molecular Biology (one of 17 user facilities at ORNL), which combines the talents of ORNL experts in neutron science, mass spectrometry, and computer science to study interactions of biological molecules such as proteins. The use of computers to discover genes in newly sequenced human chromosomes. Plans to develop an early version of a Superman suit to amplify human abilities, such as strength, speed, and endurance. The use of ORNL's radioactive ion-beam accelerator to get results that help astrophysicists accurately predict the amounts of isotopes produced when stars explode.

Integrating science requires an environment that brings together scientific leaders who are outstanding in their disciplines, who have competence and appropriate perspectives in other fields, and who are committed to collaborating across disciplines. This environment must include special experimental research facilities, advanced computational and information systems resources, educational programs that attract and develop the next generation of scientists, and partnerships that center the Laboratory within the global science enterprise. We have all this at ORNL and more, and you will see more evidence of "science at the interface" from the Laboratory in the future.

Bill R. Appleton

Bill R. Appleton
Founder of the *ORNL Review* Editorial Board

REVIEW

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The Oak Ridge National Laboratory *Review* is published three times a year and distributed to employees and others associated with or interested in ORNL.

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ORNL *Review* Web address:
www.ornl.gov/ORNLReview/

The *Review* is printed in the United States of America and is also available from the National Technical Information Service, U.S. Department of Commerce, 5285 Port Royal Road, Springfield, VA 22161

Oak Ridge National Laboratory is managed by UT-Battelle, LLC, for the Department of Energy under contract DE-AC05-00OR22725

ISSN 0048-1262

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.

Science at the Interface: A Roundtable Discussion

Exciting research opportunities exist at national laboratories because they offer major research facilities, computing tools, and a multidisciplinary mode of operation. To survive, national labs should address interesting and important problems to attract and retain highly qualified researchers and enter into productive partnerships with outside groups.

"Perhaps the greatest discovery of all this research is that we can no longer separate basic from applied science. The disciplines are connected in ways they have never been before."—Vice President Al Gore (1/1999)

Science at the interface. Discoveries of new phenomena and development of new technologies at the intersections of various disciplines, such as biology, physics, chemistry, engineering, and the measurement and computational sciences. It's the ORNL vision. To Bill Appleton, ORNL's former deputy director for science and technology, it's a national craze. "Think of advances in medicine that involved contributions from physics," he said, while moderating a roundtable discussion on "Science at the Interface" on December 17, 1999, at ORNL.

The discussion participants talked about the past accomplishments and future of multidisciplinary research and collaborations involving ORNL, especially when the Spallation Neutron Source (SNS) begins operating here in the next decade. They addressed issues such as extracting meaningful information from large amounts of data, the changing nature of collaborations and experimentation (e.g., science at a distance); attracting, training, and retaining highly qualified researchers; applying ORNL strengths to shifting trends in science and technology; and accommodating changes in the research agenda that may come with having the SNS.

The participants in the roundtable discussion and their interests were as follows: Al Trivelpiece, then ORNL director; Jacob Barhen, head of the Center for Engineering Science Advanced Research (CESAR), computational aspects of nanostructures; Don Batchelor, Fusion Energy Division, theory and computational simulation; Marilyn Brown, deputy director of the Energy Efficiency and Renewable Energy Program in the Energy Division, impact of advanced technologies on U.S. energy systems and greenhouse gas emissions; Michelle Buchanan, associate director of the Life Sciences Division (LSD), analytical chemistry and structural biology; Sheldon Datz, Physics Division, atomic and collisional physics; Eli Greenbaum, Chemical Technology Division, chemistry and nanotechnology; Linda Horton, deputy director of the Metals and Ceramics Division, who oversees ORNL metal and ceramic sciences research funded by DOE's Office of Basic Energy Sciences; Mike Kuliasha, director of the Computational Physics and Engineering Division; Doug Lowndes, Solid State Division (SSD), thin-film growth, nanostructured materials, and nanotechnology; Reinhold Mann, LSD director, collaborations involving the life sciences and computational sciences; Herb Mook, SSD, neutron scattering; Tony Palumbo, Environmental Sciences Division, bioremediation and genetic engineering; Frank Plasil, Physics Division, nuclear and high-energy physics research; Jim Roberto, ORNL associate director for Physical and Computational Sciences; John Sheffield, director of the Joint Institute for Energy and Environment at the University of Tennessee at Knoxville, all aspects of energy and the environment; Mike Simpson, Instrumentation and

Controls Division, nanoelectronics; Ed Uberbacher, head of LSD's Computational Biosciences Section, computational biology and bioinformatics; Tuan Vo-Dinh, LSD, medical applications of physics; and Thomas Zacharia, director of the Computer Science and Mathematics Division, the impact of computer technology on science.

Barhen of ORNL's Computer Science and Mathematics Division defined science at the interface as "a coherent integration and fusion of concepts, methods, and devices with the goal of achieving revolutionary advances that would not be attainable within the constraints of a single discipline." Plasil observed that scientific research needs technical solutions and that most technical solutions need scientific research. For example, teasing out information about whether free quarks were present during the earliest stage of the Big Bang requires sophisticated electronics to sort through a large volume of data coming from the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory (BNL). On the other hand, a fusion energy device that works cannot be built without the valuable information provided by materials research.


Jacob Barhen

Simpson, an electrical engineer, gave an example of how two different disciplines can help each other. Gary Saylor, a microbiologist at the University of Tennessee, came to him and asked, "How can we instrument what's going on in living cells?" "We then came up with the idea that we should think of cells as fundamentally new electronic components that could be engineered to do signal processing and other electronic functions." As a result, the two collaborated on the development of the "critters on a chip" technology in which living bacteria on an electronic chip signal the presence of nearby chemicals.

ORNL offers an intellectual interface among the traditional disciplines of physics, chemistry, biology, and engineering, Greenbaum said. "ORNL's environment encourages the convergence of ideas and concepts of separate disciplines. In our work, chemistry and physics are brought to bear on the understanding of biological systems."

Greenbaum and Simpson are involved in building an electronic logic device that uses tiny metal electrodes and photodiodes made of proteins from spinach leaves. The nature of the device is a metaphor of the meeting of disciplines—science at the interface—required to make it possible. "These new biosystems have soft condensed matter and hard condensed matter," Greenbaum said. "Only because we know the functions of individual biomolecules can we interact with each of them after they are incorporated into designed nanostructures."

Trivelpiece made an observation that triggered a discussion about the effects on various sciences of advances in measurement capabilities and data acquisition and analysis. "I've been fascinated by improvements in measurement sciences," he said. "Data collection is automated so you can now do in 10 minutes what used to take 10 weeks. If the Superconducting Supercollider had been constructed, the first shot would have produced more data than all the high-energy physics researchers accumulated in their preceding history. The data glut will be so bad that you won't take data and archive it in the same way you did in the past. Is there a future out there for doing experiments so that you don't have to collect data?"


Alvin Trivelpiece

Trivelpiece suggested that computer models of the future may be able to make instant sense out of mounds of data. He noted that there is evidence that adrenaline—the fight or flight hormone—can produce different effects in the brain. "The same chemical in microscopic quantities can trigger the rage to kill or a catatonic state depending on the circumstances," he said. He observed that, as the measurements improve and the computer models become more realistic, the ORNL-led project on the Virtual Human (see the article on p. 8) might be able to shed light on the actions and interactions of not only the heart, lungs, and kidneys but also the brain. The following are edited excerpts from the roundtable discussion:

APPLETON: Haven't improvements in instrumentation and computation and other advances aided the study of what different genes do, making functional genomics a successful example of science at the interface?

BUCHANAN: Bringing together physics, materials science, computational science, and chemistry with biology enhances what the biology community does. Advances in measurement science will some day allow us to measure chemical concentrations in the living cell in real time.

MANN: You can't do functional genomics without informatics capabilities and resources. Biology drives other sciences and these sciences also drive biology.

UBERBACHER: About 10 years ago Reinhold Mann and I developed computer technology to find genes in DNA sequences. We found the first few genes that way. By early December the entire human chromosome 22 with its 5000 genes had been sequenced. We are in the midst of analyzing the entire human chromosome 22 for genes, and we will be analyzing human chromosome 19 for the DOE complex in 2000 (see the article on p. 23). We've improved our rate of analysis by orders of magnitude by using computers in biology. We are now using a gene chip, a revolutionary biological measurement technology that allows people to look at an entire biological system at one time by making thousands of measurements across the genes being expressed in a microbial or human genome.


Ed Uberbacher

PLASIL: With engineers in the Instrumentation and Controls Division, we physicists have developed application-specific integrated circuits for the quark-gluon experiments we will be doing at RHIC. This col-


Frank Plasil

Roundtable discussion participants, from left, included Eli Greenbaum, Jacob Barhen, Ed Uberbacher, Michelle Buchanan, Herb Mook, Thomas Zacharia, Tony Palumbo, Jim Roberto (standing), Bill Appleton, Sheldon Datz (standing), Linda Horton, Mike Kuliasha (standing), Frank Plasil, Doug Lowndes, Mike Simpson, Don Batchelor, Reinhold Mann, and John Sheffield. Not pictured are Marilyn Brown and then ORNL Director Al Trivelpiece, who joined the group later. Photographs in this article were taken by Curtis Boles and enhanced by Gail Sweeden.

laboration is necessary because the amount of data we will get will be so huge that we will have trouble storing it. With high-energy collisions, we get thousands of particles, but most of them aren't very interesting. So we have to dig around for the three or four that are. This data selection must be done very fast online with specific instrumentation that really can be developed only at a national lab.

MOOK: In the early days of neutron scattering at Oak Ridge, scientists counted neutrons at a rate of 1 pixel per second. With the SNS we hope to get 5 million pixels per second. The question is, how does the user come in and get what he wants out of these 5 million pixels? The answer is he can't without the help of high-speed computing. The user may only want to measure the distance between atom A and atom B—a bond length. The way we do that now is to take a lot of data, look at the peaks, and then do modeling. What we really have to do at major facilities now is give the user a computer model into which to quickly fit the data.

Thomas Zacharia

ZACHARIA: We should do more to integrate computing into other disciplines. Computer tools are being developed at ORNL to analyze large sets of data. Someday you will be able to build into your model a simulation tool so that the computer generates the results or information you are seeking. The computer science challenges of the future are likely to be networking and data storage.

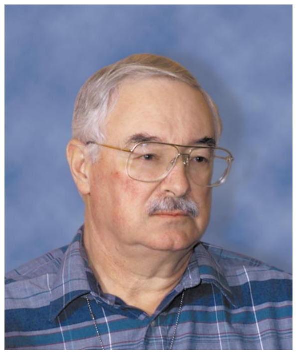
APPLETON: Are we using the unique aspects of a national lab for our research or could this work just as easily be done at a university or some industry?

GREENBAUM: Even today university research is driven by traditional departments and disciplines. Promotions within the department of chemistry are based on what is done in chemistry. National labs are driven by national missions and problems. We get beyond the disciplinary aspect of our individual training by focusing on the problem. We can move more quickly because we are not bound by traditional departments.

DATZ: A multitude of tools for analyzing and altering surfaces of materials emerged at ORNL and other national laboratories because of a marriage of vastly diverse disciplines that could not happen at universities.

BROWN: By meshing their strengths in basic research, applied and engineering sciences, and behavioral studies, national labs have a unique ability to move revolutionary ideas into the marketplace.

TRIVELPIECE: Academic institutions have more difficulty with interdisciplinary activities than national labs. This means that at national labs you have a better ability to interact with other scientists and engineers in other fields.



John Sheffield

SHEFFIELD: ORNL's work in materials is outstanding, partly because it is coupled with other programs such as energy and fusion. We couldn't have an effective energy research program without a materials research program (see the article on gas turbine power plants and ORNL's materials research on p. 16). Universities don't tend to have that kind of extent of work.

LOWNDES: At a university, a professor may be torn in several directions and forced to work in a narrow area. Many national labs are the caretakers of quite remarkable national and international user facilities so we have full-time staff working there. Despite our costs, I think we're learning how to do a better job of using postdoctoral researchers and graduate students at these facilities. The national labs are powerful places for doing big-facility research.

APPLETON: How important will collaborations be to national labs in the future?

KULIASHA: Multidisciplinary collaborations at national labs result in a synergy, or team learning, because of the data produced and the interaction of the participants.

Doug Lowndes

LOWNDES: My own feeling is that we have to collaborate with universities and use postdocs and graduate students as efficiently as we can to be highly productive. We are learning how to bring costs down while increasing our research productivity. When I came to the Solid State Division in the 1970s, we had 120 staff members and 20 postdocs. We now have an equal number of staff members and postdocs.

UBERBACHER: In the biology and genomics domain, the importance of collaborations is exploding. In functional genomics, if we're doing things with genes that have medical significance and we want to respond to National Institute of Health calls for proposals, we may need to team with medical schools or pharmaceutical and biotech companies. It's more than getting postdocs; we have to partner with the scientific leadership on the outside that can access different funding agencies and bring different perspectives.

ZACHARIA: In an age where information is so readily available and knowledge and advances are coming at a much faster rate, if we don't have a strategy of partnering with other universities and national labs as part of our planning process, I think we will be left behind.

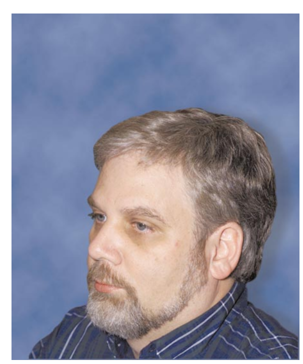
APPLETON: If this is such a good place to do science at the interface, what projects should we be looking at? What should ORNL be doing in the future that will make a difference to society?

VO-DINH: At the national labs, I see a fusion of biological and physical sciences and informatics. It used to be that basic science was very important. Recently, we see more of the dual role of technology and science. For example, scientists need a tool such as the atomic force microscope to analyze the components of a single living cell. Today we are taking a systems approach to scientific problems. That's why we need multidisciplinary research.

MANN: Systems thinking will be increasing in scope over the next 10 years in biology. In fact, systems thinking will be needed to understand the whole genome.

TRIVELPIECE: In strategic planning, researchers defend their turf, talk to people in other disciplines, and then try to find an empty circle and figure out how to combine strengths to plug the hole. As we plan, we should focus on our outrageous, unfair advantage and go to our strengths.

PALUMBO: One of our strengths is that we can use mass spectrometry to get high throughput in DNA sequencing and expression. The problem is that we can't do that yet for the task of identifying proteins and discovering their functions and interactions. We might need a brute force strategy to get high throughput. Shotgun cloning is not an elegant strategy for



Tony Palumbo

getting sequence data, but that's the one that has characterized a lot of microbial genomes.

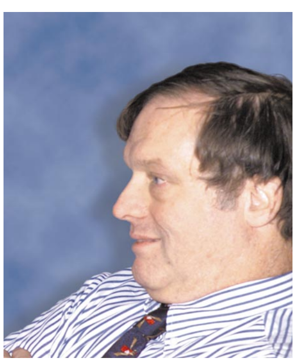

Michelle Buchanan

BUCHANAN: Fifteen years ago, mass spectrometry was not generally applied to biology. But after the development of desorption processes, including refinements made through interactions with the Solid State Division, we have techniques that allow us to use mass spectrometry to characterize DNA and proteins. Beyond using mass spectrometry to identify biomolecules, neutrons from ORNL's High Flux Isotope Reactor will soon be used to study protein-protein interactions and protein signaling processes (see the article on p. 7). The SNS and computational tools will become important for structural biology studies.

HORTON: Right now the Metals and Ceramics Division focuses on structural materials. The strength we have is in our partnerships and in applying those partnerships to merging basic, applied, and industrial science. We need to strengthen what we have been doing in the life sciences and instrumentation areas to develop functional materials, such as biomaterials, sensors, and other smart systems.

APPLETON: What are the most important scientific and technology trends of the future?

BATCHELOR: *Physics World* recently listed the ten great unsolved problems in physics. They are quantum gravity, understanding the nucleus, fusion energy, climate change, turbulence, glassy materials, high-temperature superconductivity, solar magnetism, complexity, and consciousness. We have a lot of expertise with respect to many of these problems. It seems like we should come together to try to solve these problems using our strengths in computer modeling and simulation.


Don Batchelor

PLASIL: I don't think it's a very good list.

SHEFFIELD: One of the strategic technologies forecast for 2020 by Battelle Memorial Institute is one area we actually work in, which is the issue of clean water. Water is getting more and more polluted. We are working on ways to purify water cheaply, stop pollution at its source, measure pollutant levels in water, and map water flows and pollution sources.

ROBERTO: The use of neutron scattering to study soft materials such as polymer blends and proteins will be an exciting area in ORNL's future.

GREENBAUM: We're learning what happens when soft condensed matter meets hard condensed matter, as in logic devices combining spinach proteins with metal electrodes.

KULIASHA: I heard an interesting quote. The social cry of the 18th century was "No taxation without representation." The social cry of the 21st century will be "No experimentation without simulation."

MOOK: I was surprised when I heard Vice President Gore say at the SNS groundbreaking ceremony (see the article on p. 12) that the greatest things we will do at the SNS are the things we haven't thought of yet because we have a tool to do it. I once asked John Bardeen when he was here for a superconductivity conference why the transistor was invented, how was that made possible. That was certainly a major accomplishment for any society. He said it was the people that came together at that time at Bell Labs that made that possible. They had the freedom to interact in a special way. We have to find ways to bring the best people together and enable them to interact effectively.

APPLETON: National labs offer a unique meeting place. They have major research facilities, computing tools, and a multidisciplinary mode of operation, so that's the place where exciting research is going to happen. But you have to get the people you need and you have to pick the problem.

KULIASHA: I disagree that we have to bring them here. People feel a closer affinity to their coworkers at other institutions than they do to people in the office next door. The reason people had to be close together was because the experiments were done at a few facilities. Now we have science at a distance. People are communicating by e-mail and video conference calls. I would argue that we shouldn't think about organizing around the institution but instead around the scientific problem and the multiple researchers addressing it.


Mike Kuliasha

APPLETON: I don't think any researchers are going to make a major discovery by talking to each other over the Internet. They are going to have to be in the same place.

MANN: What do we have to do to get them here? The field of genomics is moving so rapidly. We must create the right environment and have the right facilities and provide the resources. That varies from opportunity to opportunity.

DATZ: There are many tasks that require the use of many different techniques at large facilities (as in international collaborations involving ORNL researchers at CERN near Geneva, Switzerland). So you have to be able to pack a suitcase and go to a facility and do the experiment and then go home.

LOWNDES: There is no substitute for big-facility experimental research. National laboratories should be sure that facilities are being exploited to the fullest extent. We need to have interdisciplinary teams of people here putting together a new facility like the SNS. We should think carefully about the organization of research teams on site.

KULIASHA: Eighty percent of the people working at the SNS will be outside users. If you've got an exciting team, access to the exciting facility, and plenty of exciting work, people will join the team where the action is.

APPLETON: What is your personal perspective on the future of the Lab? I personally think that the national labs are in the best position they have ever been in. There is going to be more and more basic research done in this country. More of it will be done at the national labs because basic research is getting more and more complicated. You have to go to a major facility to study complex problems.


Bill Appleton

BARHEN: We live in an exciting time and enormous possibilities lie ahead. National laboratories should be national instead of DOE labs. It would be nice if we could become a resource across all science agencies. What will it take for us to be a NASA center as well as a DOE center? Collaboration across centers and institutions will be driven by how exciting projects are. We are working in areas of interest to NASA such as quantum dot computing and mobile robots for space exploration.

BROWN: Our position in the scientific world is important because we are the custodian of unique scientific equipment and facilities. We're an aging staff of scientists. Our best staff scientists are not that young. You can count our 35-year-old scientists on one hand. We have to take advantage of what I see as a trend toward distributed science. We have got to reach out and make our equipment accessible to our young collaborators all across the world so we can stay fresh. Vice President Gore said the impacts and products of the SNS will be things we have not yet identified. There had better be some advances and there had better be some good positive press because there is an underlying public pessimism about the value of science. I don't think we should focus on bringing people here as much as we should focus on getting out our ideas, accomplishments, and data using the Internet. We need to get our name out to people like graduate students so they know where there is a precious resource. Our lab should be one that can be accessed on the Web virtually.

Marilyn Brown

PLASIL: We are thinking that once our experiment is running at Brookhaven, we can control it from here. I don't know if this is the way that things will go; this is perhaps the way we would like to see them go.

We should do fundamental physics using neutrinos that will be produced at the SNS (see the article on p. 15) as well as muons that could also be produced there.

LOWNDES: In the first stage of the experiment, you will have to go to the facility. You need creative people there to help you design peripheral equipment and processing equipment. You need auxiliary equipment for biological molecules and thin films of interest. As far as the Internet is concerned, if I can sit home in my sweatsuit with my Nordic exercise machine nearby and run my experiment from my computer at home, that's great.

MOOK: When I do an experiment, I may or may not get good results, but I almost always learn something from the person next door or down the hall. I might learn about a neat experiment someone is doing using DNA. I don't see that kind of information exchange happening over the Internet.

APPLETON: If you're going to run the SNS as a distributed experimental facility, you will do things very differently than if you're going to run it as the best neutron center in the world for everyone to come to. That's the strategic decision that must be made.

HORTON: I see ORNL and the other national labs in a time of real change. ORNL historically has not been an institution focused on a single facility. We have the Holifield Radioactive Ion Beam Facility, the High Temperature Materials Laboratory, the ShaRE program, and the Surface Modification and Characterization Laboratory, and concentrations of expertise in chemistry and computing science. We have been a lot of different things to a lot of different people here. We are now becoming an institution that will largely focus, at least on the surface, on neutron science. That is a tremendous change for this institution and surviving that is something we will have to enthusiastically embrace. Or we won't make it. We can't have a neutron scattering facility for the entire world and have just a few of our researchers using it. We have to embrace the Laboratory's biology, physics, and materials science communities in neutron science projects. If you look at Argonne, you see what's happening to them. The Advanced Photon Source is becoming Argonne National Laboratory. Their basic science programs are swinging toward incorporating APS in their research in response to sponsors. It will be a dramatic and challenging time for the Laboratory.

LOWNDES: We must find a way to retain some of the best and brightest scientists.

DATZ: A good source of researchers for us is the Wigner Fellows program. Our retention rate for these Wigner Fellow postdocs is over 70%. This is an altruistic way of treating young men and women and increasing the quality of our staff. But we should be concerned that there is a paucity of young scientists coming from the U.S. and Europe. Enrollment in hard sciences and engineering is going down in this country. We should try to address recruiting good people early on so we are able to steer them into good university programs.

Sheldon Datz

LOWNDES: Through the National Science Foundation we have opportunities to introduce interdisciplinary graduate training in national labs to get over institutional barriers at universities. A proposal will be made to the NSF to build an interdisciplinary graduate education and research training program at the University of Tennessee in connection with the national nanotechnology initiative. We are seeking support for the active recruiting of good graduate students for our nanotechnology projects at ORNL.

MANN: We need to take steps like that of the old Biology Division, which was linked to the UT/ORNL Graduate School of Biomedical Sciences, which turned out 150 top graduates who are very successful around the country. A lab program connected to a graduate school has the potential of providing a pipeline for giving us staff and putting us on the map.

Reinhold Mann

SIMPSON: I've worked a lot with University of Tennessee students in the past five years. As costs rise, you have to sell your time to more and more projects. Once upon a time $400,000 of internal funding could support work in several divisions. Now it covers only equipment and one full-time employee. You run out of time to work with students or junior staff members, so they go someplace else.

Mike Simpson

PALUMBO: For some non-DOE sponsors we will need not only the SNS but also a good mass spectrometer facility to develop commercial technologies. What brings people in is not just a big facility but pockets of facilities.

APPLETON: I thank all of you for participating in this roundtable discussion. I come away from this discussion even more convinced that multidisciplinary R&D is not only productive and rewarding, but also is a mode of research that thrives in the ORNL environment. It is not just our past success that convinces me of this. It's the promising opportunities I see for the future such as the nanoscale science, engineering, and technology initiative. Additionally, I think this kind of open forum helps all of us hone our thinking. I hope ORNL can have more of such gatherings in the future.

Center for Structural and Molecular Biology Open to Users

A new DOE user facility at ORNL offers a multidisciplinary approach to studying the interactions of biological molecules.

In a multicellular organism, such as a human, cells must communicate with one another to coordinate their activities across the entire organism. Cells send messages to each other through signaling compounds that attach themselves in lock-and-key fashion to protein receptors present both on cell surfaces and inside cells. These signaling compounds include proteins, hormones, peptides, amino acids, and even dissolved gases.

An example of a signaling compound is the hormone estrogen, which swims around in circulating blood and interacts with its receptors located on the surfaces of cells within the endocrine system. Some small signaling compounds can pass through the cell membrane to interact with a receptor inside the cell, while others remain tightly bound to the surface of one cell and interact with receptors bound to the surface of a neighboring cell. Characterizing the details of these and other types of interactions of biomolecular complexes is the chief goal of a new DOE user facility at ORNL, the Center for Structural and Molecular Biology (CSMB). Michelle Buchanan, associate director of ORNL's Life Sciences Division (LSD), also serves as director of the CSMB. The CSMB includes scientists from LSD and from ORNL's Chemical and Analytical Sciences (CASD) and Solid State divisions, as well as from Los Alamos National Laboratory (LANL).

"The new center is based on our traditional strengths in neutron science, mass spectrometry, and computational sciences," Buchanan says. "Our mass spectrometry and computational sciences capabilities are now open to outside researchers."

DOE's Office of Biological and Environmental Research supports the CSBM and is providing nearly $6 million to build a biological small-angle neutron scattering (Bio-SANS) instrument, which should be functioning by June 2002. Bio-SANS will be added to the guide hall of the new cold neutron source now being constructed at ORNL's High Flux Isotope Reactor (HFIR).

"The biological SANS instrument will be designed to have both high flux and low background, which is critical to the analysis of biological materials," Buchanan says. "The upgrade of the HFIR offers a unique opportunity to provide the biological community with a SANS facility that rivals the best capabilities in the world.

"X-rays give excellent high-resolution analysis of the structure of proteins in crystals," she says. "But some very important proteins cannot be crystallized. Also, scientists use nuclear magnetic resonance (NMR) and SANS to study these proteins in their natural form, in solution. Results from the Bio-SANS will not only complement data obtained from X-ray crystallography and NMR but also will provide unique information on the interactions of biomolecules in complexes involved in the cell-signaling processes."

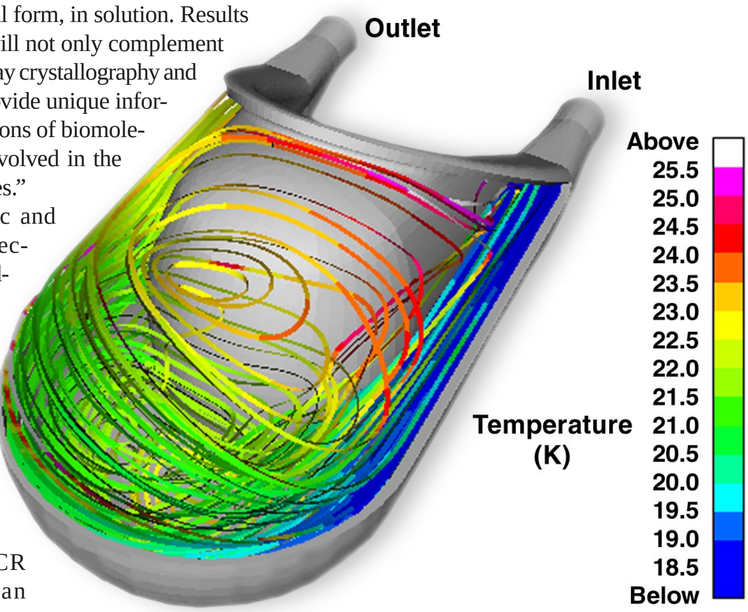
CASD's Organic and Biological Mass Spectrometry Group has added several new mass spectrometers to supplement its current capabilities, including a high-performance Fourier transform ion cyclotron resonance (FTICR) instrument.

"The new FTICR is equipped with an electrospray ionization source, which will allow us to study large proteins and protein complexes," says Buchanan. "The instrument was delivered with a 7-Tesla superconducting magnet. It will be upgraded this summer with a 9.4-Tesla magnet, which will increase the performance of the instrument with respect to both mass resolution and dynamic range. We are very excited about having this instrument for biological studies."

LSD's Computational Protein Structure Group, which predicts protein folding and threading using sophisticated computer models, will assist with interpreting data on biomolecules obtained by researchers using SANS. This group will work closely with researchers at LANL to provide users with user-friendly software for the interpretation of data.

Buchanan sees a bright future ahead for the new CSMB. "We are just beginning to get the word out about the CSMB and have already had researchers from the University of Tennessee come to use the mass spectrometry resource."

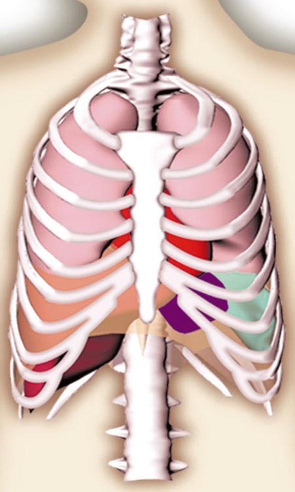
Communication between scientific facilities and users may be just as important as it is between cells in multicellular organisms.



Artist's conception of the cold neutron source–hydrogen moderator vessel, which is being built in 2000 and will be installed in 2001 in ORNL's High Flux Isotope Reactor. Neutrons from the reactor are slowed down by frequent collisions with the moderator's hydrogen atoms. Because the collisions heat up the hydrogen, it must be cooled down by a helium refrigerator to remain an effective neutron moderator. The moderator vessel cutaway (above) shows the temperature of representative hydrogen flow streams.

The Virtual Human Project: An Idea Whose Time Has Come?

A computer model of a functioning human could be the product of one of the largest multidisciplinary projects ever undertaken.



A view of the thorax of the human body based on Visible Human images. Drawing by Allison Baldwin (using thorax model by Eduardo Difilippo, Mark Lambert, and Ross Toedte).

While digging holes in his vineyard one weekend in October 1996, Clay Easterly conceived the seed of a grand vision that is spreading like a slowly growing grapevine. Easterly, a health physicist in ORNL's Life Sciences Division (LSD), saw the need for the mother of all computer models—a huge simulation of the structure and function of the human body that would integrate smaller models of individual organs, body processes, cells, and even neurons in the brain. The flesh and blood of these models would be floods of data, ranging from digitized anatomical images from the National Library of Medicine's Visible Human Project, to known electrical and mechanical properties of human tissue, to information on gene structure and function emerging from the federal government's Human Genome Project.

"I saw it as a marriage of the new biology and high-performance computing," Easterly says. "It's also a way to bring many disciplines together to organize the flood of new biomedical information, to solve complex medical problems, to identify the medical research and data collection and interpretation tools that are needed, and to drive the development of new technologies."

Easterly had returned from a meeting at Quantico, Virginia, with officials of the U.S. Marine Corps who are involved in its Joint Non-lethal Weapons Directorate. The Marines are interested in developing non-lethal weapons that are less harmful than the rubber bullets used now for such purposes as keeping people from blocking food-bearing convoys on humane missions to relieve starvation. One question raised by a Marine official at that meeting was whether researchers could computationally simulate the response of the body to rubber bullets and other kinetic weapons that may be developed. Modeling human response was seen as being preferable to actually testing it to determine if the weapons are non-lethal. "After our meeting with the Marines, my Oak Ridge colleagues Glenn Allgood, Mike Maston, Blake Van Hoy, and I had a crab and shrimp dinner," Easterly says. "We talked around the idea of modeling, but it did not dawn on me then what I would eventually consider. I think that the others may have thought about something with the magnitude of the Virtual Human Project then, but it just didn't sink into me until the next day."

When he returned to work Monday at ORNL, Easterly broached his computer model idea to Barry Berven, associate director of LSD. Berven suggested that Easterly set up a meeting with researchers who might want to pursue the vision. Among the attendees were Allgood of the Instrumentation and Controls (I&C) Division, Maston of the National Security Project Office. Richard Ward of the Computational Physics and Engineering Division (CPED), and Nancy Munro of LSD.

Ward and Munro revealed that they had both been thinking along the same lines. In the spring of 1996, they—together with Keith Eckerman of LSD and John Munro of the I&C Division—had proposed developing a model dubbed Physiological Human, using anatomic

Curtis Boles

Clay Easterly (sitting at the computer) discusses the Virtual Human project of developing computer models to simulate the body's functions with Nancy Munro and Richard Ward.

data from the Visible Human Project and physiological models from ORNL's Dosimetry Research Group and other sources.

In an earlier project Ward, Brian Worley of the Computer Sciences and Mathematics Division (CSMD), and Eckermann had used Visible Human data to build a phantom (computational anatomic model) for radiation treatment planning. The model, which used Monte Carlo calculations, was developed to help doctors decide how to deliver the maximum dose of radiation to a tumor while minimizing the exposure of normal tissue.

The Visible Human Project is a 15-gigabyte collection of digital images that shows the human anatomy in colorful detail in a three-dimensional (3D) computer model. Available on the World Wide Web since 1994, the collection consists of computerized axial tomography (CAT) and magnetic resonance imaging (MRI) scans and photographs of thousands of wafer-thin slices of two bodies donated to science. The Visible Man was an executed Waco, Texas, convict who had killed a 75-year-old man who surprised him while he was stealing a microwave oven. The Visible Woman was a 59-year-old Maryland resident who died in 1993 of a heart blockage that had no effect on the body's appearance.

As Easterly and the other meeting participants talked, the term "Virtual Human" emerged. They envisioned a project that went beyond computer visualizations of body structure. Their concept was to combine models and data to build a comprehensive computational capability for simulating the function as well as the structure of the human body. This capability will allow trauma simulations and other applications.

In 1997 and 1998 Easterly, Ward, and Nancy Munro advocated the Virtual Human idea among their ORNL colleagues. Johnnie Cannon, director of ORNL's Office of Planning and Special Projects, provided program development support and was one of the first to appreciate the value of this vision. Easterly and Maston obtained some funding from the Marines for preparatory steps leading to non-lethal weapons research involving computer modeling. In 1998 Ward obtained some internal funding for coding models of the cardiovascular system and developing an easy-to-use interface. Ward and Ross Toedte of CSMD linked the model to a Virtual Reality Model Language (VRML) graphics file of the human thorax (the body region between the neck and the diaphragm containing the heart and lungs). The user can click on and rotate the thorax on the screen, viewing it in three dimensions.

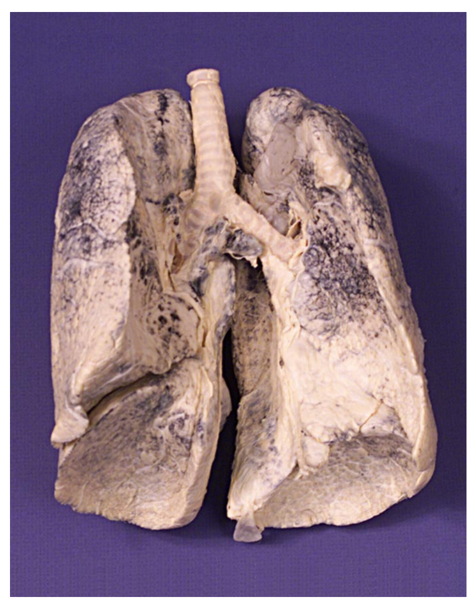
Growing Support

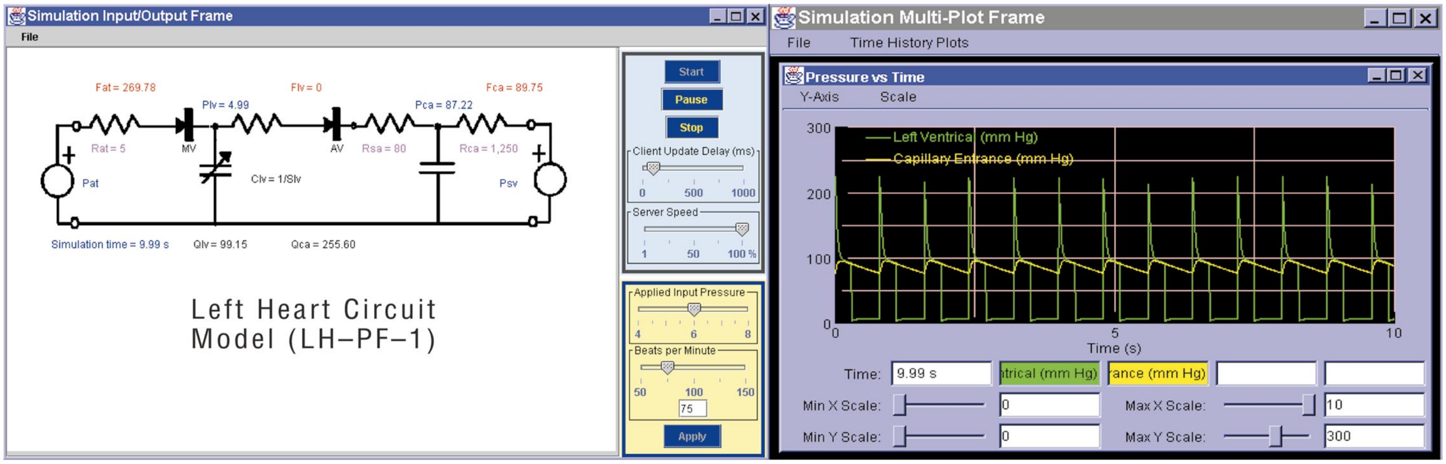
In 1999 the Virtual Human Project took a major leap forward. Easterly gained support for the idea from upper levels of ORNL management. As a result, Ward and his colleagues received internal funding for Virtual Human Project studies from the Laboratory Directed Research and Development (LDRD) Program. Most important, ORNL Director Al Trivelpiece embraced the idea. He told Easterly that the best way to get congressional support for such a massive research program, which could be on the scale of the Human Genome Project, was to get a favorable recommendation from the National Academy of Sciences. But first the Academy would have to agree to conduct a study.

On October 28, 1999, at the instigation of Trivelpiece, a Virtual Human Workshop was held at the National Academy of Sciences in Washington. The meeting was chaired by Charles DeLisi of Boston University, who helped start the Human Genome Project (and is on the LSD advisory committee). Attending the meeting were scientific leaders representing the Department of Energy, Department of Defense, National Institutes of Health, National Academy of Sciences, National Science Foundation (NSF), National Aeronautics and Space Administration, National Space Biomedical Research Institute, the White House's Office of Science and Technology Policy, several universities, four DOE national laboratories, and the private sector.

"These representatives gave solid support to the idea," Easterly says. "The meeting resulted in a

These plastinated human organs – the brain, heart, and lungs – were loaned by the University of Tennessee's College of Veterinary Medicine and used to attract attention to the Virtual Human exhibit in the ORNL display area at the Supercomputing 99 conference.





The Virtual Human Java interface, which includes a 3D model of the human anatomy (not shown here), also displays a circuit for the left side of the heart and systemic vascular system (V.C. Rideout, 1991) and plots showing changes in left ventricle and capillary entrance pressures over time. This interface allows the user to run the model on a remote server using a Web browser on the user's desktop machine.

recommendation that the National Academy of Sciences perform a study to define and scope the Virtual Human Project and make a report to Congress."

On November 8 and 9, 1999, the First Virtual Human Roadmapping Workshop was held in Rockville, Maryland. It was organized by ORNL and co-sponsored by the Joint Non-lethal Weapons Directorate.

The consensus of the two workshops is that the Virtual Human concept is "an idea whose time has come," Easterly says. "This project is seen as necessary to help manage the information explosion transforming biology and medicine by giving it organization and infrastructure. It is beginning at the right time because of the explosive emergence of information technology and supercomputing capabilities and the ability to obtain more data from the body using implantable sensors. But the project is in need of a very thorough and systematic planning process."

So far, the leadership of the project is coming from Oak Ridge. "We are beginning to think of the Virtual Human Project as a resource," Easterly says, "because it will require enormous databases, system integration, measurement systems, Web access, computer hardware, computer infrastructure, model development, analysis of individual biochemical measurements, and simultaneous analyses of hundreds to thousands of measured variables. We expect thousands of collaborators to make this massive multidisciplinary project work. It's an opportunity for biomedical researchers to put their results in the context of the human body."

"We will need researchers representing many different disciplines—anatomy, physiology, biomedical engineering, electrical engineering, computer science, physics, biophysics, systems engineering, information technology, and medical technologies," Ward says. "We are teaming with experts in universities, medical colleges, and industry to build the Virtual Human."

What ORNL Can Do

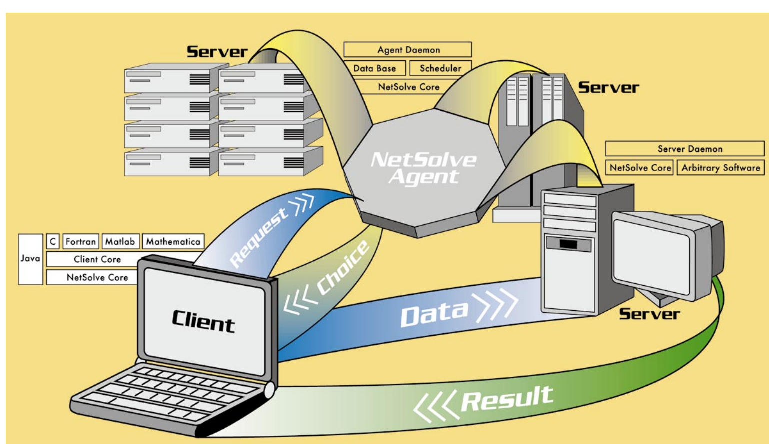
"ORNL is a leader in developing the Virtual Human resource by integrating the computer models," Easterly says. "We also will be involved in developing specific models, such as a model of the respiratory system. And we will develop implantable sensors, analytical instruments, and other methods for improving data acquisition and interpretation."

For example, ORNL researchers envision that the Virtual Human resource will give physicians access to state-of-the-art, nonlinear analysis capabilities for rapid remote analysis of patient electroencephalogram (EEG), electrocardiogram (EKG), breath sound, and other types of data. A demonstration of this capability is being planned by Lee Hively of ORNL's Engineering Technology Division (ETD) using his patented algorithms for predicting seizures from EEG data showing the brain's electrical activity.

Ward and his colleagues are involved in both model development and model integration projects. The goal of an LDRD project is to develop a Virtual Human Integrated Respiratory System Model—a computer simulation of the lung and associated structures involved in generating and transmitting lung sounds. Project participants include Allgood (I&C); Toedte (CSMD); Hively (ETD); Nancy Munro (LSD); and Kara Kruse (CPED), who is a biomedical engineer. The ORNL group is collaborating with Vanderbilt University to incorporate a lung fluid transport model.

"We plan to build a model that predicts lung disorders, such as emphysema and asthma, based on changes in breath sounds," Ward says. "We will use patient data obtained by Glenn Allgood at the Walter Reed Army Institute of Research using the lung sound monitor he helped develop at ORNL. In a collaboration with scientists at North Carolina State University and the Medical College of Ohio, we are using computational fluid dynamic methods to model the generation of lung sounds."

Here's a practical example of how the ability to monitor lung sounds to detect disorders will prove useful: The U.S. Army is interested in predicting whether a soldier's lung has collapsed as a result of a puncture wound. If the chest wound is large, a medic might not have access to the thorax area, so the best way to get a diagnosis may be to place a sensor on the throat to gather data on breathing patterns. The data could be wirelessly relayed to the medic's wearable computer, which would then feed the data into a model of the respiratory system for diagnosis of the lung injury, if any. ORNL researchers and collaborators are building such a model, which could save lives by telling a medic quickly what sort of trauma care should be administered.



NetSolve allows the client at the desktop computer to tap into supercomputing levels of power by finding appropriate computational resources, including supercomputers networked into a computational grid, and making them easily accessible to the individual user.

The lung disorder prediction model will be linked to the Human Respiratory System Model of the International Commission for Radiological Protection for predicting how much inhaled material, such as beryllium or radon-daughter products, is deposited in various parts of the lung. Visible Human data obtained from the National Library of Medicine and data from human lung casts are being used for this project.

Ward is also leading an effort on model integration, to help develop the computational infrastructure for the Virtual Human Project. A major problem impeding the progress of this effort is that computer models of various organs will be too big and complex to be stored and executed on a desktop personal computer. The idea, therefore, is to use computer technologies to allow the desktop computer user to connect with large computer servers—including high-performance computers—that can run large models and feed the results in visual form back to the user.

"We are developing a Virtual Human Portal," Ward says. "This is a Web site that can be customized to allow access by a desktop computer user to problem-solving and modeling applications on a remote server."

For this purpose CPED's Dennis Strickler modified an interface developed by Johnny Tolliver and Strickler for the Graphite Reactor Severe Accident Code (GRSAC). The original code was written by Syd Ball and Delphy Nypaver, both of the I&C Division, to simulate the operation of graphite-moderated, gas-cooled reactors. By adapting this distributed, object-oriented Java interface to physiological modeling, Strickler implemented a complex model consisting of many differential equations in a form that can be remotely controlled by the user. For example, it shows the effects that a slight change in the frequency of the heartbeat can have on cardiovascular functions, such as blood pressure.

One computer science development that will be useful is NetSolve, a client-server system that enables desktop computer users to solve complex scientific problems by tapping into supercomputing levels of power. NetSolve was developed under the leadership of Jack Dongarra, an ORNL-University of Tennessee Distinguished Scientist. "NetSolve," says Ward, "couples desktop computer software to models and problem-solving programs on a high-performance computer such as the IBM SP at ORNL." Dongarra and his collaborators are adapting NetSolve for use in the Virtual Human Portal. David Walker of CSMD is developing abstract concepts for the problem-solving environment (PSE) of the Virtual Human Portal.

Walker, Dongarra, and Ward—along with researchers from the University of Utah, Indiana University, and the University of Washington—are making an information technology research proposal to the NSF for funds to develop the computational infrastructure for the Virtual Human Project.

"This infrastructure will include a collaborative environment for model integration," Walker says, "It will permit collaborators from around the country to construct integrated models for simulating the structure and function of the human body. These models will then be executed on distributed computing resources using sophisticated scheduling mechanics that make the whole process transparent to the user."

If funded, the team would develop a generic advanced, distributed PSE, which is an integrated computing environment for composing, compiling, and running applications in a specific problem area. Created from the generic PSE, a prototype Virtual Human will facilitate developing, integrating, and solving complex 3D models of human physiology and anatomy.

"We envision developing a smart environment with intelligent agents on a remote server that would be given a problem to solve," Ward says. "The agents would find the appropriate set of models and execute them on a computational grid of high-performance computers. We will also develop a user interface to present visualization of the results of the simulation either to the client's desktop or to a room-sized immersive visualization environment called a CAVE."

What It Means to You

The beauty of a computer model of a human is that it can be customized for a specific person at any point in time. At least, that's the long-term vision shared by Easterly and his colleagues. Customization is important because of evidence that men, women, and children respond differently to various drugs, drug dosages, and other treatments, as well as environmental insults.

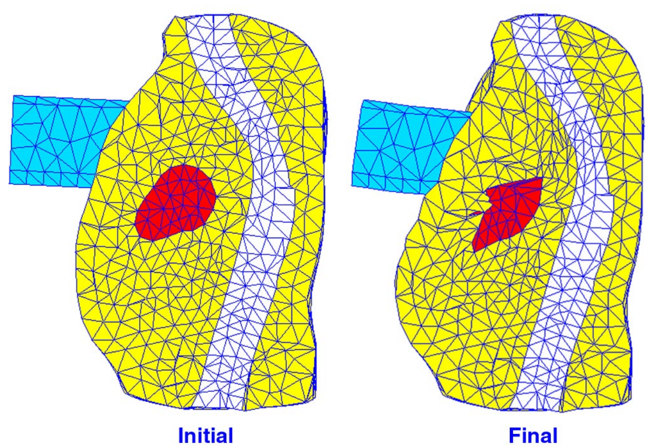
"From our earlier work in modeling children's organs," Ward says, "we see the need to build human models for different ages, sizes, and sexes. By using equations and changing some parameters, we can make the heart smaller or larger. We can make a human model or phantom grow with age." Use of a customized model—a computerized clone of you that includes your genetic makeup—will make it possible to predict how you might respond to different doses of radiation, chemicals, and drugs, or what damage you might suffer if you were in an automobile accident or airplane crash.

In fact, one of the early applications of the Virtual Human model will be the prediction of responses of the body to impacts from, say, rubber bullets. ORNL researchers doing this research can draw on some of the Laboratory's work in developing detailed models of cars and using them to predict the damage these cars will sustain in collisions at different velocities. In this case, the finite element mesh software used for cars to pinpoint the effects of pressure on material deformation will be applied to meshing the human model. This type of model can also be used to predict the tissue damage that will result from various types of car wrecks and plane crashes.

"A Virtual Human model of the lung could be useful for virtual surgery—that is, to simulate the effect of lung surgery on a patient's respiration before any surgery is actually performed," Ward says. "A model of the circulatory system could help doctors decide where to replace part of an artery to reroute the blood so it flows around a blockage. A model of a patient's hip could help a surgeon determine the effect of a hip implant on the joint's movement."

Looking ahead five to ten years, even decades from now, Easterly sees a "human model on a chip," or at least mounds of personal genetic and other medical data squeezed into a plastic 3 x 5-in. card. When plugged into a handheld computer, your card might provide you and your doctor the results of your X-rays and CAT and MRI scans, your responses to past treatments, your genetic makeup, and a list of foods and drugs you should avoid. "The more you know about your body," Easterly says, "the more you can take charge of your well-being."

The idea of the Virtual Human Project is slowly creeping through the scientific community. If the vision continues to spread, it may someday bear fruit of value to virtually every human.



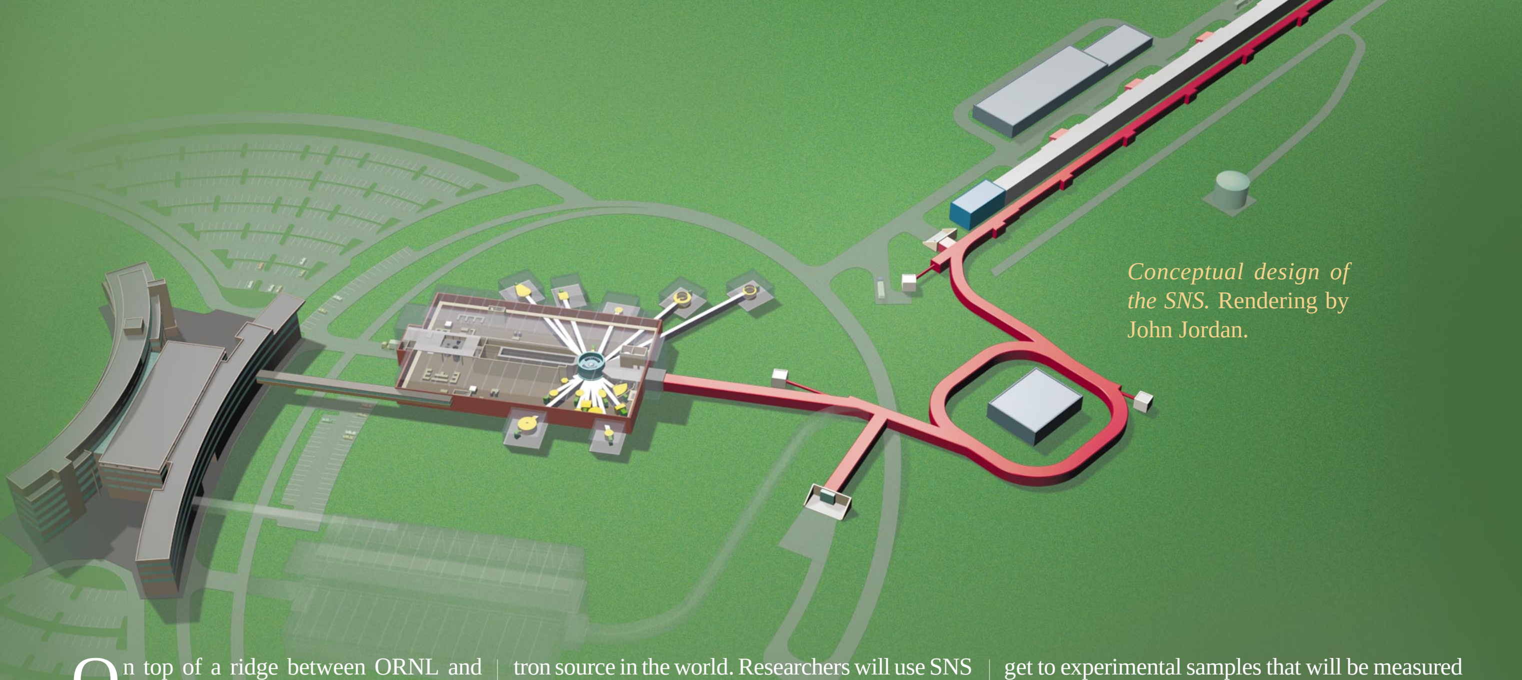
The initial and final, or deformed, shapes of a finite-element mesh model of the human body based on Visible Human data are shown here. The deformation resulted from a wood block moving at constant velocity into the chest just above the heart. The elapsed time for the simulation is 0.0001 second. The spine, heart, lungs (not shown in this view), and surrounding tissue are each assigned appropriate measures of density and elasticity. Simulations such as these can model the impacts on the body of seat belts, air bags, or objects in an automobile during an accident.

Spallation Neutron Source

SNS

A Challenging Year

The nation's largest scientific project, the Spallation Neutron Source, will be built at ORNL by a partnership of six DOE national labs. The world's most powerful pulsed neutron source is expected to begin operation in June 2006.



Conceptual design of the SNS. Rendering by John Jordan.

On top of a ridge between ORNL and the Oak Ridge Y-12 Plant, the largest civilian construction project in the United States is under way. Trees are being cleared from the construction site on Chestnut Ridge, and a one-mile-long access road connecting the ridge with Bear Creek Road is being built for hauling building materials and equipment to the site.

By 2002 a central laboratory and office complex will be built on the site to house some 300 design, construction, and project management staff for the $1.4 billion Spallation Neutron Source (SNS). The SNS is the nation's largest science project and the most recent big-science facility project sponsored by the Department of Energy's Office of Science. By June 2006 the SNS will be a magnet for scientists from many nations because it will be the most advanced, powerful pulsed neutron source in the world. Researchers will use SNS neutron beams for neutron-scattering experiments to help them better understand the structure and properties of physical and biological materials, ranging from polymers to proteins.

"The SNS will be an extraordinary tool for exploring matter and for enabling world-class science," says David Moncton, executive director of the SNS. "Information obtained from this accelerator-based facility could lead to advanced materials and products such as faster electronic devices, lubricants for more efficient cars, longer-lasting artificial joints, and more effective drugs."

The facility will include an ion source, a linear accelerator to speed up the ions, an accumulator ring to compress protons separated from the ions, a liquid mercury target for the protons, and beam lines to carry neutrons produced in the target to experimental samples that will be measured by scientific instruments. The design and construction of the SNS will be the product of a partnership among six of DOE's national laboratories with help from the principal architect-engineer and construction manager Knight Jacobs and other industry support. In addition to ORNL, the DOE teams come from Argonne (ANL), Brookhaven (BNL), Jefferson (Thomas Jefferson National Accelerator Facility), Lawrence Berkeley (LBNL), and Los Alamos (LANL) national laboratories.

Completion of the project will depend on the continued support of the President and Congress. To get it built on schedule, the SNS Project is counting on receiving the $281 million proposed in the President's budget for FY 2001. DOE plans to ask for $291.4 million for FY 2002, $224.5 million for FY 2003, $143 million for FY 2004,

$112.9 million for FY 2005, and $75 million for FY 2006 to complete the facility. Construction of the SNS will provide jobs for up to 600 construction workers over the next six years, and when operational, the SNS will employ 300 to 400 scientists and other personnel.

1999 Highlights

The high point for the project in 1999 was what Moncton called the "sweet moment" for the SNS: the December 15, 1999, groundbreaking ceremony at the SNS site. Attending and speaking at this event were Vice President Al Gore, Secretary of Energy Bill Richardson, Governor Don Sundquist and U.S. Senator Bill Frist of Tennessee, and members of the Tennessee congressional delegation. Also present was Clifford Shull, who won the Nobel Prize in physics in 1994 for his pioneering research at ORNL in neutron scattering. Other honored guests included Martha Krebs, retiring director of DOE's Office of Science, who provided direction and helped muster congressional support for the project, and Bill Appleton, then deputy director of science and technology at ORNL, who steered the project through its first few years.

"The true beauty of the SNS," said Gore, "is that no one can really know what this tool will be capable of discovering. It will bring discoveries that nobody can predict. . . We're putting America on the path of reclaiming our leadership in the neutron scattering technology that we invented here in the United States of America."

In the past year or so, DOE and the SNS Project have taken many steps to move the project forward. The project's technical, schedule, and cost baselines have been established. Cost estimates have been scrubbed, thus making it possible to double the budget for neutron scattering instruments.

Geotechnical investigation and qualification of the Chestnut Ridge were completed satisfactorily; this determination was made by a team that drilled for core samples, characterized the bedrock, assessed the site's seismic potential, and studied the area's historical record of waste disposal and other activities. The final environmental impact statement was approved and a Record of Decision was issued by the Secretary of Energy, formally establishing Oak Ridge as the SNS site.

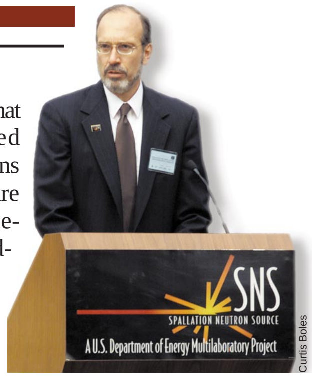
Actions to mitigate environmental impacts are under way, including the installation of a new air-monitoring tower for the Oak Ridge office of the National Oceanic and Atmospheric Administration (NOAA). The current NOAA tower in the Walker Branch Watershed, which is close to the SNS site, monitors dry deposition of airborne pollutants. These measurements could be affected by airborne dust stirred up by SNS construction. During operation, the SNS facility will emit carbon dioxide, water vapor, and heat, which NOAA likely will monitor for its studies related to global climate change. The new tower will be located far enough away from the SNS so that the facility's emissions will not interfere with NOAA measurements.

The SNS Project successfully met several management challenges presented by DOE and Congress. Moncton, director of the Advanced Photon Source at ANL, was named executive director for the SNS. In late January 2000, Tennessee Governor Sundquist signed a bill passed unanimously by the General Assembly that exempts the SNS Project from $28 million in state sales and use taxes, lowering the overall cost of the project.

Improving the Neutron End

Many ORNL researchers involved with the SNS Project are concerned with the "neutron end" of the machine. Some of those researchers are working on the design of the mercury target from which neutrons will be produced. Others are developing scientific instruments that will be used to measure the energies and angles of neutrons scattered from targets of interest.

One of the most significant technical achievements in 1999 was the completion and operation of the Target Test Facility (TTF) at ORNL. The TTF is a full-scale mercury loop in ORNL's Robotics and Process Systems Division. It has been operating with mercury since October 1999. Research at the TTF and other, smaller mercury loops under the leadership of Tony Gabriel is aimed at answering several questions: Which candidate materials for the target container are the most compatible with mercury? How can the target be designed to shield workers from the radioactivity of the proton-bombarded mercury? Can remotely operated equipment be used to safely and reliably repair and replace target components in hot cells? How can the output of neutrons be maximized for research?



David Moncton, executive director of the SNS, calls the groundbreaking ceremony a "sweet moment" for the SNS.

"Based on what we have learned from test operations at the TTF, we are improving the design before sending it to vendors who may want to bid on building the target," says Thom Mason, director of the Experimental Facilities Division of the SNS. "We will do hydraulic testing with water to simulate mercury flow. We will measure the ability of mercury to remove heat from the stainless-steel container.

"Experiments on the effects of accelerator beams on mercury targets are being done at Brookhaven and Los Alamos. We have studied stresses that have developed in mercury targets bombarded by proton beams. Based on the information we've obtained, we've concluded that mercury is the right choice for the target."

Because of the enormous power the 1-billion-electron-volt proton beam will deposit in the target, it was decided to use a liquid mercury target instead of a solid material such as tantalum or tungsten. The SNS will be the first scientific facility to use mercury as a target for a proton beam.

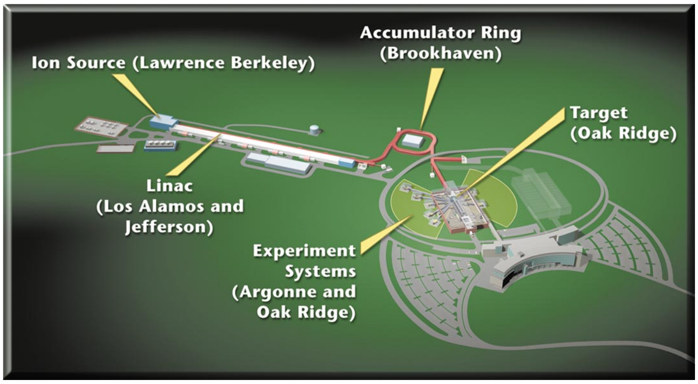
"We have been improving the target design by integrating the target group led by Tony Gabriel with the instrumentation design group led by Kent Crawford at Argonne," Mason says. "As a result of our R&D and preliminary design, we have made a number of improvements in the target, which will increase the scientific performance of the SNS for experimenters. We have adopted a more flexible

Vice President Al Gore and outgoing Office of Science Director Martha Krebs posed after the groundbreaking with directors of five of the six national laboratories participating in the SNS partnership: From left: Charles Shank of LBNL; Krebs; John Browne of LANL; Gore; Yoon Chang, ANL's interim director; Denis McWhan, who represented BNL's John Marburger; and Al Trivelpiece, then ORNL director.

shutter geometry, allowing us to install 24 instead of only 18 instruments, an increase of 33%."

According to Mason, fine-tuning moderator characteristics will significantly enhance many applications because it will allow a higher-intensity neutron beam to be produced in a temperature range of 100 K. This improvement is achieved by changing the composition of a moderator below the target by making it a composite of supercritical light hydrogen and light water. The SNS will also have two cryogenic moderators above the target. Moderators slow down the neutrons leaving the mercury target to an appropriate energy range before they enter the beam lines that deliver neutrons to the instruments.

"We also changed the composition of the reflector, which bounces neutrons straying from the target back into the moderators," Mason says. "Instead of lead only, the reflector will be made of a composite of lead and beryllium. As a result of this change, we will get sharper neutron pulses, enabling higher-resolution measurements."



Each of the participating DOE national laboratories in the six-lab SNS partnership is responsible for an important component of the accelerator-based neutron source. Rendering by John Jordan.

Taking the Users' Pulse

Mason represents the interests of the scientific community in ensuring that the overall project meets the requirements of the academic, industrial, and government research communities. He has organized workshops to ensure good communication among the users and the six DOE national laboratories participating in the design and construction of the technical portions of the SNS facility. The SNS Project has also appointed a user administrator, Joyce Shepherd, who will build up a group to work with users to ensure that the SNS Project is responsive to their needs.

"Many neutron sources were originally designed for some other purpose such as radioisotope production, so the idea of doing neutron scattering research at these sources was an afterthought," Mason observes. "The SNS partnership offers the opportunity to design a neutron source specifically optimized to meet the needs of the scientific users."

How are ORNL researchers involved in the design of neutron science instruments to be built at the SNS? "Some ORNL researchers are working at Argonne with Kent Crawford to design new instruments," Mason says. "Potential users of the SNS can influence the design of new instruments by joining instrument advisory teams, or IATs. Research groups that can get their own funding from sponsors to develop neutron instruments can form instrument development teams, or IDTs. Groups at ORNL and BNL, as well as those in Denmark and Germany, have expressed interest in forming IDTs. An IDT will get dedicated beam time for its scientific program in return for its contribution toward the construction and operation of the instrument."

Several groups at ORNL have expressed interest in writing proposals to get funding for instruments and for experiments to be performed at the new facility. In the Physics Division, there is interest in pursuing fundamental physics studies with cold neutrons and in making measurements of interest to the astrophysics and nuclear structure communities. DOE's new Center for Structural and Molecular Biology at ORNL plans to seek funding for a neutron-scattering instrument to study the structure of biological molecules. And a group in the Metals and Ceramics (M&C) Division is working with the SNS Experimental Facilities Division and outside researchers to prepare the scientific case for and define the essential characteristics of a neutron diffractometer to study residual stress in engineering materials.

The Ion End of the Machine

The SNS design calls for an accelerator system consisting of an ion source being developed at LBNL, a full-power linear accelerator being developed by LANL and the Jefferson Lab, and a proton accumulator ring being developed at BNL that will deliver a 2-megawatt (MW) beam to the mercury target (being developed at ORNL). The facility has been designed with the flexibility to provide additional scientific output in the future.

A prototype negative hydrogen (H-) source has already been tested at 45 milliamperes (mA). It will be developed further to achieve the 70 mA needed to support 2-MW operation. The ion beam will be delivered to a linear accelerator that will use radiofrequency radiation and magnetic fields to accelerate, focus, and steer the ion beam toward the accumulator ring. The decision to use superconducting technology to power the accelerator will reduce its footprint from five to three football fields in length. In this design, the beam is injected into the ring through a foil that strips the two electrons off each negatively charged hydrogen ion, making each one a proton. The protons circulate in the ring about 1000 times before being extracted as a pulse of less than 1 microsecond for delivery to the liquid mercury target.

Nurturing the Six-Lab Partnership

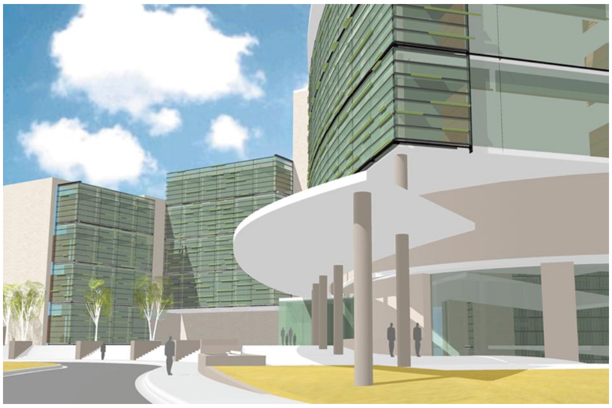
The large-scale, six-lab partnership needed to design and build the SNS is unique in DOE history. What must be done to ensure that the six national lab partners work together successfully on the design and construction of the SNS?

"The keys to making this partnership work," says Carl Strawbridge, administrative director of the SNS, "are the commitment of the six lab directors in the partnership; various tools such as the interlaboratory Memorandum of Agreement; and a strong, experienced SNS management team working with the DOE project team."

What must be done to ensure congressional funding and support for the SNS partnership over the next seven years? "We are fortunate that no one in the scientific community and the political system questions the scientific need for the SNS," Mason says. "The materials science applications of the SNS are seen as important by everyone. We recently enjoyed endorsements from the National Academy of Sciences' Solid State Sciences Committee and the American Physical Society Council.

"It is important that potential users of the SNS all over the nation speak or write to their congressional representatives about the need for support for the SNS. It is crucial that we get the appropriation of $281 million for the next fiscal year so we can begin procuring accelerator components and initiate significant construction activities onsite. We hope we can continue to enjoy strong support for this national project."

Now that construction of the SNS has begun on top of the ridge, SNS supporters have even higher hopes for the project.



Artist's conception of the central laboratory and office complex of the SNS to be built on the Chestnut Ridge site in two years.

Neutrino Detector Laboratory To Be Proposed for ORNL

The proposed Oak Ridge Laboratory for Neutrino Detectors could help unlock mysteries in astrophysics.

Do neutrinos streaming from the sun have mass or not? It's one of the puzzles of physics. Confirming that neutrinos have mass could help astrophysicists account for part of the missing matter in the universe, possibly providing insights into the fate of our rapidly expanding cosmos.

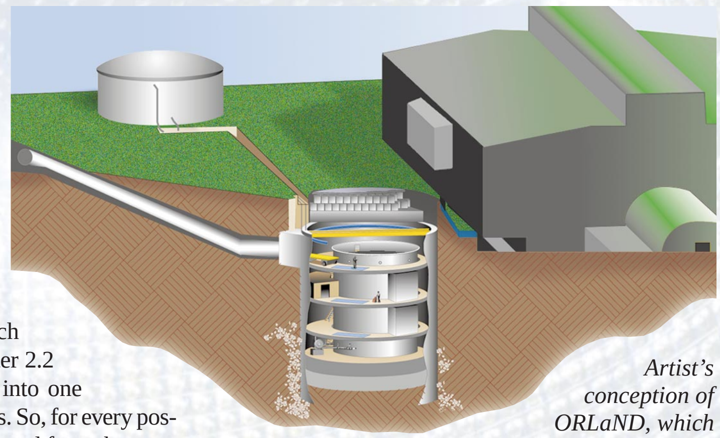
A neutrino is an electrically neutral subatomic particle that penetrates steel, concrete, our bodies, and the earth itself. Neutrinos are produced by stars, including the sun, by the decay of radioactive isotopes, and by nuclear reactors.

In June 1998 an international team of scientists at the Super-Kamiokande detector in Japan—a specially constructed underground lake of highly purified water surrounded by a huge array of light detectors (background image)—reported evidence that neutrinos have mass. It is important that scientists at other neutrino facilities verify this finding and accurately measure neutrino properties.

A proposal for a detector facility that could bring scientists even closer to a definitive answer to the question of whether neutrinos have mass will be made to DOE by mid-2000. The approximately $50-million facility, called the Oak Ridge Laboratory for Neutrino Detectors (ORLaND), would be built near the Spallation Neutron Source (SNS) (see previous article). The ORLaND proposal is being prepared by a group of nearly 100 scientists from universities and national laboratories in the United States and abroad. Frank Avigonne, professor of physics at the University of South Carolina, is the spokesman of the ORLaND collaboration.

The SNS will be the source of the world's most intense, pulsed beams of neutrons for use in neutron scattering research. The SNS facility will include a liquid-mercury target for bombardment by beams of protons from the SNS accelerators and beam lines to carry neutrons produced in the target to experiment stations. It is the target stage of the SNS that interests physicists like Yuri Efremenko, a University of Tennessee research professor of physics based in ORNL's Physics Division. He, along with Frank Plasil, an ORNL corporate fellow in the division; Glenn Young, a Physics Division section head; and Ken Carter from the Oak Ridge Institute for Science and Education, are helping draft the neutrino proposal and leading the ORNL effort to construct the facility.

"When the protons interact with the mercury atoms in the target," Efremenko says, "not only neutrons, but also unstable subatomic particles called pions are formed. After 26 nanoseconds, each pion decays into a neutrino and a negatively charged particle called a muon. Each muon is unstable, and after 2.2 microseconds, it decays into one electron and two neutrinos. So, for every positively charged pion produced from the mercury target, we get three neutrinos."



Artist's conception of ORLaND, which could be located near the SNS.

The advantage of the SNS as a source of neutrinos is that it does not produce a steady stream of neutrinos as do the sun and reactors. The neutrinos (like the neutrons) will be produced in pulses whose on and off times are known. Thanks to computers, the arrival times of the neutrinos at the ORLaND detector can be predicted accurately. Therefore, scientists will know exactly when to expect a neutrino signal in the detector. If they see weak signals in between the pulses, they will attribute them to background radiation such as cosmic rays hurtling through the atmosphere. Thus, they will be able to separate real events from spurious ones.

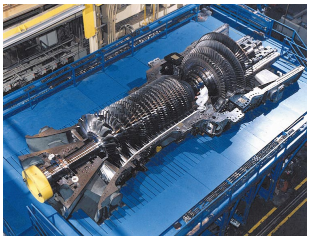
The main detector of the ORLaND facility will be a cylindrical tank placed in a 33-m- (110-ft-) deep bunker near the SNS target building. The detector itself will be about 15 m (50 ft) deep and 15 m in diameter. On top of it will be 4.5 m (15 ft) of large steel and concrete blocks to reduce the intensity of cosmic rays coming through. The facility will provide space for outside groups of researchers to assemble their own special detectors as part of an international research effort on neutrino measurements.

"ORNL's 2000-ton liquid scintillation detector will be 25 times smaller than the Japanese detector," Efremenko says. "It will contain mineral oil mixed with an additive that emits light when struck by charged particles. The emitted light will be detected by an array of thousands of photomultipliers, each about 20 cm (8 in.) in diameter." Despite its small size, the proposed ORLaND detector will still be the world's most effective neutrino facility because of the large neutrino flux produced by the SNS during routine operation.

When a neutrino strikes a proton in the hydrogen- and carbon-containing mineral oil, a positively charged electron (positron) and a neutron are produced. The neutron then interacts with another proton, thereby emitting a gamma ray with a total energy of 2.2 million electron volts. The gamma-ray photons, in turn, collide with electrons, imparting to them a recoil energy. It is these scattered electrons that finally produce light in the oil-additive liquid scintillator, resulting in the indirect detection of the neutrino.

"Our main goal," Plasil says, "is to look for neutrino oscillations, in which one type of neutrino changes to another type. If we detect neutrino oscillations, then we will know that neutrinos have mass. If they have mass, the universe will be heavier than we thought, and our current understanding of subatomic particles embodied in the so-called Standard Model will have to be revised. We also plan to conduct experiments to determine the probability with which neutrinos interact with different types of nuclei. This research will be of great interest to the astrophysics community."

Turbine Renewal: Shaping an Emerging Gas-Fired Power Source



The gas turbine is evolving into the workhorse of electricity production in the 21st century, and ORNL materials research is helping to boost its efficiency and reduce its emissions.

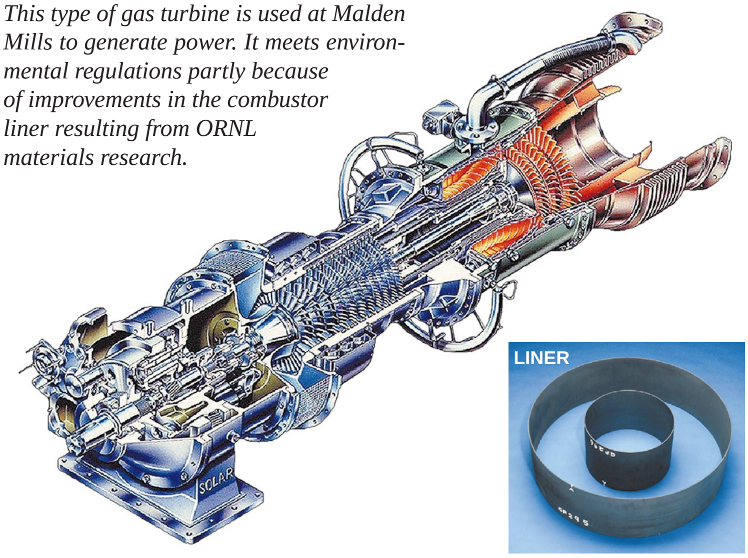
In 1995 three buildings of Malden Mills, the maker of Polartec climate control fabrics, burned down in a major industrial fire. But instead of shutting down operations and dismissing the employees of this major manufacturer in Lawrence, Massachusetts, Aaron Feuerstein, president and owner of Malden Mills, decided to rebuild the mill buildings and re-employ the workers. For this decision in the age of corporate "rightsizing" and relocation of plants to countries where labor is cheaper, he received international acclaim and awards for his humanitarian treatment of employees. President Clinton cited him for corporate responsibility.

In his decision to build a highly efficient cogeneration power plant to replace the inefficient one in which the fire started, Feuerstein faced a problem. Under Environmental Protection Agency (EPA) rules, a new power plant must meet stringent limits on the exhaust gas concentrations of pollutants such as nitrogen oxides (NO_x) and carbon monoxide (CO). To help solve this problem, the Department of Energy (DOE) decided to make Malden Mills a demonstration site for a power plant featuring a gas turbine, the type of engine that in different forms flies airline passengers across oceans and drives M-1 tanks across battlefields. The gas turbine is evolving into the workhorse of electricity production in the 21st century.

The old Malden Mills power plant was to be replaced with a cogeneration plant that combines a natural gas-fired turbine with a steam recovery boiler for the production of electricity and heat. This combined heat and power (CHP) plant uses fuel 25 to 40% more efficiently than do today's coal-fired plants and emits about 40% less carbon dioxide, a greenhouse gas.

A Centaur 50 gas turbine engine built by Solar Turbines, Inc. was to be used in the power plant. The problem was that, although this engine is highly efficient, it would discharge too much NO_x, violating EPA regulations. So, DOE provided funding for technical support to help upgrade the Solar Turbines engine so that it would meet emissions specifications. DOE asked

The Malden Mills power plant in Lawrence, Massachusetts, has a Solar Turbines gas turbine engine (Centaur 50S SoLoNOx Engine) that has been improved partly because of materials research results from ORNL.



This type of gas turbine is used at Malden Mills to generate power. It meets environmental regulations partly because of improvements in the combustor liner resulting from ORNL materials research.

material scientists in ORNL's Metals and Ceramics (M&C) Division to help determine which ceramic composite and protective coating would work best in liners of the combustion chamber (combustor) for use in the rebuilt plant's gas turbine.

After an intensive 24-month effort involving Solar Turbines, ORNL, Pratt and Whitney, DOE's Argonne National Laboratory, B. F. Goodrich, and Honeywell Advanced Composites, a turbine outfitted with ceramic composite combustor liners was put into operation in August 1999. In a November dedication ceremony at Malden Mills, Secretary of Energy Bill Richardson declared that this power generation unit has the "lowest emissions of any industrialized heat and electric combined facility in the United States—and possibly the world."

According to DOE, natural gas turbines are expected to make up more than 80% of the power-generating capacity to be added in the United States over the next 10 to 15 years. Of the more than 200 new power plant projects announced recently in the United States, 96% plan to use natural gas and most will employ gas turbines. The global turbine market is also promising, with estimates of worldwide power generation acquisitions approaching $100 billion over the next 10 years.

How a Land-Based Gas Turbine Works

A turbine is a rotary engine that uses a continuous stream of fluid to turn a shaft that drives machinery, such as the rotor of an electric generator. In a steam turbine, high-pressure steam is forced through turbine wheels to rotate a shaft driving a generator. Fossil fuel power plants and nuclear power plants, which heat water to make steam, use steam turbines to drive large electricity generators.

A gas turbine generally consists of a compressor, combustor, and turbine. Part of the turbine drives the compressor, which sucks in large quantities of air, compresses it, and feeds the high-pressure air into the combustor. There the air is mixed with a fuel, such as natural gas, kerosene, or gas derived from coal. The mixture is burned, providing high-pressure gases to drive the turbine.

In a CHP plant, the hot exhaust gases from the gas turbine are used to generate steam in a heat recovery boiler and the steam is used in the industrial process. As a result, less fuel is needed. The CHP plant not only spins an electric generator but also supplies heat, making it a cogeneration facility.

In another type of power facility, the combined cycle gas turbine (CCGT) plant, the exhaust heat from the gas turbine is used to produce steam for a power-producing steam turbine. Combining the output of the gas and steam turbines generates more electricity for the same amount of fuel. A CCGT may also have a recuperator, or heat exchanger, which uses some of the energy in the gas turbine's exhaust gases to preheat the air entering the combustor. In this way, the energy efficiency of the CCGT is improved.

Conventional land-based gas turbines used for power generation are 33 to 40% efficient when used in "simple cycle" mode—that is, without a recuperator or steam generator. How can a CCGT both be made at least 60% efficient and meet the goals of lower emissions and lower energy costs set in DOE's Advanced Turbine Systems (ATS) Program? U.S. turbine manufacturers working in the program concluded that turbine inlet temperatures must be over 1427°C (2600°F) and that the amount of air typically bled from the compressor to cool turbine components must be reduced. These two criteria, coupled with the large size of the turbine engines involved, severely challenged the gas turbine industry.

"For gas turbines to hold up under these sustained temperature and pressure extremes, changes had to be made in the materials used in them and in the ways they are manufactured," says Mike Karnitz, manager of the gas turbine project in the M&C Division. "ORNL materials research played a key role in identifying improvements in turbine components to meet DOE goals."

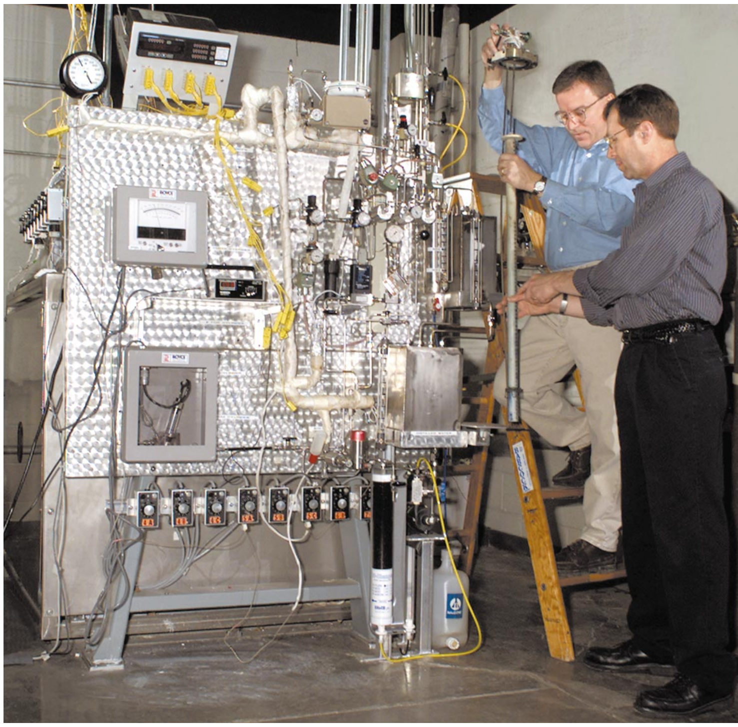
How ORNL Helped

Gas turbines use fuel more efficiently because they can be operated at higher temperatures than can other power sources currently available. But high-temperature operation can result in the formation of NO_x from nitrogen in the fuel and in the air. Large amounts of preheated air are pulled into the combustor, and additional lower-temperature air is pumped through holes in the metallic interior walls of the combustor to cool them as combustion occurs inside. The pumped-in air mixing with the combustion gases creates hot spots that trigger the formation of NO_x through high-temperature reactions between nitrogen and oxygen in the air. To reduce NO_x formation, one route is to replace the metal combustor liners with ceramic liners. Because they can withstand more heat, ceramic liners should require less cooling; therefore, they can be designed without cooling holes, reducing the tendency to create hot spots. If less air is used and fewer hot spots are present, less NO_x is produced, making it possible for the gas turbine to meet the air quality standard. In addition, reducing the need for air cooling also saves energy, making the gas turbine more efficient.

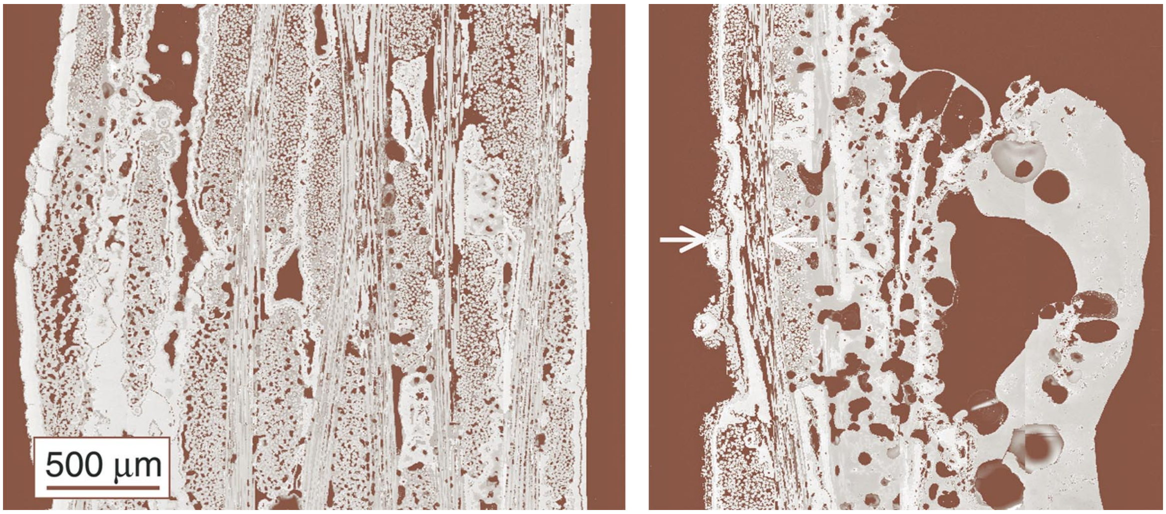
Selecting the best ceramic liner material for the Solar Turbines' gas turbine for Malden Mills required two years of testing. Among the primary candidate materials in this study were numerous variations of silicon carbide (SiC)-based composites. To produce these composites, continuous SiC-fibrous preforms were densified by one of two processes, chemical vapor infiltration or Si-melt infiltration, both of which create a relatively dense SiC matrix. The resulting continuous fiber-reinforced ceramic composites (CFCCs) are strong and have an acceptable fracture toughness and a noncatastrophic failure mode.

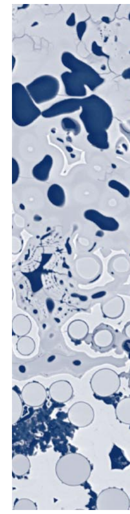
All SiC-based composite materials have a problem: They degrade at elevated temperatures in a combustion environment. Although SiC-based materials are relatively resistant to oxidation, significant concentrations of water present in high-pressure combustion gases can accelerate corrosion in these materials at temperatures typically encountered in a gas turbine combustor (~1200°C). These problems are exacerbated by

J. W. Nave



Jim Keiser and Mike Howell (on ladder) prepare to install samples in the Keiser Rig. This ORNL test furnace is used to expose samples of CFCC combustor liner materials and coatings to high-pressure water vapor similar to the combustion gases in gas turbines.





Significant materials recession (loss of liner thickness) was accompanied by subsurface microstructural damage on the working surfaces of a CFCC combustor liner. This outer liner ran in a Solar Turbines Centaur 50S engine for >5000 hours at the Texaco, Bakersfield, California test site without a protective environmental barrier coating.

the presence of boron-containing and other constituents introduced during the composite fabrication process.

To understand and fully evaluate this water vapor effect on different SiC-based composites, a team of M&C researchers was assembled to examine this phenomenon and ultimately help select the most stable CFCC material to use for combustor liners. Karren More, Peter Tortorelli, Matt Ferber, and Jim Keiser brought to the team extensive experience from previous work on microstructural characterization, high-temperature corrosion, and mechanical reliability of ceramics and CFCCs. Particular use was made of the "Keiser Rig," a unique high-temperature, high-pressure exposure facility developed by Jim Keiser and Irv Federer in the early 1990s to examine corrosion of candidate heat exchanger materials.

The Keiser Rig enabled the ORNL team to simulate the high water-vapor pressures encountered in land-based gas turbines such as Solar Turbines' engine. Microstructural characterization by More of composites exposed in the Keiser Rig and the same materials exposed in actual engine tests for comparable times revealed similar modes of material degradation. The root cause of the CFCC microstructural degradation in both laboratory and actual engine exposures was attributed to high water-vapor pressures. Using the Keiser Rig, the ORNL researchers screened the different CFCC materials, provided insight into the degradation mechanisms for the different CFCC compositions, and reliably estimated the degradation rates for each composition.

"The corrosion reactions in the hot combustion gas rapidly convert the silicon carbide–based materials to silicon dioxide, silicate glasses, and volatile products," More says. "As a result, there is a loss of sound liner thickness, making the liners prone to premature failure. To protect the walls from this surface recession, it was necessary to identify an oxide coating that could serve as an effective environmental barrier to oxidation. Protective coatings for the CFCC liners have been and continue to be evaluated at ORNL."

The ORNL research, coupled with extensive field testing by Solar Turbines and materials improvements and coating development by the different materials manufacturers, laid the foundation for the selection of the best CFCC composition and coating system for the combustor liners used in the low-emission Centaur 50 engine installed at Malden Mills. This collaboration allowed the demonstration project at Malden Mills to proceed and meet the EPA limits for NO_x and CO. The liners have run without problems for more than 4000 hours.

J. W. Nave

Karren More and Larry Walker use the Hitachi HF2000 transmission electron microscope to study fiber-matrix interfaces in continuous fiber-reinforced ceramic composites (CFCCs). These composites are similar to the CFCC combustor liners used in gas turbines for power production. More and Walker also use the JEOL 733 electron microprobe to analyze CFCCs after exposure to high-pressure water vapor in the ORNL test furnace and after actual engine tests.

The Appeal of Gas Turbines

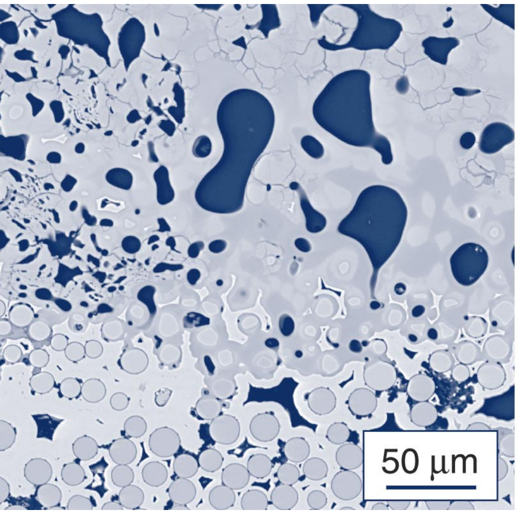
Rod Judkins, manager of ORNL's Fossil Energy Program, says that coal-fired power plants provide 56% of the nation's electricity even though a new coal power plant has not been built by a U.S. electric utility since the 1970s without a government subsidy. In the future, he said, U.S. utilities are interested in building power plants that use natural-gas-combined cycles.

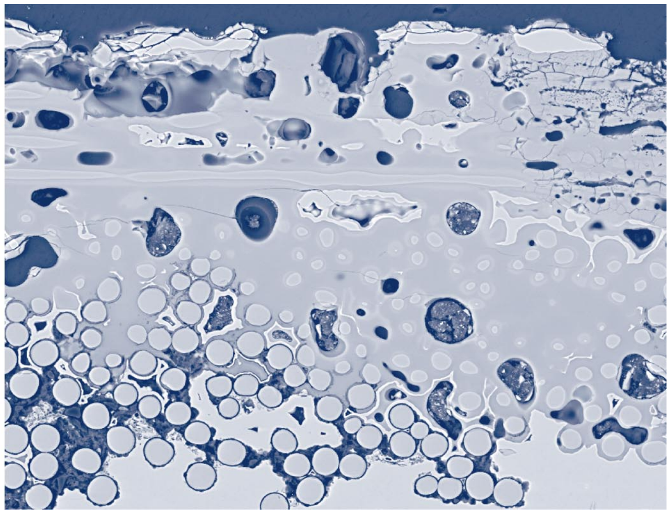
"There are many reasons why utilities like gas turbines for future power production," Judkins says. "Besides being more efficient and producing less carbon dioxide than coal-fired power plants, gas turbines cost $500 per kilowatt less, lowering the cost of electricity by 10%. Also, gas turbine plants can be built faster, and they come in a wide range of sizes, offering flexibility."

CCGTs are steadily becoming even more appealing. One reason is that partnerships involving DOE, national laboratories, electric utilities, natural gas companies, gas turbine manufacturers, and universities are rapidly boosting the efficiency and reliability of natural-gas-combined cycles while lowering their emissions.

The first U.S. application of a utility-sized advanced CCGT engine to result from the efforts of DOE's ATS Program was announced in December 1999. Sithe Energies of New York City, one of the world's largest independent power producers, announced it was building a power plant near Scribna, New York, that would incorporate two 400-megawatt (MW) versions of the DOE-supported natural gas-fired Frame 7H CCGT built by General Electric (GE) Power Systems. The first of these units, about the size of a large locomotive, passed a critical verification test in February 2000 and was to be shipped from GE's Greenville, South Carolina, manufacturing facility to New York a few weeks later.

It is predicted that these new CCGTs, which are currently in the testing stage, will discharge





The microstructural degradation observed on the working surface of a CFCC inner liner after 1000 h in an engine test at the Texaco test site (left) was similar to the damage observed for a CFCC sample co-processed with the liner exposed for 1000 h in the ORNL Keiser Rig at a high water-vapor pressure (right). Comparison of results from laboratory and engine exposures for several different CFCCs demonstrated that the Keiser Rig provided a valid simulation of the CFCC microstructural damage at a rate comparable to that observed in actual combustor environments.

half the NO_x typical of existing utility-scale turbines. They will also emit 20% less carbon dioxide than was produced by turbines available only eight years ago.

These GE turbine engines and similar utility-scale power systems being developed by Siemens-Westinghouse are now emerging from DOE's ATS Program. An industrial-sized advanced gas turbine developed under the ATS Program—the Solar Turbines Mercury 50—has already been announced. This engine has an efficiency improvement of some 15% compared with the state of the art before the ATS Program was initiated.

Improvements in turbine designs, cooling systems, materials, and manufacturing technologies achieved through the ATS Program by the gas turbine manufacturers and the materials and component suppliers have made possible higher turbine operating temperatures. As a result, advanced gas turbine technology is ready to attain significantly improved power plant efficiency.

The workhorse of electric utilities today is the highly centralized coal-fired power plant steam turbine, which typically has a fuel efficiency of less than 40%, although over 45% efficiency is claimed for advanced steam plants in Europe. CCGTs designed for utilities under the ATS Program, such as the new GE turbines, are exceeding 55% net efficiency (using the definition of efficiency applied to coal-fired steam plants) or 60% efficiency in terms used for gas turbines. Because fuel represents the largest single cost of running a power plant, a 10% increase in efficiency can reduce operating costs by as much as $200 million over the life of a typical gas-fired 400-MW combined cycle plant.

ORNL's contribution to the DOE-GE project was to manage the program in which two companies—Howmet Corporation in Whitehall, Michigan, and PCC Airfoils in Cleveland, Ohio—developed an improved manufacturing process for fabricating single-crystal nickel-based superalloy turbine blades, or "airfoils." These airfoils make the turbine spin when they are pushed by high-temperature gas. Single-crystal components are preferred over conventionally used materials because they are stronger at high temperatures. Thus, turbine blades made of this material are required to withstand the higher-temperature conditions needed to increase engine efficiency.

Single-crystal blades were first developed for use in aircraft. Turbine blades used in current civil aircraft today typically weigh up to 2.3 kg (5 lbs.), but blades for advanced land-based gas turbines, which must also be grown as single crystals, can weigh 18.2 kg (40 lbs.). Howmet and PCC Airfoils are developing the manufacturing technologies for these very large single-crystal airfoils. Five years ago, single-crystal turbine airfoils of this size could not be produced. Under the auspices of the ATS Program, efforts aimed at improving the yield of these castings are continuing. ORNL's Mike Karnitz has provided management support and technical oversight to this project.

The new GE gas turbine produces power at 60% efficiency.

Meeting Other Materials Challenges of Industrial Turbines

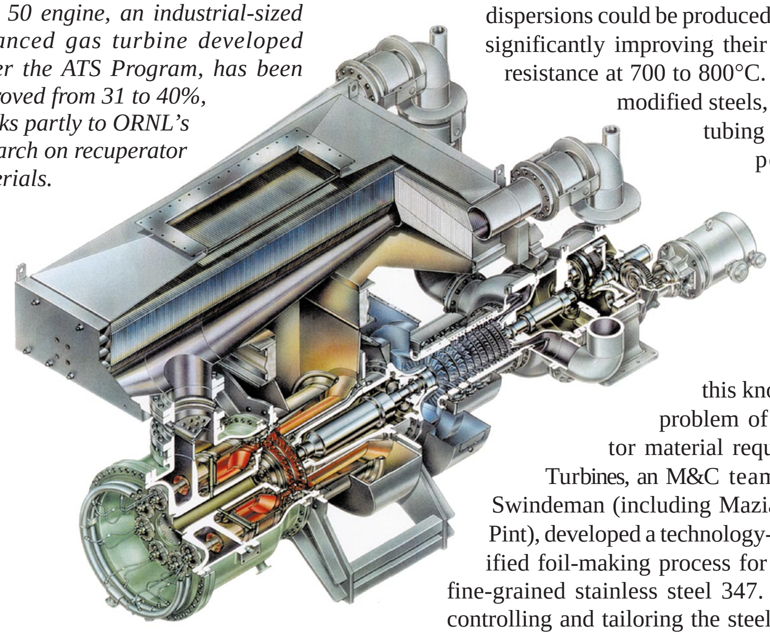
Bond coats. In other ATS materials and manufacturing programs managed by Karnitz, Siemens-Westinghouse and Pratt Whitney have improved thermal barrier ceramic coatings for use on turbine airfoils to enable increases in turbine rotor inlet temperatures needed to achieve ATS efficiency goals. This effort has been strongly supported by a team of researchers in ORNL's M&C Division that includes Matt Ferber, Allen Haynes, Michael Lance, Karren More, Bruce Pint, Glen Romanowski, and Ian Wright. Thermal barrier coatings (TBCs) have two layers. A ceramic top coat provides insulation to help keep the single-crystal alloy blades from getting so hot that they melt. The second layer is a metallic bond coat that serves to "glue" the ceramic top coat to the metal blade and also provide resistance to oxidation and corrosion. At the high temperatures of the gas leaving the turbine combustor, the alloys used for the airfoils can degrade rapidly through oxidation unless they have a protective bond coat.

ORNL's TBC Program has two main goals, according to Wright. "The first is focused on maximizing the ability of the metallic bond coats to resist thermal oxidation," he says. "The second involves learning how the complete TBC system degrades during service."

One of the keys to maximizing TBC lifetime is to minimize the rate of growth of the oxide scale formed on the bond coat while maximizing its adherence to the bond coat when exposed to the turbine environment. ORNL efforts in this area involve using model alloy systems to quantify improvements made possible through various alloy modifications. A specially developed coating rig is used in the laboratory to explore ways to incorporate these improvements into actual bond coatings. Collaboration with the gas turbine industry participants in the ATS program results in rapid assimilation of such developments and the examination of production-related issues relative to modified TBCs.

An understanding of the actual modes of degradation of TBCs is essential to the development of models that can be used to predict service lifetimes. The ORNL effort in this area

The efficiency of Solar Turbines' Mercury 50 engine, an industrial-sized advanced gas turbine developed under the ATS Program, has been improved from 31 to 40%, thanks partly to ORNL's research on recuperator materials.



involves the development and application of techniques to identify and characterize the processes involved in TBC degradation. Crucial insight into mechanisms at work is being gained through the application of the M&C's Division's comprehensive suite of advanced surface analysis techniques.

Recuperator foil. Small, industrial-sized turbines intended for simple-cycle use can meet ATS goals by using a recuperator. The material used to make a recuperator to recover heat from turbine exhaust gases must be able to operate reliably at 593°C (1100°F) for a long time. Thus, the material selected for the Solar Turbines Mercury 50 engine recuperator—type 347 stainless steel—had to be modified to improve its creep strength, which is its ability to resist deformation during long exposure to high temperatures.

Here's the problem: The recuperator is made of a stainless-steel foil folded into a unique corrugated pattern to maximize the surface area for efficient heat transfer. Hot incoming air and exhaust gases pass through the channels in the foil under different pressures and temperatures, so they must remain separated. If the steel foil gets too hot, the channels can deform and collapse, blocking the flow of the gas. If the foil cracks or corrodes through, leakage of the gas can also cause it to fail. The goal of the ATS Program was to modify the material so that it will have sufficient creep strength to last for more than 30,000 hours or longer, if possible.

About 15 years ago ORNL's Phil Maziasz was trying to develop austenitic stainless-steel alloys that would be resistant to radiation damage for possible use in fusion reactors. He discovered that ultrafine, stable metal carbide dispersions could be produced in such steels, significantly improving their creep-rupture resistance at 700 to 800°C. Tests of those modified steels, such as boiler tubing for fossil-fuel power plants, showed that they are indeed highly creep-resistant. Applying this knowledge to the problem of the recuperator material required by Solar Turbines, an M&C team led by Bob Swindeman (including Maziasz and Bruce Pint), developed a technology-specific, modified foil-making process for strengthening fine-grained stainless steel 347. It does so by controlling and tailoring the steel's microstructure, ensuring its corrosion resistance. Small pieces of foil were cold-rolled and then heated to partially dissolve niobium carbide (NbC) particles already present in the material from previous processing. During creep testing or service at 650 to 700°C, stable precipitates of NbC form in the stainless steel microstructure. The strengthened steel recuperator channels should not close up or corrode under the high temperatures of the gas turbine environment.

This work was done under a cooperative research and development agreement (CRADA) between ORNL and Solar Turbines, with the material supplier, Allegheny Ludlum, as an integral team member. Using the M&C Division's unique infrared furnace containing high-intensity tungsten halogen lamps, the ORNL researchers simulated the conditions on Allegheny Ludlum's continuous-annealing line. Using ORNL results, Allegheny Ludlum is modifying the process for producing large amounts of coils to be used to make test recuperators. Solar Turbines takes the foil produced by the modified process and fabricates folded foil for commercial recuperator air cells at its TurboFab plant in Houston. When recuperators made from this foil have been completely tested, the modified processing will be used to manufacture recuperators for Solar Turbines' new Mercury 50 gas-turbine engine. The new recuperator technology, which is an essential part of ATS gas turbines, helps increase the energy efficiency of the Mercury 50 engine from 31 to 40%.

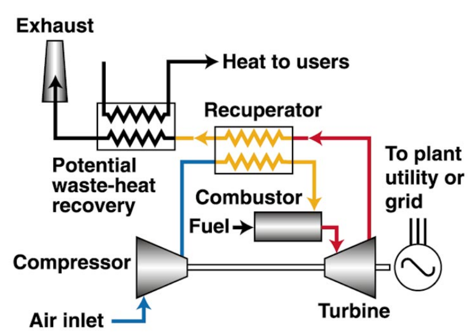
Turbine Materials Research at ORNL: The Outlook

Microturbines are a new class of gas turbine of growing commercial interest. They generate 75 kilowatts of electricity or less; by comparison, larger industrial gas turbines generate 3 to 30 MW and CCGTs produce power up to 400 MW. Currently, microturbines are about the size of large refrigerator-freezers, and the number of manufacturers is growing. One market for these microturbines may be commercial businesses that want to use them to power their building appliances and provide excess electricity they can sell back to their electric utility company. Because the efficiency of current microturbines is just under 30%, DOE's goal is to make advanced engines that are 35 to 45% efficient.

ORNL researchers are testing a wide range of materials necessary to improve microturbine efficiency. They are studying ceramics such as silicon nitride, which will be needed for the highest temperatures anticipated in future gas turbines. They are evaluating foils of advanced, heat-resistant metals, which will be needed for near-term use in turbine recuperators.

As a world leader in materials research and as DOE's largest energy research laboratory, ORNL is making a major contribution toward ensuring that tomorrow's dominant source of electricity will be low in emissions and high in efficiency.

Photograph and schematic of a microturbine, which could be used by a small business to generate power.



Heat Pumps: More Energy Bang for the Buck?

ORNL is playing an important role in developing heat pumps for air conditioning and water heating.

Natural gas is enjoying a resurgence in popularity these days for several good reasons. It's a clean-burning fuel. When burned, it gives off 40% less carbon dioxide than coal used to provide electrical power. And it's abundant and affordable.

To make natural gas even more affordable, ORNL has been funding the development of a highly efficient gas-fired heat pump for providing air conditioning and heating. Working with commercial partners, Bob DeVault, Patricia Garland, Abdi Zaltash, Phil Fairchild, and others in ORNL's Energy Division have guided the development of the generator-absorber heat exchanger (GAX) technology, a heat pump that is designed to use 30 to 50% less energy than other systems.

In mid-1999, the first pre-production GAX absorption air conditioners were installed in model homes in the new Village Green subdivision in Southern California. The test began following a ribbon cutting on May 13, 1999, at Village Green, that was attended by ORNL's DeVault, Ron Fiskum (DOE program sponsor), and Dan Reicher (DOE Assistant Secretary for Energy Efficiency and Renewable Energy). The 183-unit Village Green subdivision is being constructed in phases over a projected two-year period. By the end of 1999, more than 50 homes, all with GAX absorption air conditioners, were under construction. For comparison, several comparable homes using conventional heating and cooling units will also be monitored to obtain baseline data. Although it is too early to have seasonal test results from Village Green, the new GAX absorption air conditioners have received the standard independent product certifications required of all residential air-conditioning systems. The GAX air conditioners were independently certified as being 29% more efficient than the single-effect absorption air conditioners that have been produced for decades.

Village Green home with GAX heat pump during ribbon-cutting ceremony in 1999.

Robur Corporation of Evansville, Indiana, the manufacturer of the old single-effect Servel air conditioners, has introduced both 3-ton and 5-ton residential and light-commercial GAX absorption air conditioners into the marketplace. Robur plans to convert its absorption air conditioner production entirely to the new GAX technology during 2000.

In a separate, parallel industry cost-shared effort, ORNL and its commercial partner, the Unitary Gas Heating and Cooling Products Consortium (a gas industry limited liability company created by a consortium of gas utilities and pipeline companies), continue to develop prototype GAX absorption air conditioners and heat pumps. Support for the ORNL-DOE program comes from Southern California Gas Company (the largest gas utility in the United States), Southwest Gas Corporation (the fastest-growing gas utility because Las Vegas and Phoenix are in its service territory), Mississippi Valley Gas Company, Texas Gas Transmission, and others.

ORNL researchers in the Buildings Technology Center are also supporting the development and field testing of a novel type of electric heat pump for heating water that produces hot water twice as efficiently as conventional units. "Water heating accounts for about 17% of the energy consumed in a typical household, so it's a good candidate for energy savings," says ORNL's John Tomlinson. "But conventional electric water heaters are reaching their efficiency limits. We need to apply heat pump technology instead of resistance heaters to water heating."

A prototype of the heat pump water heater. Image enhanced by Rosemary Adams.

Tomlinson, Randy Linkous, and others in the Energy Division are providing technical support to Enviromaster International, a small company located in upstate New York, for the development and field testing of a heat pump water heater designed for the large electric water heater replacement market. The researchers will also aid in promoting the technology through DOE's Energy Star Program.

An electric heat pump water heater (HPWH) uses about half as much electricity as conventional water-heating units. Nevertheless, HPWHs have not sold well because the technology is unfamiliar, the cost of each unit is high, and early models were unreliable and difficult to install. The new electric HPWH is designed to be more attractive to consumers.

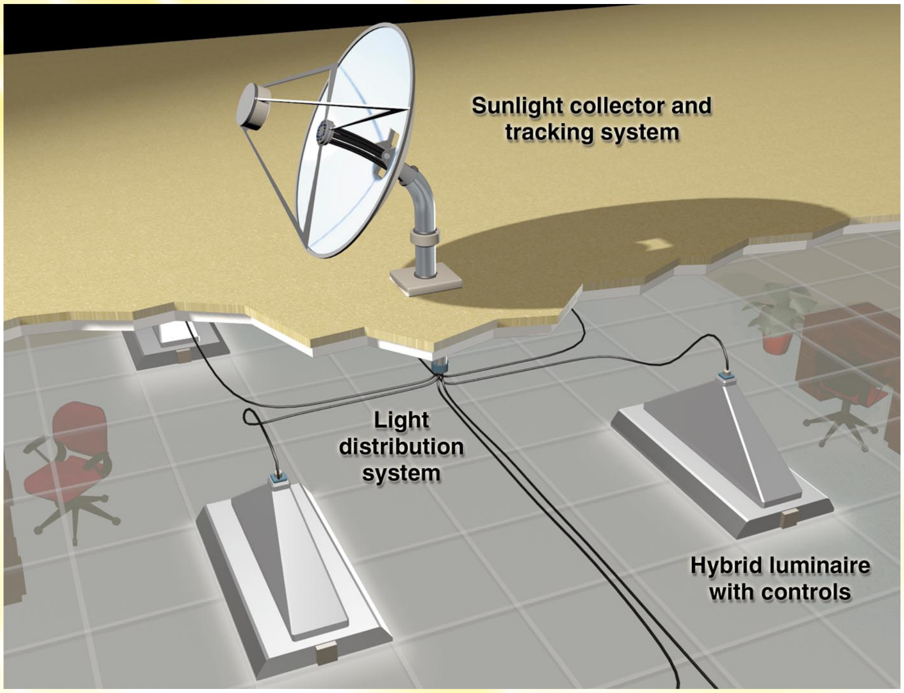
Unlike earlier HPWH models, the new drop-in model can easily be installed by a plumber to replace the existing water heater. The installed cost of the new HPWH will be about $400 more than that of a conventional 50-gallon water heater, but for many families, the energy savings in two years will cover this additional cost.

Round-the-clock durability testing of the HPWH design was scheduled to begin at ORNL in the spring of 2000. These accelerated tests will continue for nine months, subjecting the HPWH to the equivalent of 10 years of real-world use. In addition, a field study of the HPWH will begin this summer at 18 test sites located across the country. These tests are being conducted in partnership with a number of large and small utilities. Commercial launch for the new design is anticipated in early 2001.

Once these new heating and cooling devices are commercialized, it is hoped that many consumers will get pumped up about the energy savings these technologies will bring.

Combined Solar Light and Power for Illuminating Buildings

The sun's rays can light a room directly through optical fibers and indirectly by powering the room's light bulbs, thanks to a bright idea from ORNL.



Artist's conception of the combined solar lighting and power system showing the cutaway of the inside of a building illuminated by sunlight and lighting fixtures powered by solar energy. Drawing by John Jordan.

How many ways can you light a room, besides screwing in an electric light bulb? You could pipe in sunlight through optical fibers connecting the roof and the room. That would work wonderfully well during the day, especially a cloudless one. Or you could use a more efficient approach invented at ORNL: Maximize the use of the sunlight's energy by piping in the visible portion of the spectrum while turning the nonvisible, infrared part into solar electricity to power the light bulb. That way you could provide hybrid lighting to the room.

Part of the light would come from the sun and part would come from the electric light bulb. To keep the room at a constant lighting level, smart sensors could be used to dim the electric light when the incoming solar light is bright. And the electric light could be turned up to its highest level at night.

In 1999 Jeff Muhs and his colleagues in ORNL's Engineering Technology Division devised this full-spectrum solar energy system, using a winning combination of existing technologies. They now call the concept "combined solar light and power."

"While we were doing our hybrid lighting studies, we realized that visible light contained only half of the energy of sunlight and that we were simply throwing the rest away," Muhs says. "We were not fully using what's available in sunlight. We decided we could collect the nonvisible light and use it to generate electricity or heat water while using the visible light to light the building's interior."

ORNL is negotiating with two industrial groups to license the system so that it can be further developed and marketed as a commercial product. ORNL and 10 companies have formed the Hybrid Lighting Partnership. Each of the companies manufactures one of the different components of the combined solar light and power system.

The heart of the system is a parabolic dish concentrator (primary mirror), which collects and separates the incoming sunlight. The concentrator, which resembles a satellite dish, is supported by a penetrating pipe that contains a bundle of very large optical fibers. The sunlight striking the concentrator is reflected to an attached secondary optical element positioned above the dish. This element consists of a spectral filter and a silicon-based photovoltaic cell.

The spectral filter reflects the visible light into the pipe containing the optical fibers, which channel the visible light into the building's interior. The spectral filter also transmits the infrared light into the photovoltaic cell, which absorbs this invisible light and turns 20% of its energy into electricity.

"It is four times more efficient to light a room using visible light from the sun and electricity from the photovoltaic cell than it is to use traditional solar electricity only for lighting," Muhs says. "It is more sensible to use visible light from the sun directly for illumination of building interiors than to convert sunlight into electricity and turn around and reconvert only 30 to 40% of it to light."

The development was funded by DOE's Office of Building Technologies, State and Community Programs. This DOE office and DOE's Office of Power Technologies are expected to jointly support further research. It is hoped that the system can be commercialized in two or three years.

ORNL's full-spectrum solar system may also be used with other technologies to better manage carbon emissions from power plants. Because "carbon-eating" algae growth rates require much less light per unit area than is available naturally on a sunny day, it may be possible to drastically reduce the required acreage needed to sequester carbon from power plants. A team including Ohio University and ORNL have proposed a 10-acre chamber capable of replacing a 250-acre lake. The system contains closely spaced vertical sheets of algae illuminated by self-illuminating large-core optical fibers that glow like fluorescent lamps but use ORNL's collector technology. The infrared portion of the spectrum is captured by photovoltaic cells to produce several megawatts of electricity to operate pumps and conveyor belts needed to grow and harvest the algae.

ORNL's combined solar lighting and power concept appears to have a bright future.

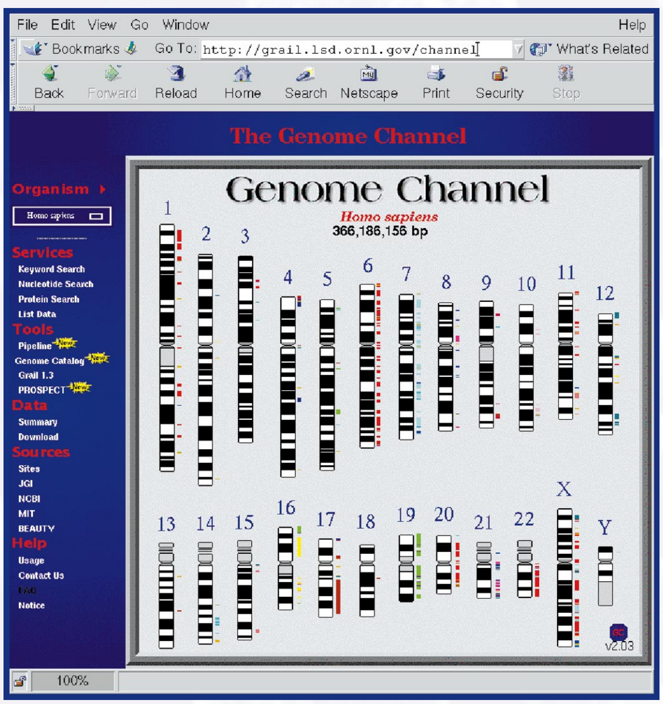
What's in a *Chromosome?* Tune in to the Genome Channel

ORNL supports DOE's human chromosome sequencing efforts by computationally analyzing DNA sequences to locate known genes, predict unknown genes, and estimate gene functions.

In April 2000, in Walnut Creek, California, researchers from three DOE national laboratories completed the draft sequencing of human chromosomes 5, 16, and 19 for the Human Genome Project. These were not the first chromosomes to be sequenced; the first was chromosome 22, whose order of DNA bases was published in December 1999 by a group of institutions funded by the National Institutes of Health (NIH). However, these were the first human chromosomes to be sequenced by DOE's Joint Genome Institute (JGI), which integrates the genome centers at the Lawrence Berkeley, Lawrence Livermore, and Los Alamos national laboratories with informatics and functional genomics capabilities at ORNL.

ORNL supports JGI by computationally analyzing DNA sequences to locate known genes, predict unknown genes, and estimate the functions of many of these genes. It is known that chromosomes 5, 16, and 19, which make up roughly 11% of the human genome, contain genes that are linked to kidney disease, various cancers, hypertension, and diabetes.

In addition, through its Web site, called the Genome Channel, ORNL provides new information every month on the latest DNA sequences obtained experimentally (including partial and whole sequences of human chromosomes) and their computationally identified genes.



A view of the Genome Channel home page on the World Wide Web.

The Genome Channel is a Web browser tool that provides a comprehensive sequence-based view of parts of the human and mouse and several complete microbial genomes. This information resource is being used by many people worldwide, ranging from biomedical researchers at NIH and the Massachusetts Institute of Technology to scientists who are developing drugs at some of the world's largest pharmaceutical companies. The Genome Channel, which has about 100,000 hits per month, was listed among five "hot pick" Web sites in the December 17, 1999, issue of *Science* magazine.

A researcher interested in developing a drug to control Parkinson's disease or cancer can get relevant information from the Genome Channel by typing in a class of genes, such as "caspase," in the search space. "Caspase genes control cell death," says Ed Uberbacher, head of the Computational Biosciences Section in ORNL's Life Sciences Division. "In Parkinson's disease, cells die when they shouldn't, and in cancer, cells grow and spread instead of dying when they should."

Regulatory proteins are of interest to researchers because they control the activity of a host of genes, turning some on and others off, thus affecting the types and levels of proteins produced. The Genome Channel provides information on regulatory proteins as well as up-to-date lists of many important gene types, based on the most recent ORNL analysis.

Uberbacher was one of the developers of the Gene Recognition and Analysis Internet Link (GRAIL) computer program. Among other things, GRAIL is known for having helped researchers locate the gene responsible for Adrenoleukodystrophy (related to the disease featured in the movie *Lorenzo's Oil*). The updated version of GRAIL, called GRAIL EXP, is available to users of the Genome Channel.

"Using ORNL's IBM SP supercomputer, our programs search the databases for expressed sequence tags," Uberbacher says. "These are fragments of gene sequences that resemble or match DNA sequences we are interested in analyzing. Using these sequences as evidence, we can identify and locate genes along the human genome. By knowing the gene sequence, we can then predict the amino-acid sequence of the gene's protein product. By matching the sequence to known protein sequences in a database, we can often predict the biochemical function of the protein.

"We link gene sequences computationally to genetic maps of chromosomes showing markers, or known locations along a chromosome, that are tied to known biological functions. By doing this data mining, we can predict a function for a particular gene sequence of interest."

According to Uberbacher, ORNL researchers will estimate two-thirds of the functions of the genes that make up the sequenced chromosomes. "We will be able to predict that a gene's protein product catalyzes a particular biochemical reaction," he explains. "But to find out what the gene actually does in the organism, we will rely on ORNL biologists studying the effects of mutations of a similar gene in the equivalent chromosome in mice. For example, the biologists might find that the gene affects embryonic development."

To get updates on the latest findings concerning human chromosomes 5, 16, and 19, stay tuned to the Genome Channel (compbio.ornl.gov).

Microbial Functional Genomics and Waste Site Bioremediation

By learning the functions of genes in bacteria, researchers may learn better ways to keep toxic metals out of the environment.

Researchers in ORNL's Environmental Sciences Division (ESD) are seeking to understand the genetic structure, functions, regulatory networks, and mechanisms of bacteria that might help keep toxic metals out of the environment. To do this, they are integrating genomic, biochemical, and physiological approaches to explore whole genome sequence information. One of the genomic technologies being used by ESD researchers is DNA array, or DNA microchip, technology. Basically, genes are laid down in rows and columns on a glass slide in the order in which they once existed in, say, a microorganism.

"We are using this exciting new technology to study gene function and gene regulation in bacteria capable of reducing metals," says Jizhong Zhou, an ESD researcher. "Such bacteria may be useful for bioremediation of the Department of Energy's waste sites." DNA microarray technology is also being developed and used by Ken Beattie, Mitch Doktycz, and other researchers in ORNL's Life Sciences Division engaged in functional genomics research and development.

Zhou, Tony Palumbo, and other ESD researchers are studying *Shewanella oneidensis MR-1*, a group of bacteria that are found virtually anywhere, including in water and soil, and at sites of infection. Just as humans breathe in oxygen, these bacteria respire oxygen, nitrates, cobalt, chromium, and uranium (U) to obtain energy. They move electrons from each food molecule (e.g., organic compounds), changing the charge state and the state of the respired material (e.g., U ions) on which they dump electrons.

For example, when a *Shewanella* bacterium respires a soluble U^{6+} ion in contaminated streams, it dumps two electrons on it to create an insoluble U^{4+} ion, which sinks to the sediments. DOE is interested in bacteria with this capability because they could help keep water-borne uranium from leaving DOE sites.

About 99% of this bacterium's sequence is known, thanks to work by the Institute for Genomic Research (TIGR) in Rockville, Maryland, funded by DOE's Office of Biological and Environmental Research. Using ESD's new genomic microarray equipment, the ORNL researchers will lay down some 6 million bases and 6000 genes from the *Shewanella oneidensis* bacterium on the gene chip. In the meantime, while sequencing is being completed, the ORNL researchers are also working with smaller subsets of the genes.

The goal of ORNL's first DOE-funded project on microbial functional genomics and ecology is to identify the genes in the bacteria that are responsible for metal reduction, especially reduction of uranium to convert soluble ions into insoluble ones. This work is being done in collaboration with the California Institute of Technology and Michigan State University.

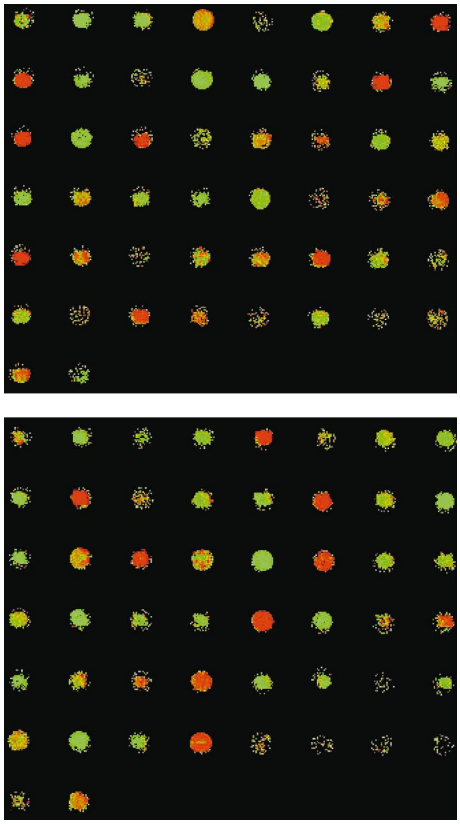
In a pilot study, ESD researchers optimized the hybridization conditions with a partial gene chip containing about 200 genes. "We are among the first groups to show that microarray technology can be used to analyze gene expression in bacteria for environmental applications," Zhou says. "We are using it to help us define gene functions and gene regulatory mechanisms in microorganisms."

To determine which bacterial genes are important in the respiration of metals, ESD researchers grew the bacteria in oxygen and on metals. They exposed some *Shewanella* bacteria to oxygen only and stained them with a red fluorescent dye. They exposed other *Shewanella* bacteria to metals only and dyed them green. Some genes turned on in the presence of oxygen and other genes turned on when exposed to metal. These expressed genes produce messenger RNA, which carries the dye (see image).

"Working with 200 selected genes, we compared microarrays to see which genes were turned on under different conditions," Zhou says. "Once we found out which of those genes turn on in response to the presence of metal, we deleted two of these metal-reduction genes from this bacterium to generate mutants using the genetic vectors we recently developed. We will expose the mutant to uranium to see if it still reduces uranium. If not, that suggests those missing genes are important to uranium reduction."

More research will be needed to determine the precise function of each metal-reducing gene by examining the role its protein product plays in the organism. To carry out this research, ESD researchers are collaborating with a group at Argonne National Laboratory. There various tools are being used to find differences in proteins produced by normal and mutant *Shewanella* bacteria and to characterize enzymes that regulate gene expression by turning some genes on and others off through mutagenesis.

ESD researchers have also used DNA microarray technology to analyze the community structure and activity of bacteria of environmental importance. "We are the first group," says Zhou, "to demonstrate that DNA microarray technology works well for analyzing complicated environmental samples."



The red dots on the gene chip represent bacterial genes expressing themselves in the presence of oxygen. The green dots indicate bacterial genes expressing themselves when exposed to metal. The yellow dots denote genes expressed by bacteria under both sets of conditions.

Human Improvement

Using robotics and intelligent machine technologies, ORNL researchers will devise a "suit" to make humans faster, stronger, tougher, and smarter.

Exerting 10 pounds of force on a joystick-type handle, François Pin uses ORNL's Advanced Telerobotics Technology Demonstrator to hoist an unarmed 5000-pound bomb.

Tom Cerniglio

When Sylvia joined her military unit, she didn't realize that she was going to become faster, stronger, and smarter in a hurry. The military was training her to wear an early version of a Superman suit. Sylvia stepped into a "soldier amplification exoskeleton," which "lifted" her weight and the weight in her backpack. As a result, she could run much faster and for much longer.

With the exoskeleton's attached long arm, she could lift heavy objects that she would not normally have been able to hoist. Her smart exoskeleton sensors would warn her if she was being exposed to hazardous gases or if enemy forces were nearby. Additionally, the information provided almost instantly by her wearable "talking" computer boosted her memory, helped her solve mathematical problems, and guided her in making wise decisions. Her perceptive abilities were enhanced, too. She could see better in the dark and through fog and smoke, thanks to night-vision and multispectral goggles.

François Pin, corporate fellow in ORNL's Robotics and Process Systems Division (RPSD), believes the first prototype Superman suit, described in the above scenario, will be devised for the U.S. military at ORNL within the next five years. The ORNL-developed system will be even better and less bulky than the robot suit that Sigourney Weaver strapped on to make her a gigantic kickboxer in the movie *Alien II*. And the multidisciplinary talents at ORNL will help make possible the engineer's old dream of human amplification.

In the late 1990s, Pin, John Jansen, and others from RPSD developed the Advanced Telerobotics Technology Demonstrator (ATTD). This device multiplies human strength using a preselected amplification ratio in the electrical control system. As a result, with 10 pounds of force on a joystick-type handle, one person can move and control a mechanical arm to lift and put in place a 5000-pound payload while sensing all the forces that act on the payload, such as inertia, friction, or impacts. For example, with this machine, you could easily hoist very heavy objects—such as an automobile engine you wanted to put in a car—and assemble them precisely. The machine senses the motion and forces exerted by your hand and then duplicates the motion while amplifying the forces. It also allows you to "feel" what happens to the payload.

In 2002, largely because of the ATTD's success, ORNL researchers will work on a follow-on project for new Air Force and Navy programs. These will be focused on developing human-amplifying machines to increase the abilities of diverse recruits in a time when fewer people are volunteering to serve in the U.S. military.

Because of improvements in robotics and intelligent machine technologies, the U.S. Defense Advanced Research Projects Agency (DARPA) has established an $80 million program to support the development of soldier amplification capability. ORNL has received some DARPA funding to study the feasibility of building within the next three to five years an exoskeleton that is safe and user-friendly. The goal is to amplify the strength, endurance, and speed of soldiers.

John Jansen operates the actuation system of ORNL's human-strength amplification machine which resembles the torso of a human with an extra-long arm. Photo enhanced by Gail Sweeden.

Curtis Boles

"Use of such an exoskeleton could also improve the safety and productivity of workers in the construction, mining, and manufacturing industries," Pin says. "Exoskeletons could also be worn to make rescue operations safer and faster, for example, when extracting people from rubble left from earthquakes or terrorist bombs."

As a precursor to the exoskeleton slated to be developed, Pin, Jansen, Joel Chesser, Dave Connor, John Rowe, and Lonnie Love, all of RPSD, in collaboration with Terry Tiegs of ORNL's Metals and Ceramics (M&C) Division and Marc Simpson of the Instrumentation and Controls Division, developed a prototype of a torso with a long arm. The prototype was the outcome of a 1999 project sponsored by internal funding from the Laboratory Directed Research and Development Program at ORNL.

"This human amplification machine testbed includes changeable parts that can be made of different materials and have different control and sensor systems," Pin says. "We have shown that we can amplify the strength and reach of a human using components made of lighter materials than have traditionally been used."

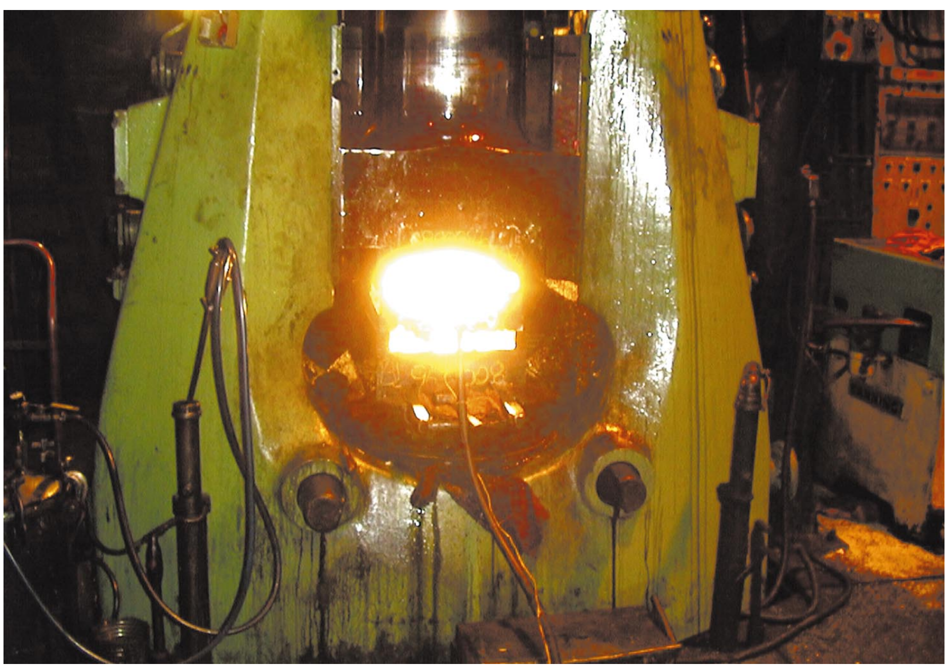
The RPSD researchers are now trying to achieve a factor of 10 drop in payload-to-weight ratio. Their goal is to create an exoskeleton of stronger, lighter materials, such as special alloys developed by the M&C Division or carbon nanotubes produced by the Solid State Division. In this multidisciplinary project, they will rely on researchers from other ORNL divisions for smaller and faster computing and electronic technology, smarter sensors, and smaller power sources and motors.

Researchers from RPSD have also demonstrated "human de-amplification" using manipulators that assemble microgears into micromachines. "We use a less-than-one amplification ratio in the control system to manipulate such tiny objects safely," Pin says. "In this case, gravity is not the dominant force, but surface tension and electrostatic attraction are very important. This work could lead to assembly of nanosize components to create micromachines."

For Pin, thinking small is part of thinking big in the world of robotics.

ORNL's Infrared Processing Center: Industrial Interest Heats Up

Using infrared heating technologies, ORNL is helping industry reduce repetitive stress injuries among workers and improve the quality of medical implants.



A woman takes a polymer boot, heats the edge of it with a new electric infrared heater about the size of a toaster, and slips it easily on part of a car steering wheel assembly. She still remembers those days when she had to shove the boot on the component to protect it. Some of her colleagues at General Motors' Delphi Automotive Steering Systems in Athens, Alabama, had suffered repetitive stress injuries from this work. But now she and her co-workers like their jobs better because they are benefiting from a new infrared heater developed at ORNL. The new heater expands the leading part of the polymer boot so it can be more easily mounted onto a metal housing in the automotive rack-and-pinion steering assembly. As a result, the number of repetitive stress injuries among workers at the plant has dropped sharply.

According to Aly A. Badawy, director of research and development at Delphi Automotive Steering Systems in Saginaw, Michigan, "The infrared boot heater virtually eliminates the force required to install the boot. This reduction in force results in the elimination of the ergonomic problems associated with placing the boot on the steering assembly." The Delphi managers also like using the ORNL heater in the fabrication process, because when the boot cools, a better seal is made than if the boot had been forced on without heating it.

Since ORNL's polymer boot heater was first tested in November 1998 at the Delphi plant, some two million boots have been mounted using the original prototype infrared boot heater; today twelve newer units are in use there. Interest in the new heater continues to grow. Now, the Ford Visteon automotive parts plant in Indianapolis is considering installing some infrared heaters.

Top: This ORNL-developed infrared boot heater being used at Delphi Automotive Steering Systems has eliminated repetitive stress injuries linked to placing the boot on a car steering assembly. Bottom: This ORNL-developed infrared insert heater preheats dies at the KomTek plant before medical hip implants are forged.

Fabricating hip and knee implants to help people walk without pain is an action-filled process. At the KomTek, Inc., plant in Worcester, Massachusetts, dies used to form a medical implant are incorporated in hammer forges. In this process, a skilled worker uses long tongs to pick up a solid piece of a cobalt-based alloy from a furnace that has heated it to approximately 2400°F. The worker then inserts the piece between two dies and steps on a pedal. A pneumatic hammer smashes the top die against the bottom die with a driving force of up to 25 tons.

Why is such a violent hammering process needed to make an implant? "You can't pour hot liquid metal into a mold to make an artificial hip because the casting will have neither grain flow nor directional strength, allowing the possible formation of metallurgical defects," explains Craig Blue, a metallurgical engineer in the Metals and Ceramics (M&C) Division and a co-inventor of the polymer boot heater. "Hot forging surpasses casting in producing parts that are predictably strong and, therefore, safe and reliable for human use."

However, hot forging has two problems if the dies are cold. The hot metal hitting the cold metal will not always fill the mold, making the implant shape defective. Secondly, hot metal in contact with cold metal causes the die to wear, crack from the thermal shock, and fail prematurely.

At KomTek a $50,000 set of hip dies lasts only a few days, producing approximately 1500 hip implants before rework is needed on the dies. "Unless the dies are preheated to 400°F before the solid metal is introduced," Blue says, "the manufacturer will initially get bad implants and the dies will fail prematurely, cutting into the profit margin. Some medical implant companies have tried using conventional electric or gas heating to warm their dies, but it takes four hours and degradation of the dies can result, so most just use cold dies."

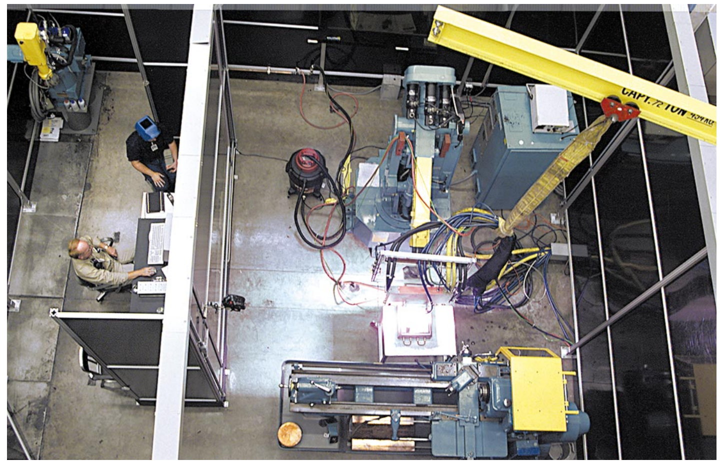
But Blue and his associates have developed a possible solution for KomTek: an infrared heater containing tungsten halogen lamps that preheats the dies in 10 minutes, not 4 hours. The ORNL heater, which is 30 cm (12 in.) wide and 45 cm (18 in.) long, has worked well for more than six months at KomTek, indicating that it is industrially robust. It is almost twice as energy efficient as the standard electric heaters used in hot forging.

"Our goal is to show that infrared heating improves product quality and extends the life of dies," Blue says. "Early results show this is the case."

"We are extremely pleased with results of the ORNL system," says Michael C. Maguire, vice president for product and process development at KomTek.

When Blue was a doctoral student at the University of Cincinnati, he was involved in a NASA project in which he had to find a way to join silicon-based microsensors. Because he needed to get them to high temperatures fast, he used tungsten halogen lamps, which go from cold to full power in 0.75 s and can be shut down instantly. This type of electric lamp provides radiant heating by emitting infrared radiation from a fine tungsten filament resistively heated in a quartz envelope containing argon or a halogen gas. Blue then began designing furnaces using tungsten halogen lamps for different materials projects.

J. W. Nave



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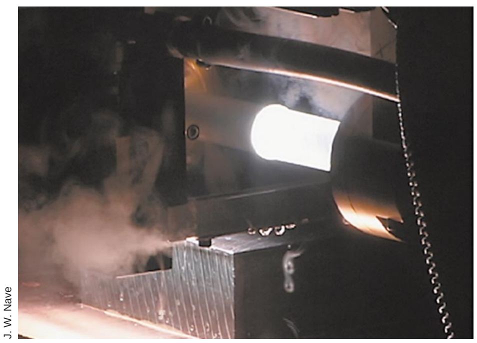


Views of the powerful plasma arc lamp at ORNL's Infrared Processing Center.

When Blue came to ORNL in March 1995 as a postdoctoral researcher, he worked with group leader Vinod K. Sikka and many others in the Materials Processing Group to guide the construction of a tungsten halogen lamp furnace. The furnace was built by Barry Whitson, Kenneth Byrd, and Larry Smarsh of ORNL's Plant and Equipment (P&E) Division. The start of this project was made possible by programmatic support from ORNL's Advanced Industrial Materials Program, managed by Peter Angelini, and from the M&C Division. Because of this equipment, Blue, Sikka, Evan Ohriner, Srinath Viswanathan, and Ted Huxford, in cooperation with many others, have brought in $3.7 million in industrial and DOE funds to support infrared heating research projects. Now Sikka's Materials Processing Group and other engineers are further developing the technology for materials research.

Blue spearheaded the development of ORNL's first-generation Infrared Processing Center. Additions to the center are continuously being made. The heart of the center now is a plasma infrared system capable of delivering 3500 watts (W) per square centimeter. It was installed by Whitson, John Norris, and Bill Fellows of the P&E Division.

In addition to the polymer boot heater and the die heater, Blue and his M&C colleagues Sikka, Ohriner, Viswanathan, P. Gregory Engleman, and David C. Harper are developing coatings to extend the life of industrial dies for casting automobile parts. The coating research and other work have required the development and installation of the world's most powerful lamp. This 300,000-W stabilized plasma source of radiant heating, built by Vortek Industries of Canada to meet ORNL specifications, is now attracting even more industrial interest in the Infrared Processing Center. For example, Caterpillar and B. F. Goodrich representatives have already visited it.

"We are using the plasma arc lamp to develop coatings for casting dies," Blue says. "Coatings are needed for aluminum dies used to make auto parts. These dies are fitted with H-13 steel pins used to make holes in the cast part so they don't have to be machined in, saving money. These dies are placed in an H-13 steel housing. The problem is that when liquid aluminum is injected into the dies, it reacts with the H-13 steel, degrading it and gradually making the die unusable."

Using the plasma source, Blue and his colleagues have come up with a chromium carbide coating that protects H-13 steel from attack by liquid aluminum. "We are finding that by using our powerful plasma lamp to precisely and rapidly heat a precursor material on the H-13 steel, we can make coatings that fuse with the substrate without changing the base material properties," Blue says. "Because the intense radiant heating sets up large temperature gradients so fast, the iron in the H-13 steel will have almost no time to dissolve. Thus, heat treating of the coated component will not be necessary. We are testing these coated dies at Tennessee Tools to see if the coating allows the dies to last longer."

Besides making medical implants and automotive parts, the U.S. forging industry, a $6 billion enterprise, provides truck, aerospace, and agricultural equipment parts; valves; fittings, and industrial tools, all of which are essential to the U.S. economy. Degradation of dies and other tools used by the custom forging sector of the industry is a major economic problem. As the Infrared Processing Center at ORNL finds ways to extend the life of dies, the custom forging and die casting industries are likely to warm to the DOE user facility.

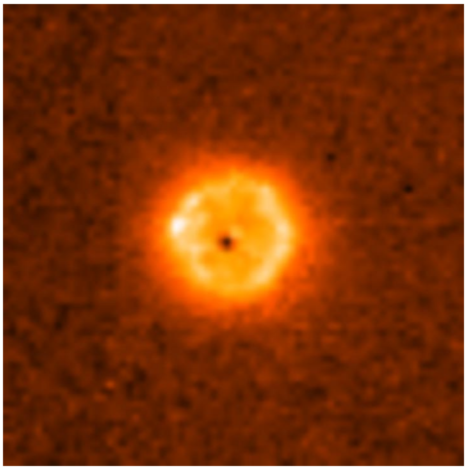
How Much Stuff Is Made in Stellar Explosions? ORNL's Answer

By using new experimental results from the Holifield Radioactive Ion Beam Facility in an astrophysics computer model, ORNL researchers have more accurately predicted the amounts of 87 different isotopes produced by exploding stars.

Imagine a large explosion on the surface of a star. Trillions and trillions of swirling hydrogen and fluorine nuclei race past each other, propelled by the exploding star's soaring temperatures. In maybe one in a million close encounters, an unstable, radioactive fluorine-17 (^{17}F) nucleus will collide with and scatter off a hydrogen nucleus, like a cue ball glancing off a smaller billiard ball. In one in a trillion close encounters, an ^{17}F nucleus will capture a hydrogen nucleus (proton), and the fused particles will form a neon-18 (^{18}Ne) nucleus.

Such energy-releasing nuclear reactions involving radioactive isotopes in stars are thought to be crucial to the production and dissemination of elements that sustain life on the earth. In our terrestrial environment, unstable ^{17}F spontaneously decays within a couple of minutes to oxygen-17 (^{17}O). However, at the high temperatures and densities in stellar explosions, there is a small probability that a nucleus of ^{17}F can capture an additional proton before it decays, forming ^{18}Ne. A series of such fusion reactions in stellar explosions can synthesize heavier isotopes, such as the iron that circulates in our blood.

The probability that this fusion reaction will occur varies greatly with the relative velocities of the ^{17}F nucleus and the proton. Theorists have predicted that certain relative velocities will correspond to an excited quantum state in ^{18}Ne, where the fusion rate will be dramatically enhanced. They have also predicted the energy and lifetime of this ^{18}Ne quantum state, but the results of nine experiments using stable nuclear beams did not support this prediction. However, in 1999, the first published data from ORNL's Holifield Radioactive Ion Beam Facility (HRIBF) showed that the Nuclear Astrophysics Research Group, led by Michael S. Smith, in ORNL's Physics Division, was the first to confirm the existence of and determine the properties of this ^{18}Ne quantum state.



The expanding gas ring was ejected into space by a giant stellar explosion on the surface of a white dwarf star (bright spot in the center) in the galactic nova system QU Vulpeculae. The gas in the ring is glowing in the light of hydrogen atoms excited by ultraviolet radiation. This image of Nova QU Vul was obtained by an infrared camera on the Hubble Space Telescope. (Photograph courtesy of the University of Wyoming and the Space Telescope Science Institute.)

Bombarding a hydrogen-containing polypropylene target with a high-quality ^{17}F beam from HRIBF, the team measured the number of ^{17}F ions scattered off the target at different angles for different beam energies. The number of protons scattered at each beam energy was counted in a second detector. When they shifted from one beam energy to another, the researchers noticed a significant change in the proton scattering rate. This beam energy can be correlated with a star temperature range that may be critical for the synthesis and expulsion of particular isotopes. Postdoctoral research associate Dan Bardayan, the principal investigator on this experiment, was then able to calculate the probability that ^{17}F ions will fuse with protons to produce ^{18}Ne ions at various stellar temperatures.

"We determined that the properties of the neon-18 quantum state do significantly enhance the rate at which fluorine-17 nuclei fuse with hydrogen under some conditions occurring in stellar explosions," Smith says. "We recently put this reaction rate into an astrophysical model that runs on a supercomputer. It calculates the amounts of 87 different isotopes produced in the stellar explosion. When we examine the prediction using our new rate, our preliminary results indicate that a number of isotopes are produced in significantly different quantities than previously thought. The new prediction and older predictions differ in some cases by a factor of 1000."

The model of the synthesis of isotopes in nova explosions was written by postdoctoral research associate W. Raphael Hix, Smith, ORNL theoretical astrophysicist Anthony Mezzacappa, and two outside collaborators. It predicts that roughly 800 times more oxygen-18, 40 times more carbon-13, 30 times more carbon-14, 70 times more nitrogen-15, and 3 times more nitrogen-14 were produced than previously predicted. Many isotopes were produced in far smaller amounts than previously predicted, including many which are radioactive isotopes that later decay to stable isotopes. The team will continue their investigation by varying the temperatures and densities describing the explosion in their model.

It took the HRIBF staff a number of years to achieve the very difficult feat of generating a high-quality ^{17}F beam for the 1999 experiment. The beam current was 8000 particles per second and the beam energy was 10 to 12 million electron volts. Since that experiment, they have increased the beam current by a factor of 100. ORNL physicist Jeff Blackmon led an experiment in January and February 2000 in which the more intense beam was used to study another important reaction in astrophysics.

"Our measurements are having important astrophysical implications," Smith says. "It is exciting that we can make measurements in the laboratory that help us better understand the details of what happens when stars explode."

Electronic License Could Reduce Drunken Driving

If the American public can learn to accept electronic driver's licenses and smart ignition systems in cars, drunk driving would be discouraged and highway safety would be improved.

He has two drunken-driving offenses but the judge allowed D. P. to keep his license under several conditions. First, he had to pay $250 for the installation in his car of a smart ignition system. Then D. P. was given an electronic driver's license that resembles a credit card but contains a computer chip. On this chip is stored driver information about D. P., including the provision that the car not start until he passes a test.

Instead of a key, he inserts the card into a card reader in the KitteLock computerized ignition system invented by Fred Goldberg of Sweden, a materials researcher whose 18-year-old stepdaughter Kitte was killed by an unlicensed driver on a university campus in Stockholm. The monitor on the dashboard reads, "D. P., breathe into the alcohol breath tester." D. P. exhales into the built-in instrument and passes the test. Then the monitor reads, "D. P., please start the car." D. P. pushes a button and the car starts.

Pat Hu of ORNL's Center for Transportation Analysis (CTA) would like to see a small-scale U.S. demonstration project in which persons repeatedly convicted of driving under the influence (DUI) might continue to drive but only on the condition that they have an electronic license, as in the above scenario. "These drivers are a danger to themselves and to others," she says, recalling a friend who lost his wife and two children in a car crash caused by a drunk driver during their trip to the airport to pick him up. Mothers Against Drunken Driving and the American Automobile Association agree.

In 1997 in the United States, more than 16,200 people were killed and one million were injured in vehicle crashes involving intoxicated drivers—almost 39% of all traffic fatalities. It is estimated that one-third of suspended drivers lose their licenses for drunk-driving offenses and that up to 80% of DUI offenders continue to drive after their licenses are revoked. A California study suggests that drivers whose licenses have been suspended or revoked are four times more likely to be involved in crashes than drivers with valid licenses.

In late 1998, under the leadership of Hu, CTA and the National Highway Traffic Safety Administration (NHTSA) of the U.S. Department of Transportation cosponsored the Workshop on Feasibility of Electronic Driver's Licenses for Improved Highway Safety, held in Irvine, California. Attending were 43 stakeholders representing vehicle manufacturers, the insurance industry, the highway safety community, law enforcement, state departments of motor vehicles, the legal and liability profession, federal agencies, national laboratories, and universities. They discussed technological solutions, socioeconomic issues, and institutional barriers.

The workshop focused on KitteLock because it is the only operational system that integrates smart card technology, an ignition interlock device, and an alcohol breathalyzer. The attendees had a chance to try out a Volvo S-70 sedan outfitted with the KitteLock system. This demonstration vehicle was then shipped to ORNL and driven for six months in 1999. As a result of this field test, ORNL drivers made a number of suggestions for improving the system. One frequent suggestion was that the monitor giving driver instructions be dropped below the dashboard to make it less distracting.

"American society historically resists excessive government intervention and Big Brother programs that threaten to invade privacy," Hu says. "One of the biggest challenges to implementing electronic driver's licenses will be to secure widespread public acceptance and community support." Hu thinks that the U.S. public will be more likely to accept this technology if it is first demonstrated on high-risk drivers. "Targeting a demonstration project at drivers who might have fewer privacy 'rights,' such as convicted DUI offenders, might reduce public concern about invasion of privacy," she says. "Electronic driver's licenses require that drivers with previous DUI convictions must continually demonstrate their ability to safely operate a vehicle in order to be 'granted' driving privileges."

If the electronic license and smart ignition system becomes more acceptable to the public and more widely implemented in American cars of the future, it could improve highway safety in other ways besides preventing drunk driving. It could keep a person with a suspended license from driving. It could ensure that drivers of commercial vehicles do not exceed their legal limit on driving time each day. It could reduce the number of car thefts, especially if combined with a fingerprint identification sensor. And it could improve the accuracy of accident reporting by recording on the card chip the driving speed when the accident occurred. Someday the key to increased highway safety could be a chip-carrying plastic card.

Curtis Boles

Pat Hu inserts her electronic driver's license in the Kittelock smart ignition system inside the Volvo S-70 sedan. This car was driven at ORNL during a six-month field test in 1999.

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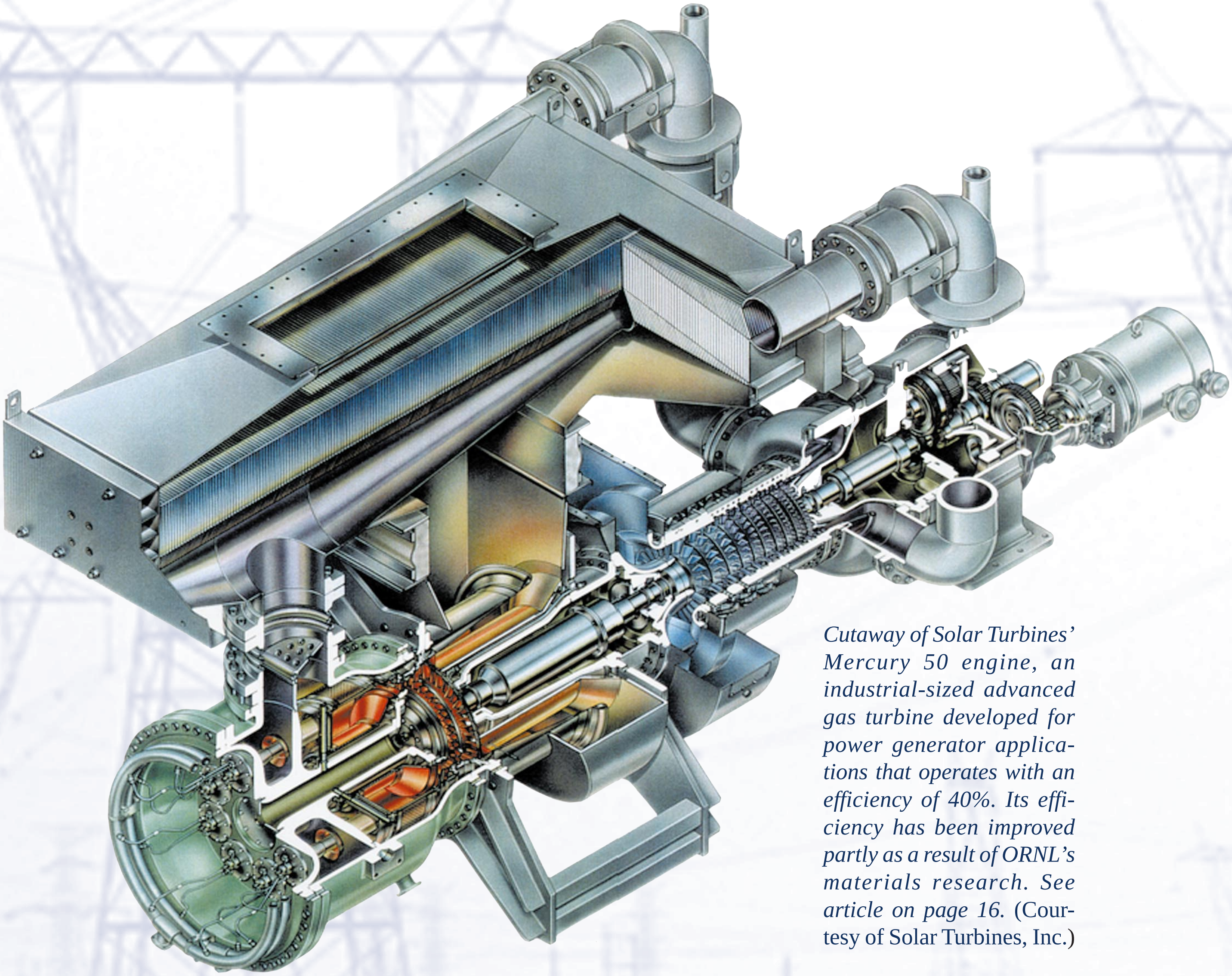

Cutaway of Solar Turbines' Mercury 50 engine, an industrial-sized advanced gas turbine developed for power generator applications that operates with an efficiency of 40%. Its efficiency has been improved partly as a result of ORNL's materials research. See article on page 16. (Courtesy of Solar Turbines, Inc.)