Breakthroughs

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WINTER 2007

Environmental Renaissance

PNNL researchers master the art of predictive sciences that use environmental stories of the past to paint a balanced future

Pacific Northwest National Laboratory

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Breakthroughs

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editor's screen

Tomorrow's environmental health depends on today

Life is really about consequences—whether it's those extra pounds brought on by eating junk food in front of the television or landfills piling up with indestructible junk. If we pause for a moment to look back, the causes for these situations become incredibly clear. We learn from the past.

In putting together this issue, I was struck by how much the future of our ecosystem and human health hangs in a delicate balance today. As technology develops at exponential rates, who is answering the question "How will this affect the future?"

Centuries ago one of the great art masters, Leonardo DaVinci, sketched the Vitruvian Man, also known as the "Renaissance Man." He couldn't have known how symbolic this work of art would become to science in representing balance, human health and the environment.

In an age of computers and high-speed electronics, we have the ability to use information from our past to gain insight into the future. Using their expertise in what is known as predictive science, PNNL scientists are creating state-of-the-art modeling tools for the environment to understand trends—from melting snow packs to genetic mutations in fish—and surmise what the future holds. With this knowledge, government decision makers, industry and even the average citizen can make more enlightened decisions about how to live today.

Using science and modifying our behaviors, we all can change what tomorrow looks like… and ensure worthy subjects for artists of the future. — LT

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At a *glance*

PNNL veteran named director of microproducts group

Landis Kannberg

Landis Kannberg, a program manager at Pacific Northwest National Laboratory, has been appointed director of the Microproducts Breakthrough Institute (MBI). A collaboration of PNNL and Oregon State University, the MBI is a partner in and shares space with Oregon's first signature research center, the Oregon Nanoscience and Microtechnologies Institute (ONAMI).

To date, the MBI has collaborated on more than $10 million in research and development, including a technology used in a heat-activated, portable cooling unit and a micro-scale blood filter for a portable kidney dialysis device.

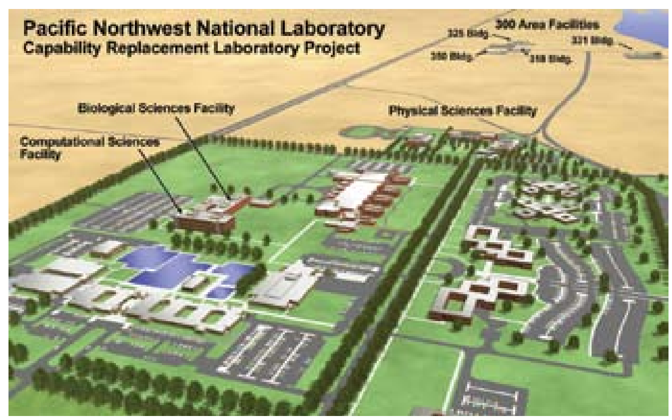
MBI's goals are three-fold: first, to become a nationally and internationally reputed center for microtechnologies; second, to accelerate the commercialization of microtechnologies—particularly for chemical and energy applications; and third, to increase collaborative microtechnology research and development with academia, national laboratories and industry. ●

DOE approves new PNNL facility study

Study defines strategy for new construction and extending use of existing facilities

The Department of Energy has approved the results of an essential study that will shape the future for Pacific Northwest National Laboratory's future facilities. Authorized and conducted in December 2006, the study outlined a strategy for new construction and extending the use of some existing facilities in the Hanford Site 300 Area.

The Physical Sciences Facility will be built on the Horn Rapids Triangle, just north of the Laboratory's central campus, and will consist of three separate modules: chemical processing and materials science and technology, ultra-trace, and radiation detection. ●



PNNL receives national safety award

Left to right: Vern Madson, Cindy Caldwell, Steve Smith, all of PNNL, and Roger Briggs, DOE Pacific Northwest Site Office, accept the award on behalf of PNNL.

Pacific Northwest National Laboratory has been recognized as one of America's Safest Companies as featured in *Occupational Hazards* magazine's November 2006 issue. Each year, the honor is given to a group of companies that demonstrate their management-supported safety processes, involvement from staff and innovative solutions to safety challenges.

The winning organizations must demonstrate solid safety performance and a commitment to safety education and communications. "They (PNNL) get the symbiotic relationship between productivity, profits, morale, and employee retention," said Sandy Smith, chief editor of *Occupational Hazards*.

PNNL is the first Battelle-managed laboratory and multi-program national laboratory to win this respected award. Previous winners include Alcoa, Bechtel Group Inc., Dow Chemical Co., and DuPont. ●

Science of doing business

From Russia with love

Russian research capabilities are advancing the hydrogen economy

Ensuring that hydrogen-burning engines are explosion-proof is one of the barriers to establishing a hydrogen economy. A tiny Russian-designed hydrogen sensor that can quickly detect and warn of a gas leak may be one of the technologies to help catapult the world into the hydrogen age.

A research and business collaboration among Apollo, Inc., of Kennewick, Washington, scientists from the Karpov Institute of Physical Chemistry in Moscow, Russia, and Pacific Northwest National Laboratory has resulted in the design and commercialization of a miniature hydrogen gas sensor that is more reliable, works faster, and costs less than other sensors currently in use.

PNNL initiated this relationship through the DOE National Nuclear Security Administration Global Initiatives for Proliferation Prevention (GIPP) program. The GIPP program creates opportunities for scientists who worked in the weapons technology field during the Cold War era to redirect their research toward peaceful and profitable endeavors. Professors Leonid Trakhtenberg, Genrikh Gerasimov and Vladimir Gromov were using nanoscale materials for sensing reactive gases at the Karpov Institute. GIPP provided the technology transfer mechanism to convert their nanoscale approach into a commercially available product and introduce it to the marketplace.

The collaboration among the Karpov Institute, PNNL and Apollo began about five years ago according to Brian Opitz, the Laboratory's GIPP nanometals sensor project manager. PNNL, already working with the Russian team, began searching for a U.S. business partner to commercialize the technology. "Our original visionary for this project at PNNL, Dom Cataldo, approached Apollo with the idea of working with the Russian scientists to design and build a better hydrogen gas sensor," Opitz said. "Two years later, a CRADA was signed to develop, test and produce sensors that would detect and measure various gases."

A CRADA, Cooperative Research and Development Agreement, is a contractual agreement that provides the unique opportunity to use new technologies evolving from federal research programs in a collaborative way. The collaborating parties share costs and pool the results of their research and development program.

In this case, Battelle, which operates PNNL for DOE, exclusively licensed patent applications based on certain inventions derived under the CRADA to Apollo, and Apollo applied for the global patent on the hydrogen gas sensor. Apollo Sensor Technology (AST), a division that Apollo, Inc., created to commercialize the sensor, will pay Battelle royalties derived from sales of the technology. Under the provisions of the GIPP program, Battelle will then share such royalties with the Karpov Institute.

Dan Briscoe, AST vice president for business development, said industry is looking for the next level of leak detection technology. The new sensors can detect tiny amounts of hydrogen in the parts-per-million range, which is essential for the technology to be effective because concentrations of only 4 percent of the gas can result in an explosion.

AST anticipates marketing the sensors to industries that manufacture, store and use hydrogen in their production processes, such as power plants and petroleum refineries where hydrogen gas is involved in processing heavy crude to light crude. Hydrogen also powers some emergency backup systems used at microwave towers, radio stations and hospitals.

A similar nanotechnology approach used for the hydrogen sensor is capable of detecting and measuring other gases as well, including ammonia, methane, carbon dioxide, and carbon monoxide. Research is already under way to design similar sensors to detect gases in indoor environments, leading to computerized continuous monitoring systems for better air quality in office buildings, schools, hospitals, and cruise ships. ●

Photo courtesy of Shell Hydrogen.

Apollo's new tiny Russian-designed hydrogen gas sensor would be ideal for safety detection systems in futuristic hydrogen-powered cars.

Newly discovered plague proteins could help fight bioterrorism and disease

The Black Death, the great pestilence, bubonic plague—familiar names for a disease documented since antiquity that has at times caused epidemics throughout the world, most notably during the Middle Ages when it wiped out roughly one-third of Europe's population.

Caused by the bacterium *Yersinia pestis*, which can infect humans through the bite of a rat flea carrier, plague did not disappear into the dusty pages of history but still exists today. In fact, the Centers for Disease Control and Prevention considers *Y. pestis* a high-priority organism for study because of its potential use for bioterrorism. The bacterium is a potent human health threat that has the power to overcome its host's immune defenses. To improve detection and enable the design of new vaccines and treatment, the biological processes that determine the bacterium's life cycle and ability to cause disease need to be identified. At Pacific Northwest National Laboratory, scientists recently discovered unique proteins in *Y. pestis* specifically related to their growing environment that are potential biomarkers for use in detecting the disease and intercepting its progress.

Biomarkers are indicators of change in a biological system that can yield information about the state of a disease, susceptibility and exposure. PNNL scientists Mary Lipton and Kim Hixson, along with colleagues at Lawrence Livermore National Laboratory, re-created the growing environment for *Y. pestis* in flea carriers and mammal hosts using unique proteomic equipment (a proteome is a survey of proteins in a cell) and cultured the bacteria to express virulence-related proteins. They compared abundance changes of 992 proteins under four different growth conditions at two different temperatures with and without calcium. An increase in temperature and decrease in calcium concentration are two known regulators that trigger the expression of proteins related to the organism's ability to cause disease. Changes in these two conditions simulate changes the bacteria encounter condition. A hypothetical protein is defined by the Institute for Genomic Research as one identified by a gene-finding algorithm whose sequence matches that of no other known protein and for which there is no other evidence showing it to be a gene product.

Scientist Kim Hixson used a mass spectrometer such as the one shown here to discover protein biomarkers. The William R. Wiley Environmental Molecular Sciences Laboratory, located on the PNNL campus, is home to some of the most powerful mass spectrometry instruments available.

as they are transmitted between flea and host. Identifying abundance changes of proteins under the environmental conditions that promote or inhibit the disease can provide insights into the bacterium's life cycle.

Lipton and Hixson found 176 proteins and likely proteins in *Y. pestis* whose numbers rise and fall according to the disease's virulence. Of these, 89 were found to have similar changes in abundance to 29 proteins known to be linked to virulence, indicating they are biomarkers related to virulence. The scientists also uncovered another 87 "hypothetical" proteins as unique biomarkers associated with disease

These unique biomarkers have promise for use as detection tools in public health, medical and defense applications. Drug and vaccine designers could potentially use these biomarkers to develop new agents to disrupt a biological pathway and intercept the bacteria's ability to infect a host.

The approach used in this research is also being applied to search for biomarkers across a wide range of biological systems, from other infectious bacteria such as *Salmonella* to soil microbes of interest for cleaning up toxic waste. This research study was published in the November 2006 *Journal of Proteome Research*.

Fuel cell researcher powers path to the future

Subhash Singhal

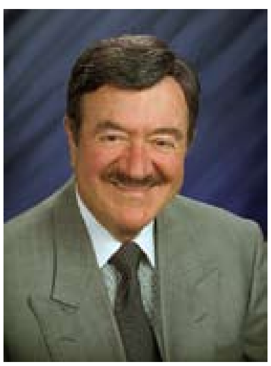
Fuel cell pioneer Subhash Singhal has received the Christian Friedrich Schoenbein Gold Medal for his contributions to the development and promotion of solid oxide fuel cells for clean and efficient power generation.

The biennial award is the highest honor presented by the European Fuel Cell Forum, an international organization commissioned to promote innovative fuel cell technologies. The gold medal is named for the Swiss scientist credited with identifying the fundamental chemistry of fuel cells and later for the collaborative creation of the fuel cell in 1839.

As director of fuel cell research at Pacific Northwest National Laboratory, Singhal provides senior technical, managerial and commercialization leadership to the Laboratory's fuel cell program. Singhal's research supports the Department of Energy's Solid State Energy Conversion Alliance Program. Projects currently under way include the development and use of thermomechanical and electrochemical computer models that predict fuel cell performance and assess the reliability and lifetime, fuel use, and thermal and flow characteristics of the cell. His work emphasizes embedding fuel cell solutions into strategies working to establish a sustainable energy future.

Singhal is one of five PNNL scientist who have been named a Battelle Fellow, the organization's highest recognition for individual achievement in science and technology. ●

Mass spectrometry expert recognized



Jean Futrell

Pacific Northwest National Laboratory's Jean Futrell has been awarded the 2007 American Chemical Society (ACS) Frank H. Field and Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry. This award is the highest recognition given by the ACS for fundamental contributions to mass spectrometry.

Futrell was selected for his work developing and modifying mass spectrometry instrumentation for specialized research purposes. His invention of tandem mass spectrometry is deployed in nearly every commercial mass spectrometer available. Futrell's research has answered several fundamental questions about mass spectrometry, including a detailed analysis of the mechanisms of ions.

Co-author of nearly 300 peer-reviewed journal articles, Futrell is internationally recognized for his significant scientific contributions. He holds the distinction of Battelle Fellow, the organization's highest technical appointment for international scientific leadership. ●

PNNL scientist wins Humboldt Research Award

Lai-Sheng Wang

Lai-Sheng Wang, a long-time researcher at the Environmental Molecular Sciences Laboratory situated on the Pacific Northwest National Laboratory campus, has received the Humboldt Research Award for his achievements in nanoscience. This award is bestowed annually to the top 100 internationally renowned scientists. Recipients are invited to research a project of their choosing in Germany for up to a year.

Dr. Wang is touted as a world leader in nanocluster research. His work helped create hollow nanoscale cages of gold atoms, which are the first known metallic equivalent of the buckyball—a hexagon of rigid, natural molecules composed of exactly 60 carbon atoms. Wang also helped pioneer the study of multiply-charged negative ions.

A physics professor at Washington State University Tri-Cities, Guggenheim Fellow, and member of several scientific societies, Wang has authored more than 250 publications, including features in *Nature* and *Science*. ●

NOTABLE Achievements

Five PNNL scientists awarded fellowship by AAAS

Five scientists at Pacific Northwest National Laboratory have been named Fellows of the American Association for the Advancement of Science (AAAS). James Fredrickson, Richard Smith, S.K. Sundaram, William Weber, and John Zachara were officially named at the Association's national meeting in San Francisco in February. The fellowships were given for their meritorious efforts to advance science; each recipient received a certificate bearing a blue and gold rosette as a symbol of their accomplishments.

AAAS is the world's largest non-profit, general scientific society. Its mission is to advance science through projects, programs and publications in the areas of science policy, science education and international scientific cooperation. Founded in 1848, AAAS has grown to include more than 250 affiliated societies and academies of science, serving 10 million individuals.

The organization publishes *Science* magazine, first established by Thomas Edison in 1880, which showcases several top research papers in the biological and physical sciences field. *Science* has the highest paid circulation—more than one million—of any scientific journal worldwide.

James Fredrickson, Ph.D. and PNNL Fellow, was elected to the biological sciences section. A chief scientist in the Biological Sciences Division within PNNL's Fundamental Science Directorate, Fredrickson has made significant contributions within the field of microbial ecology and environmental microbiology. In addition to his Laboratory role, he serves as chief scientist for the Department of Energy's Genomics: Genomes to Life program, whose mission is to study fundamental biological processes and ultimately understand how living systems operate.


Fredrickson

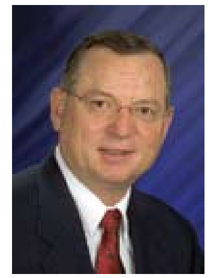
Richard Smith, Ph.D. and Battelle Fellow, was inducted into the chemistry section. Smith is chief scientist in the Biological Sciences Division. His fellowship recognizes his leadership in analytical chemistry, specifically in the deployment of advanced separation methods with high-performance mass spectrometry for the study of proteins. In addition, Smith serves as director of the National Institute for Health Research Resource Center for Integrative Proteomics. He is an adjunct professor of chemistry at Washington State University, the University of Idaho and the University of Utah.


Smith

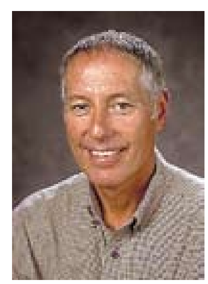
S.K. Sundaram, Ph.D., was elected to the engineering section. Sundaram is chief materials scientist in PNNL's Advanced Processing and Applications Group in the Environmental Technology Directorate. His fellowship rewards his leadership and innovative contributions to a diverse cross section of materials science, particularly new tools for synthesis and characterization of novel materials, diagnostics and nanomaterials. Sundaram serves as adjunct faculty member in the School of Mechanical and Materials Engineering for Washington State University and has visiting appointments at MIT, Harvard and Princeton.


Sundaram

William Weber, Ph.D. and PNNL Fellow, was named to the physics section. A scientist in the Laboratory's Fundamental Science Directorate, Weber was recognized by the AAAS for his continued work and research on the defects, ion-solid interactions and radiation effects in ceramics, especially pertaining to modeling and simulations of radiation damage processes. Weber also serves on PNNL's Council of Fellows as chairman and on the Laboratory's Publication Advisory Committee.


Weber

John Zachara, Ph.D., was inducted into the geology and geography section. Zachara is senior chief scientist for environmental chemistry in the Laboratory's Chemical & Material Sciences Division. The fellowship acknowledges his contributions to environmental science, predominantly for work on the chemical and microbial processes affecting subsurface contaminant transport at the Hanford Site in Washington state. Zachara, chief scientist for in-ground contaminants at Hanford, is widely recognized for leading a multi-organizational team to resolve important science issues pertaining to contaminant fate and transport in Hanford's vadose zone and groundwaters.


Zachara

SPECIAL REPORT:

Environmental Renaissance

Dr. Rod K. Quinn is the director of the Environmental Technology Directorate (ETD) at Pacific Northwest National Laboratory. Under his leadership, the directorate applies scientific expertise to solve current and future environmental challenges in our own backyard and around the world. ETD contributes to the cost-effective cleanup of contaminated nuclear weapons sites, protecting human health and the environment from the effects of contaminants, improving knowledge on the impacts of climate change, and deploying air- and water-neutral technologies for energy generation.

▲ ETD Director Rod K. Quinn

Rod addresses how PNNL is revolutionizing the state of the art with predictive science—solving existing environmental problems and creating a safer and cleaner environment for the future.

What are your thoughts on global environmental challenges?

There is an overwhelming global realization that we—as individuals, corporations and government—must do things right the first time in terms of environmental citizenship. If we don't, the consequences are evident in devastating events, from industrial accidents such as Chernobyl or the Valdez oil spill to natural disasters such as hurricanes and tsunamis amplified by human activities.

In many cases, we've acted and then cleaned up the consequences. With demands constantly taxing the environment—and increasing—this is no longer a viable option. We have complex environmental concerns to address now, and new ones are rapidly and consistently emerging. As our nation seeks to ease national dependence on foreign oil, the environmental impacts of alternative energy solutions must be a top priority.

Where do the nation's greatest environmental challenges lie?

Our greatest challenge is time and information. As a country, we need sound scientific research to explain and even anticipate the environmental cost and consequences of human behavior. We are discovering things that generations ago we didn't think would affect our environment the way they are. For example, researchers at PNNL's Marine Sciences Laboratory on the Olympic Peninsula in Washington state found that human contraceptives could impact the fertility of trout; the synthetic estrogen in birth control pills eventually enters the municipal wastewater system. We've come to find out that trout populations are affected; beyond that, this discovery has forced us to consider greater human health impacts of everyday life. How are compounds that enter the soil, groundwater and air affecting us long-term in the water we drink, the food we eat and the air we breathe? Answering these questions will help decision makers balance the needs of our ecosystem and human health along with economic realities.

As we gain these insights, there is understandably a sense of urgency about finding solutions faster. Recognizing the rich resources the Pacific Northwest holds and their ties to the economic health of our region, Washington Governor Gregoire and Oregon Governor Kulongoski have made finding this balance a legislative priority. This is another great example of how working together, we can achieve more. We can meet the challenges with solutions and head off future impacts.

How will today's research affect the environment 10 years from now?

Everything humans do impacts the environment—from what we dispose of in landfills to the chemicals used in our daily activities that are released into our ecosystem—mainly soil, water and air. Add in impacts from industrial and government operations, and the outlook for the environment is hazy.

Driving toward a predictive science model, we can make this picture clearer. This model is based on mechanisms to pinpoint negative effects presymptomatically, rather than relying on overt symptoms. In the medical field, health practitioners use high blood pressure as a potential indicator of heart disease. However, often by the time high blood pressure is detected, the body already shows signs of damage. We're looking at these things differently to avoid that. Researchers at PNNL are striving for new ways to predict the effects of our actions so we can minimize or eliminate the stresses to the environment. Predictive science can teach us how to create new technologies and modify our behaviors today so we are not negatively impacted in the future.

One area we are just beginning to understand is how nanoparticles might affect the human respiratory system. Nanotechnologies offer promising solutions ranging from cancer treatments to sustainable energy and clean water. But a potential downside may be the release of tiny particles into the environment. Our three-dimensional virtual respiratory tract model demonstrates how pollutants enter, travel and collect in the body. By studying this, we are beginning to understand human health effects of nanotechnologies.

What other kinds of environmental research are under way to reverse future impacts?

Water management is another key environmental priority for the United States. This precious resource is a central element to consider as we search for new energy solutions, particularly water-intensive options like coal recovery. The Laboratory is partnering with the states of Washington, Oregon and Idaho to understand and predict how the Pacific Northwest water system will be impacted by climate change and new energy resource development.

Also of significant regional importance to the Pacific Northwest is the cleanup and prevention of pollution in the Puget Sound. This critical body of water, which hosts large shipping ports and the major urban areas surrounding Seattle, is being threatened by historic practices; continued population growth is another challenge. PNNL's expertise in restoring and managing water resources, from the mountain snowpack to the salt water, is resolving some of these issues and preventing unfavorable impacts.

How is PNNL meeting these challenges?

Because global environmental problems are incredibly complex, we must bring together the best scientists and engineers in the field. PNNL is proud of its outstanding reputation and vast experience in an array of scientific disciplines, including environmental sciences. The Laboratory's network of partnerships involves stakeholders at the federal, state and local levels. We are working together to identify and determine the best path forward on environmental issues.

I think with our history, we are particularly well-poised to make a difference. For more than 40 years, the Laboratory has undertaken complex issues at the

Hanford Site, a former plutonium production area in southeastern Washington. Our geologists, hydrologists, chemists, physicists, and computer scientists have characterized unique waste streams, designed treatment methods and storage forms, and helped remediate the soil and groundwater.

Over the years, we have applied that knowledge and expertise to other projects. For example, our work in separating problematic elements out of radioactive waste led to an understanding of how to remove radionuclides that could enter the body from a dirty bomb explosion. Currently, we're investigating chitosan, obtained from lobster, crab and shrimp shells, as an agent to bind radionuclides in the body to stop them from damaging the liver, kidneys and other organs.

Additionally, our decades of experience in subsurface science may serve to reduce the amount of greenhouse gas carbon dioxide—implicated in global climate change—emitted by coal-fired power plants. That expertise has positioned us to discover ways to capture carbon dioxide deep underground. By developing methods for making carbon sequestration safe and affordable, PNNL will contribute to stabilizing atmospheric levels of carbon dioxide. This is but one part of how the Laboratory is contributing to the development of environmentally-friendly and economically viable energy solutions.

What does PNNL envision for the future?

We are focused on driving toward scientific solutions that will help address environmental challenges before they turn into a devastating event. At PNNL, we are well-positioned and committed to blazing a new path forward—one that cleans up waste, prevents future environmental insults and uses natural resources responsibly. I believe that if we stay focused on this mission, PNNL will greatly contribute to ensuring a better quality of life for future generations.

vironmental Renaissance

Forecasting future water supplies leaves stakeholders soaked in uncertainties

Apple orchards, vineyards, hydroelectric power, municipal water supplies, and salmon runs all depend on the same oversubscribed resource—water. Even in the snowy Northwest, water is a finite resource with an infinite number of competing demands.

Global climate change furthers the region's water problems. Water availability is dominated by seasonal release and storage from mountain snowpacks. Scientific models suggest several climate change effects, including significantly reduced snowpack, wetter winters, drier summers, and changes to river temperatures and flows that are tough on migrating salmon.

Moreover, the Clean Water Act, the Endangered Species Act, and other water appropriations and permitting requirements impose strict limitations on how stakeholders can impact water issues.

Balancing Needs and Resources

To combat this dilemma, Pacific Northwest National Laboratory is developing an integrated research agenda. Balancing the region's water availability and needs, energy requirements and desire for a sustainable ecosystem, the Laboratory is assisting stakeholders in making better water allocation decisions. This approach taps into PNNL's expertise in integrated earth and energy systems modeling, water treatment technologies and scientific decision support systems.

Understanding the interdependence of energy and water for alternative energy source development is central to achieving a regional water balance. Therefore, stakeholders need to better forecast water availability to make better usage decisions. These forecasts are needed at geographical scales ranging from local irrigation diversion points to the entire Columbia Basin.

Understanding Future Water Resources

The Northwest Regional Collaboratory, a PNNL-led, NASA-funded collaboration of two national laboratories and four regional universities, works to combine satellite images into watershed models in order to fill in the gaps between immediate weather forecasts and estimates based on historical data.

These models support streamflow forecasting and can be used to refine decisions about water releases from reservoirs for salmon, irrigation and municipal use as well as for the production of electricity.

Growing Demands, Diminishing Resources

Ensuring future water supplies meet the Northwest's growing population and vibrant agricultural base, as well as the water and energy needs for both, is vital. Citizens and industry alike are seeking out more electricity to maintain their livelihoods. Hydropower—while an attractive and clean way to supply energy—adds an additional demand on water resources. More energy = more water.

The interdependence of water and energy lies squarely in the center of major environmental and economic problems in the region. Population growth and economic development are placing higher demands for energy to access and distribute water supplies; this includes pumping more groundwater to meet irrigation requirements. The development of alternative energy resources such as coal-bed methane and oil shale has raised major concerns for water consumption, quality and management.

Teaming for Solutions

With so many variables pressing this one single resource, PNNL's approach to addressing the issues is to team with other interested parties and stakeholders. The Northwest Regional Collaboratory is but one example of the Laboratory's collaborations with other science and technology institutions to address regional water issues.

PNNL and the Idaho National Laboratory are investigating the integration of hydropower and wind energy to meet water and energy needs of agriculture. The case study will help develop strategies for alternative energy sources as our region faces increasing demands for both.

Water is the common currency of our economy and an essential part of the Northwest's quality of life. The science and technology community must provide a sound foundation for the sustainable use of this limited resource. PNNL is working with regional partners to provide the science and technology necessary to meet this crucial need.



Digging into dirt: Subsurface science at PNNL

Imagine drinking water that has dripped through the sponge you've just used to clean the breakfast dishes. This is happening around the world. Rain and snow pass through soil polluted with pesticides, poisonous metals and radionuclides into the underground streams that supply rivers, lakes and drinking water.

"We need to understand this system better to protect our groundwater and, by extension, our drinking water," said Pacific Northwest National Laboratory's Applied Geology and Geochemistry Group Manager, Wayne Martin.

PNNL builds synergistic teams of experts, including biologists, statisticians, hydrologists, geochemists, and computer scientists. These teams study the complexities of the whole environment, not just the soil or groundwater. The teams provide regulators with answers to make complex decisions and design innovative technologies to capture or convert pollutants.

Dealing with Arsenic and Lead at Old Fertilizer Plants

In the mid 1800s, fertilizer manufacturers began obtaining the plant nutrient phosphate by processing apatite ore with sulfuric acid. Pyrite ore, with traces of arsenic and lead, was a feedstock used for the onsite production of sulfuric acid. Waste fluids and solids from acid and fertilizer production were disposed of at the sites.

Over a century later, researchers at PNNL are helping ConocoPhillips and others deal with the long-term legacy of contamination and costly cleanup problems at sites in South Carolina and Massachusetts. The teams locate contaminated areas, evaluate the site to determine the physical and geochemical processes controlling migration of the dangerous metals, help design customized remediation methods, and assist with long-term monitoring.

Stopping Radionuclides at a Nuclear Weapons Site

Beneath the Hanford Site, a former plutonium production complex in southeastern Washington, lie about two million curies of radionuclides. One concern is a persistent plume or smear of uranium that is moving through the subsurface toward the Columbia River bordering the Site on the east.

PNNL researchers have taken a holistic approach to understanding where the uranium will move and how it will react. By looking at the whole of the environment, not just the soil, researchers can develop methods that stop the migration of uranium and protect the river.

To reliably and cost-effectively test for uranium in the hyporheic zone, where the groundwater bubbles into the river, PNNL researchers are looking at that ecosystem, including microbes and fungi that make up common rock slime, which grows at the river's edge. By including ecologists, biologists and computer scientists, this team is searching for genes, proteins or metabolites that indicate the ecosystem has encountered uranium.

Mapping the Results of Pesticide Dumping

DDT and other pesticides are, by definition, toxic to insects that can destroy food crops and carry malaria or other diseases; however, when companies dispose of these chemicals improperly, the consequences can be devastating to humans and the environment. Just how devastating is what PNNL's geostatisticians helped determine.

Geostatistics combines geology and mathematical statistics and can be used to understand the spatial distribution of one or more pollutants through a complex environment.

When high levels of pesticides were discovered on southern California's coastal shelf, PNNL Staff Scientist Chris Murray was asked to produce maps showing the thickness and contaminant concentrations of the polluted sediment. The Environmental Protection Agency used the maps to evaluate cleanup options.

Looking Ahead

The future of subsurface science may be up in the air, literally. Researchers at PNNL are working to safely incorporate the greenhouse gas carbon dioxide into the subsurface. As part of a large consortium, the researchers are looking at the feasibility of pumping the gas deep underground. There, it would react and become harmless minerals within the soil.

Balancing oil and environment... responsibly

As the price of oil continues to fluctuate unpredictably and nears the brink of depletion, pursuing unconventional oil supplies, such as oil shale, oil sands, heavy oils, and oils from biomass and coal, has become increasingly attractive. Of particular significance to the American way is that our continent has significant quantities of these resources.

Tapping into these new resources, however, requires cutting-edge technologies for identification, production, processing, and environmental management.

Pacific Northwest National Laboratory and fellow Battelle-managed national laboratories are pooling their expertise to deliver these solutions. Collaboratively, the laboratories are integrating their research and technologies for industry leaders. While tackling the problem as a team will give the United States a competitive edge in leading the way toward global solutions, researchers recognize that it is all for naught if these resources are tapped at cost to the environment.

Fortunately, PNNL is home to some of the world's leading environmental experts. One team, led by Wally Weimer, the Laboratory's industrial market sector leader for the oil and gas industry, is working hard to understand the opportunity and responsibly engage in unconventional oil recovery.

"Industry has the ability to transition our technology discoveries and innovations into working solutions," Weimer said. "It's very exciting to see how government-sponsored research can come together for industrial clients to address an issue that's important to all of us."

The basic research has been under way for years, and PNNL has emerged as a leader for addressing several environmental aspects of this project, including the protection of surface water and groundwater resources. As it turns out, unconventional oil resources tend to locate near areas that are water-limited, creating an enhanced need for protection of these resources. Another area of environmental concern is carbon emissions. The development and utilization of unconventional resources will release carbon dioxide into the atmosphere; these emissions over time could potentially impact global climate and air quality. Researchers at PNNL are using predictive computer modeling to understand these effects and to develop technologies that can stop the problems before they start.

A rescue is being attempted. With the collaboration among its peer national laboratories, PNNL plans to be part of the solution that solves the problems with new sources for oil…and at the same time protects the environment.

Biomarkers: Transforming human health and the environment

You've seen it in the news headlines: ***Anthrax discovered in the mail… SARs outbreak… Norovirus outbreak… Potential for an avian flu pandemic looms… Obesity and diabetes threaten Americans' health… Demand for water on the rise, while water quality falls.*** What do they have in common? All of them clearly illustrate the link between how environmental stressors affect human and ecological health.

As concerned citizens, we've utilized preventive measures where we can, including using hand sanitizers, taking vitamins and eating well, getting immunizations, using disinfecting wipes and in-home water filtration systems. However, for every ounce of prevention we take, we still are vulnerable to the broad spectrum of biological and chemical agents in the environment that threaten our health. And we don't usually realize it until we start to feel sick.

We cannot escape the fact that human health is always impacted by our environment and how our

Scientists at Pacific Northwest National Laboratory are developing a new class of materials that can be engineered to attract and trap CO_2 and other gases into their molecular cages. These breakthroughs will enable alternative fuel sources to burn clean.

Carbon capture made easy

Gasification plants may be one of the keys to a hydrogen economy, if capture and sequestration of carbon dioxide (CO_2) becomes technically and economically feasible. These plants would transform fossil fuel feedstock, including coal, biomass and municipal wastes, into clean-burning hydrogen gas where the only byproduct is water.

But there are problems to solve. In addition to producing hydrogen, coal gasification produces CO_2. Current methods for CO_2 capture use large volumes of chemical solvents that must be cycled through dramatic changes in pressure and temperature to absorb and then release CO_2. These pressure and temperature swings use a lot of energy and increase costs of electricity production by 15 to 30 percent.

Researchers at Pacific Northwest National Laboratory are developing a new class of materials for CO_2 capture that aims to significantly reduce the energy penalty for CO_2 capture. The PNNL process does not require dramatic pressure and temperature swings, making it more energy-efficient. And the concept integrates CO_2 capture with a water-gas shift reaction into a single, more efficient unit, reducing costs and creating a near-zero emissions system. Integrating the process improves the efficiency of the water-gas shift reaction, which converts carbon monoxide to CO_2 and hydrogen by reacting with water vapor, ultimately producing more CO_2 and more hydrogen, the desired product.

A unique nanomaterial will be instrumental in the integrated process. “We are working with a nano-structured material called an organic clathrate that can be engineered to attract CO_2 and other gases into its molecular cages,” said Laboratory Fellow Pete McGrail, who is leading the carbon capture work. Organic clathrates can hold several gas molecules in each of their cavities. The material is a solid that could be packed into an absorber column to collect CO_2 from the gas stream.

“The water-gas shift reaction of interest takes place at 230 to 260 degrees Celsius,” said Praveen Thallapally, who is leading the materials synthesis work. “We have created a new clathrate material that can absorb CO_2 at 220 degrees Celsius so we believe it’s possible, with additional research, to create materials that will perform at the temperatures necessary for this application.”

McGrail and his team also are using molecular dynamics simulations in their studies. Instead of the time-consuming conventional method of constructing a material, synthesizing it and evaluating it, they are using computer simulations to help guide their materials development and discovery effort.

bodies react to it—from the air we breathe, the food we eat and the environment we live in. Wouldn’t it be great to know these stressors were affecting our health before the symptoms set in?

Pacific Northwest National Laboratory scientists are transforming how we assess and manage our health and environment by applying system science and pattern recognition to the discovery of biomolecular signatures. Biomolecular signatures, a set of genes, proteins, metabolites, and/or lipids, present a unique pattern of change in an organism that can be used to identify an exposure or response to a specific environmental stressor.

The ability to identify these biosignatures will lead to the transformation of environmental and threat assessment from a measurement science to a predictive science. To get started, they are focusing on three stressors: biological agents associated with terrorist threats, potential toxicity of nanoparticles used more and more in everyday products, and protection of our river environment from contaminants.

“We are identifying environmental biomarkers—which are the earliest indicators of biological changes based on the response to—not just to the exposure to—environmental stressors,” said Dr. Terri Stewart, who leads PNNL’s Environmental Biomarkers Initiative. “As with any preventive measure, the earlier, the better which is a driver for the team to find these biomarkers.”

By identifying and understanding these early indicators of illness and other environmental damage, scientists will be better able to intervene before human health or the environment are negatively affected. This vital intervention may lead to new preventive measures to ensure cleaner water, an overall cleaner environment and a better quality of life.

An ounce of prevention

When you think about it, Americans go to great lengths to be healthy these days. This generation is far more knowledgeable about the benefits of a healthy lifestyle than generations past. In addition to paying attention to diet and exercise, many regularly take precautions to avoid illness and disease. Today, taking vitamin supplements, eating foods rich in antioxidants and applying sunscreen are almost as commonplace as brushing teeth in the morning. After all, an ounce of prevention is worth a pound of cure.

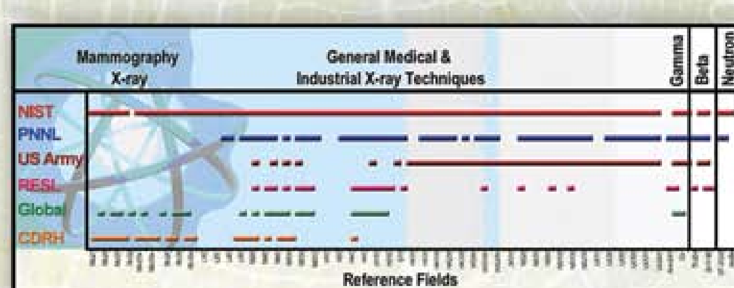
But what if we could do more to prevent environmentally induced diseases, such as those resulting from exposure to ionizing radiation? Keep in mind that everyday sources of radiation exposure such as passing through airport security, watching TV or standing in front of a microwave have not been linked to cancer. Only high-frequency radiation (ionizing radiation and ultraviolet radiation) has been proven to cause genetic damage, which can lead to cancer.

Certain professionals, such as emergency personnel, astronauts, medical professionals and radiation workers, can have a higher risk of exposure to ionizing radiation. The exposure itself may not be preventable, but medication to prevent the potential genetic damage that can lead to cancer is an exciting possibility.

Through radioprotectant and molecular biology research projects, scientists at Pacific Northwest National Laboratory have developed novel approaches for identifying certain cellular molecules that can reduce the deleterious effect of radiation exposure by increasing the body's DNA repair function. PNNL's extensive radiation facilities can deliver multiple kinds of radiation exposures to cells (beta, alpha, x-ray, gamma-ray, and neutron fields). Such facilities, combined with proteomic, genomic, metabonomic, DNA repair assay, and systems biology capabilities, are allowing scientists to study the efficacy of radioprotectants at the cellular level over a wide range of dose levels and radiation types.

The human body is a remarkable machine that regularly works hard to maintain its health—there are approximately 10,000 to 1,000,000 genetic lesions per cell that must be repaired daily! Such repair is essential in all life forms, and failure to make these repairs can eventually result in a major disease, including cancer. PNNL's newest efforts should lead to not only the ability to enhance this daily repair of normal genetic lesions but also the ability to repair even the more difficult lesions caused by high radiation dose such as those sustained by cancer therapy patients, astronauts and first responders to emergencies.

Some day in the not too distant future, individuals might take a daily supplement that triggers the cell's DNA repair function to enter a hyperproductive state, thereby reducing the mutagenic or carcinogenic impact of exposure from radiation or chemical contaminants. For example, emergency personnel responding to terrorist or natural catastrophic events could protect themselves by boosting their DNA repair function before entering environments with exposure potential.



The ionizing radiation capabilities provided by the National Voluntary Laboratory Accreditation Program-accredited laboratory at PNNL comprise the broadest range of accredited capabilities available in the country outside of the National Institute of Standards and Technology. (US Army Dosimetry Center, Redstone Arsenal, AL; RESL is DOE's Radiological & Environmental Sciences Laboratory, Idaho Falls, ID; Global Calibration Laboratory, Cleveland, OH; CDRH is the Center for Devices & Radiological Health, USDA, Rockville, MD)

Ionizing radiation is used in a host of medical procedures and is an effective treatment for certain kinds of cancer. Ironically, however, these high doses of radiation may adversely cause DNA mutations in surrounding healthy tissue that can lead to the development of another cancer. Pretreatment with a radioprotectant may someday eliminate this secondary damage.

Most exciting of all to PNNL researchers are the unimaginable future discoveries that may result from interdisciplinary studies that take advantage of premier capabilities in ionizing radiation with new proteomic, genomic and metabonomic tools in systems biology. Through the benefits of further research, the general public may eventually be able to add a DNA-repair boosting supplement to its beach bag of sunscreens, hats and antioxidant-rich snacks.

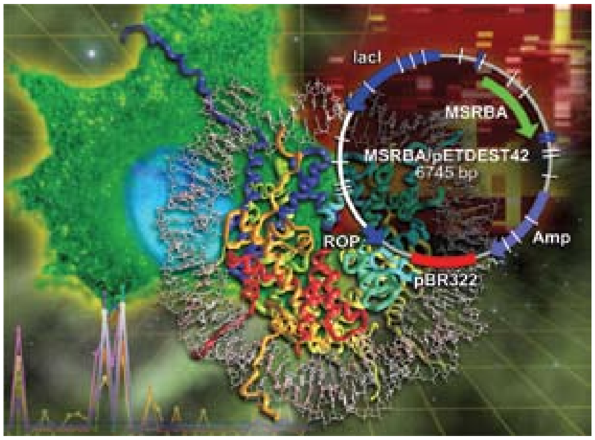
Data-intensive computing key to predictive science

The ability to protect the nation from terrorist attacks, discover the hidden secrets of genes and monitor and control the electrical power grid requires the ability to process and analyze massive amounts of data and information in real time.

“The power to make breakthroughs and solve complex problems lies in our ability to successfully manage the increase in data, extract valuable knowledge from the multiple and massive data sets, and reduce the data for understanding and timely decision making,” said Deborah Gracio, deputy director of Computational Sciences and Mathematics.

Gracio leads the Data-Intensive Computing Initiative (DICI) at Pacific Northwest National Laboratory. The four-year initiative is aimed at creating a computing infrastructure that will integrate data-intensive computational tools with domain science problems such as national security, biology, environment, and energy, to facilitate the next frontier—predictive science.

According to Gracio, the computing infrastructure will enable predictive systems that aid scientists in the development of predictors or means for understanding the precursors to an event. “They can start to identify the biomarkers in the environment that could cause contamination or be able to observe a pattern in the way terrorists interact, opening the possibility to change the outcome.”



Data-intensive computing advances scientific discovery to understand the fundamentals of complex systems and provides insight into systems biology.

Staff scientist Ian Gorton, a recent recruit from Australia (see “Meet” below), is the chief architect for creating the computing infrastructure. Gorton, whose goal is to develop a robust, flexible integrated system architecture encompassing both hardware and software, calls the project Medici, alluding to the Florentine architects of the Italian Renaissance and playing on DICI.

“The focus of Medici is the construction of software tools, or the underlying plumbing, that will allow applications to be plugged together so that scientists and application developers can create complex, data-intensive applications,” Gorton said. “Our primary aim is to create technologies that provide scientists the ability to create various applications on a single underlying architecture. And, once created, these applications will run fast and reliably, and they’ll be able to adapt in certain ways to changes in their environment while they’re actually executing.”

Gorton has worked for nearly two decades in the software architecture research world. “The types of applications I tend to build always involve many distributed computers and databases. They’re incredibly difficult to build for various technical reasons, so it’s always been a fascination of mine to try and build and use technology to make integrating all these different types of systems easier.”

Gorton’s team had the opportunity to demonstrate the Medici technology at Supercomputing 06. “Using our very first version of Medici, we plugged together a set of network sensors and analytical tools that were developed by various researchers at the Laboratory for cyber security purposes,” he said. “And it all worked beautifully.” ●

Meet Ian Gorton, Chief Architect

Ian Gorton, a staff scientist at Pacific Northwest National Laboratory and chief architect of PNNL’s Data-Intensive Computing Initiative, has 17 years experience in research and development and consulting in software architecture.

He has held senior positions at IBM Transarc and Australia’s National Science Agency, the Commonwealth Scientific and Industrial Research Organization. Gorton had worked previously at PNNL, leading research and consulting projects that created new methods and technologies for building complex software systems.

“I enjoy the opportunity to work with different people you find in a national laboratory, such as biologists, the people in cyber security and the environmental scientists,” Gorton said. “The potential diversity of applications that we have to provide the underlying infrastructure for is useful because it enables us to really understand what people want to do in their own application domain.”

Gorton has written two books on software architecture and is a member of the IEEE Computer Society, ACM and a Fellow of the Australian Computer Society.

Ian Gorton

Sailing for science

When most people think of an ocean cruise, they think of buffets and relaxing in deck chairs. For Pacific Northwest National Laboratory researcher Philip Long, an expedition cruise aboard the Joint Oceanography Institutes Deep Earth Sampling (JOIDES) Resolution research vessel meant 12-hour workdays examining ocean floor core samples for methane hydrate.

Physical property specialists Philip Long (PNNL) and Anne Tréhu (Oregon State University) operate an infrared camera on the catwalk of the JOIDES Resolution. The infrared camera helps the scientists identify which portions of the core contain gas hydrate.

Methane hydrate is an ice-like substance made of water and methane (natural gas) that occurs beneath ocean floors. It looks like ice, but it burns when ignited. A single liter of methane hydrate equals the energy of 164 liters of natural gas, by volume. This fact, coupled with estimates of the abundance of methane hydrate worldwide, has piqued interest in its potential as a fuel source. However, these ice pockets in the ocean sediment melt quickly when brought to the surface and release methane into the atmosphere.

Researchers are investigating the role that these deposits have played in ancient global climate change and the possible effects on future climate change. The icy hydrates serve to cement the ocean floor sediments, stabilizing the sea bottom. If the methane hydrates melt due to a warming climate, destabilized sediments could shift in undersea landslides.

Unassuming deposits of methane hydrate hold vast potential as an alternative fuel source.

The National Science Foundation and the Department of Energy Office of Fossil Energy sponsored two hydrate expeditions for the JOIDES Resolution—one along the Oregon Coast and the other off Vancouver Island. Long's role on the scientific team for both expeditions was to scan core samples for hydrates using infrared thermal imaging.

Long and fellow PNNL scientist H. Todd Schaef embarked on another expedition last summer to locate deposits of hydrates in the Indian Ocean and Andaman Islands. The Indian government sponsored the expedition to study possibilities of retrieving and storing methane gas to offset its demand for new sources of energy. ●

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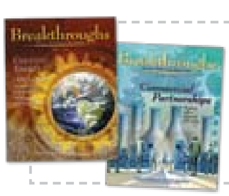

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