Pacific Northwest
NATIONAL LABORATORY

FY 2008

KEY ACCOMPLISHMENTS

Fundamental & Computational Sciences Directorate

Atmospheric Sciences & Global Change

Natural terrestrial sequestration options, such as reforestation of land, could contribute to meeting greenhouse gas emission goals under four different climate policy scenarios.

USING MOTHER NATURE to Reduce Greenhouse Gases

RESEARCH showed that adopting low-cost land management practices that naturally sequester carbon dioxide could contribute up to 20% of the carbon mitigation needed worldwide in the first half of this century. For the first time, Pacific Northwest National Laboratory's scientists included terrestrial sequestration in computer simulations of the cost and technology options necessary for stabilizing greenhouse gas concentrations by 2100. Land management changes studied included reducing tillage on crop land, changing grassland grazing patterns, and converting land to forests.

Thomson AM, RC Izaurralde, SJ Smith, and LE Clarke. 2007. "Integrated Estimates of Global Terrestrial Carbon Sequestration." *Global Environmental Change* 18(1):192-203.

Sponsors: U.S. Climate Change Technology Program, building on research supported by DOE's Office of Science, Integrated Assessment Research Program, Climate Change Research Division; and NASA

U.S. CLIMATE CHANGE Effects Revealed

The most extensive examination ever conducted of the impacts of climate change on U.S. ecosystems over the past few decades and into the near future reveals that the effects of human-caused climate change in the United States are more widespread and significant than previously thought. The bottom line: climate change is already affecting forests, water resources, farmland, and wildlife—and will continue to do so.

With leadership and contributions from Pacific Northwest National Laboratory scientists, the national assessment was released in May 2008 under the U.S. Climate Change Science Program. To write the assessment, 38 researchers from a variety of fields conducted an exhaustive review, analysis, and synthesis of the scientific literature, surveying more than 1,000 publications. The findings point to measurable effects—many of them negative—from global warming and higher carbon dioxide concentrations. And, the future doesn't look much brighter, with the assessment predicting "profound effects."

The report is significant in two ways. First, it brings a sense of urgency because the changes are evident today, not just years from now. And, it establishes a scientific baseline for how the nation will need to cope.

In addition to Dr. Tony Janetos' role as convening lead author, Dr. César Izaurralde and Allison Thomson contributed to the assessment. All three are with the Joint Global Change Research Institute, a partnership of Pacific Northwest National Laboratory and the University of Maryland. In addition to Janetos, the other lead authors were Peter Backlund of the National Center for Atmospheric Research and David Schimel of the National Ecological Observatory Network.

Backlund P, A Janetos, and D Schimel. 2008. *The Effects of Climate Change on Agriculture, Land Resources, Water Resources, and Biodiversity in the United States.* U.S. Climate Change Science Program, Washington, D.C.

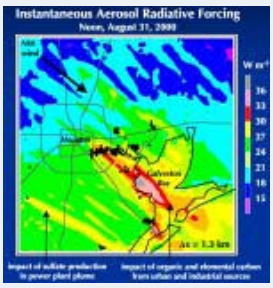
Sponsor: U.S. Department of Agriculture

ADDING CHEMISTRY to the Relationship

Scientists at Pacific Northwest National Laboratory have enhanced a computer model that is used worldwide in predicting climate change. The improved Weather Research and Forecasting model, released in April 2008, includes important climate feedback processes, such as interactions among human-made or natural trace gases and particulates, simultaneously with changes in meteorology.

In contrast with climate models that cover the entire planet, the flexible grid structure in WRF permits simulations on smaller scales suitable for understanding effects of climate change at regional and local levels.

WRF is publicly available and is being used by hundreds of researchers worldwide. Preliminary versions have been used by scientists in Chile, India, England, and Germany as well as at institutions in the United States, including Pacific Northwest National Laboratory, the National Oceanic and Atmospheric Administration, the National Center for Atmospheric Research, Princeton University, and North Carolina State University.



This map, generated using the Weather Research and Forecasting model, shows the effect of different pollutants in the air over Houston, Texas.

Gustafson WI, EG Chapman, SJ Ghan, RC Easter, and JD Fast. 2007. "Impact on Modeled Cloud Characteristics Due to Simplified Treatment of Uniform Cloud Condensation Nuclei During NEAQS 2004." *Geophysical Research Letters* 34:L19809, doi:10.1029/2007GL0300321.

Sponsors: National Science Foundation, National Oceanic and Atmospheric Administration; Pacific Northwest National Laboratory's Laboratory Directed Research and Development program

Results from PNNL researchers and their colleagues indicate that biogenic secondary organic aerosols—like α-pinene—may condense as a separate phase, possibly a "coating."

REMODELING Organic Aerosols

A significant discrepancy exists between how organic aerosols may form in nature and the approach commonly used in climate change models, according to a study led by Pacific Northwest National Laboratory that employed EMSL instrumentation. The current approach makes assumptions on how the organic gases may partition between the gas and particulate phases. Because atmospheric aerosols influence the climate through cloud formation and other factors, such discrepancies could have large implications for global models that simulate the effects of organic aerosols on climate.

Song C, RA Zaveri, ML Alexander, JA Thornton, S Madronich, JV Ortega, A Zelenyuk, XY Yu, A Laskin, and D Maughan. 2007. "Effect of Hydrophobic Primary Organic Aerosol on Secondary Organic Aerosol Formation from Ozonolysis of α-pinene." *Geophysical Research Letters* 34:L20803.

Sponsors: Pacific Northwest National Laboratory's Laboratory Directed Research and Development program; DOE's EMSL

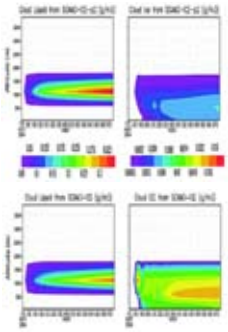
ARCTIC CLOUDS GET a Reality Check

In recent decades, the Arctic has been experiencing warming twice as large as the global averages. However, the uncertainty in climate model simulations and future climate projections is larger in the Arctic than the rest of the globe. A new method developed by scientists at Pacific Northwest National Laboratory and Lawrence Livermore National Laboratory improved the accuracy of climate models by more realistically representing clouds and resulting energy feedback.

Liu X, S Xie, and SJ Ghan. 2007. "Evaluation of a New Mixed-Phase Cloud Microphysics Parameterization with the NCAR Single Column Climate Model (SCAM) and ARM M-PACE Observations." *Geophysical Research Letters* 34, :L23712, doi:10.1029/2007GL031446.

Xie S, J Boyle, SA Klein, X Liu, and S Ghan. 2008. "Simulations of Arctic Mixed-Phase Clouds in Forecasts with CAM3 and AM2 for M-PACE." *Journal of Geophysical Research D* 113(D4):Art. No. D04211.

Sponsor: DOE's Office of Biological Environmental Research



Simulations of cloud liquid water content and ice water content as a function of altitude and time show significant differences with respect to cloud temperature and altitude.

STUDYING ARCTIC AEROSOLS Sheds Light on Clouds and Climate

The Arctic is an ideal location to study climate change because it displays dramatic evidence of shifts, such as melting sea ice. In April 2008, an 80-person team of U.S. and Canadian climate scientists completed a month-long field study over the North Slope of Alaska. Packing 40+ specialized instruments into a research aircraft, they sought to precisely measure aerosol and cloud properties.

Scientists from Pacific Northwest National Laboratory participated in the leadership and instrument teams for the field study, called the Indirect and Semi-Direct Aerosol Campaign. "Our objective was to obtain a data set that will allow scientists to compare and contrast Arctic aerosol and cloud properties from the spring and fall," said Pacific Northwest National Laboratory's Dr. Beat Schmid, aerial vehicles program technical director for the campaign.

"It turns out that aerosols act as 'hosts' on which cloud droplets and crystals form," said Dr. Steven Ghan, a Pacific Northwest National Laboratory climate physicist and lead scientist for the campaign.

According to Ghan, the size and composition of these particles affect the type and longevity of the subsequent clouds. They also affect how much heat is reflected into space or absorbed by the clouds. Ultimately, these factors contribute to the climate of our planet.

In measuring the aerosol particles, one instrument, the SPLAT II, generated considerable excitement on its maiden voyage. Dr. Alla Zelenyuk designed SPLAT II at EMSL to measure fundamental chemical and physical properties of individual particles down to the nanoscale level. It's the most precise and sensitive instrument of its kind in the world.

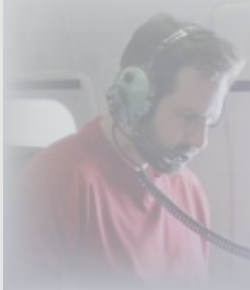
Early results show that certain kinds of airborne dust and metal particles tend to attract ice crystals, forming clouds.

I CAN SEE CLEARLY NOW

A new method, devised by scientists at Pacific Northwest National Laboratory, reduces cloud-induced glare by as much as ten-fold in some cases when satellites measure atmospheric pollution on cloudy days. Satellites monitor the pollution level in the atmosphere by measuring the amount of reflected sunlight. But, sunlight bouncing off clouds and tiny particles of air pollution "blinds" instruments trying to determine how much the sky is actually reflecting. Researchers found that combining measurements of reflected light at several wavelengths can eliminate the cloud effects, making measurements much more accurate, reducing uncertainties, and improving models of climate change and its impacts.

Kassianov EI, and M Ovtchinnikov. 2008. "On Reflectance Ratios and Aerosol Optical Depth Retrieval in the Presence of Cumulus Clouds." *Geophysical Research Letters* 35(6):L06807.

Sponsors: DOE's Office of Biological & Environmental Research; NASA



Sponsor: DOE's Atmospheric Radiation Measurement Program, with contributions by the Atmospheric Science Program, Environment Canada, and the National Research Council of Canada

Biological Sciences

At PNNL, scientists discovered that diverse bacteria produce an identical set of proteins known as the core proteome.

PROTEIN RESEARCH Uncovers Surprising Similarities in Diverse Bacteria

DIVERSE bacteria have more in common than previously thought. Bacteria as diverse as metal-reducing ***Shewanella oneidensis*** and bubonic plague-causing *Yersinia pestis* produce identical proteins, according to scientists from Pacific Northwest National Laboratory. Called the "core proteome," their research, done at EMSL, represents 6 years of gathering and evaluating proteomics measurements.

Knowing what proteins lie outside of the core proteome, and thus are unique to a bacteria, may present an opportunity to identify proteins that signal environmental stress and to identify targets to treat infectious diseases. For example, with the core proteome data, the team created a list of potential therapeutic targets for the disease-causing *Salmonella typhimurium.*

Callister SJ, LA McCue, JE Turse, ME Monroe, KJ Auberry, RD Smith, JN Adkins, and MS Lipton. 2008. "Comparative Bacterial Proteomics: Analytics of the Core Genome Concept." *PLoS ONE* 3(2):e1542.

Sponsors: DOE's Office of Biological & Environmental Research; National Institute of Health's National Institute of Allergy and Infectious Diseases and National Center for Research Resources

NOW IT'S MOLECULAR: New Understanding of Radiation Effects on Cells

New molecular data from scientists at Pacific Northwest National Laboratory indicate that dysfunctional mitochondria cause elevated reactive oxygen species (ROS) in the offspring of cells that survived radiation exposure. These results bring molecular-based evidence to a previously cell-based area of radiation research.

Mitochondria are the power generators in cells. ROS have important roles in cell signaling. However, environmental stress, such as radiation exposure, can cause ROS levels to increase through a mechanism that can be passed on to the progeny of cells that survive radiation exposure. Some of these cell lines with persistently high levels of ROS also exhibit sporadic changes in their DNA.

Radiation can also cause genomic instability that can be expressed in the daughters of irradiated cells. Genomic instability is thought to play a role in cancer development. Scientists do not yet understand the mechanisms of radiation-induced genome instability; however, many cell lines that exhibit chromosomal instability also show persistently elevated levels of oxidative stress. The Pacific Northwest National Laboratory team hypothesized that the genomic instability could result from ROS-induced DNA changes.

Previous work at the University of Maryland on radiation-induced genome instability showed that some unstable cells had persistently elevated levels of ROS likely caused by dysfunctional mitochondria. To further investigate this, scientists from Pacific Northwest National Laboratory, Washington State University, and the University of Maryland performed quantitative high-throughput mass spectrometry proteomics studies on samples enriched in mitochondrial proteins from three unstable cell lines and their stable, unirradiated parental cell line. Out of several hundred identified proteins, they collected sufficient data on 74 mitochondrial proteins to test for statistically significant differences in the abundance between unstable and stable cell lines.

Two of the unstable cell lines investigated had elevated ROS levels, and both lines showed significant differences in mitochondrial proteins when compared with control cell lines. The investigators suggested that this molecular data from these two lines complement their cellular data in suggesting that persistently elevated ROS levels resulted from mitochondrial dysfunction. The profiles of altered mitochondrial proteins are completely different for the two cell lines, which suggests that different types of dysfunction at the molecular level give rise to similar cellular phenotypes. The researchers now plan to investigate the mitochondrial proteome in genetically stable cell lines with elevated ROS and unstable cell lines with normal levels of oxidative stress.

Miller JH, S Jin, WF Morgan, A Yang, Y Wan, JS Peters, and DL Springer. 2008. "Profiling Mitochondrial Proteins in Radiation-induced Genome-unstable Cell Lines with Persistent Oxidative Stress by Mass Spectrometry." *Radiation Research* 169(9):700-706.

Sponsor: DOE's Office of Biological & Environmental Research

MOBILE ELEMENTS Identified in *Shewanella oneidensis* MR-1

The common microbe ***Shewanella oneidensis*** MR-1 quickly adapts to changing environments. Researchers at Pacific Northwest National Laboratory are studying how the microbe acquires or evolves new functions to eventually harness the microbe for cleaning up toxic waste.

In 2008, the team mapped nearly 300 mobile genetic elements of ***S. oneidensis*** MR-1. Mobile DNA or genetic elements that move throughout the organism can interrupt genes and prevent functional proteins. Also, they can acquire genetic material from other organisms that encode beneficial functions, such as resistance to toxic materials. In addition, the team identified 200+ mutated genes that might prevent the bacteria from producing needed proteins.

While the researchers' goal was to better annotate the genome of ***S. oneidensis*** MR-1, their efforts led to new discoveries about how this organism has evolved and continues to evolve in response to changes in the environment.

Romine MF, TS Carlson, AD Norbeck, LA McCue, and MS Lipton. 2008. "Identification of Mobile Elements and Pseudogenes in the *Shewanella oneidensis* MR-1 Genome." *Applied and Environmental Microbiology* AEM.02720-07.

Sponsor: DOE's Office of Biological & Environmental Research

SOPHISTICATED MONITORING Array to Address Mystery of Uranium Plume

Why does uranium contamination persist in groundwater under the south end of the Hanford Site, a former plutonium production complex, even after completing traditional cleanup activities?

To provide answers for DOE, Pacific Northwest National Laboratory has installed an innovative system for field experiments to better understand this complex site and to support future cleanup decisions. The elegant, yet adaptive, site allows scientists to study the effects of groundwater level, flow direction, and composition on uranium concentrations in groundwater, and uranium migration to the nearby Columbia River.

Photo credit: Bob Brawdy, *Tri-City Herald*

The site is one of three Integrated Field Research Challenge, or IFRC, locations established to investigate fundamental science issues important to contaminant fate and transport and groundwater remediation.

Positioned within a ~100-meter plot of contaminated ground, the array of 35 monitoring wells, each equipped with sophisticated instrumentation, is near where large volumes of contaminated wastewater were disposed. The waste originated from nuclear fuel fabrication facilities that supported the nation's weapons program decades ago. The Hanford IFRC allows researchers to perform injection experiments using waters of different temperature and composition pumped from other locations in the 300 Area groundwater plume. The variability permits scientists to probe and map migration pathways through the subsurface and examine factors that control uranium release from the historically contaminated sediments.

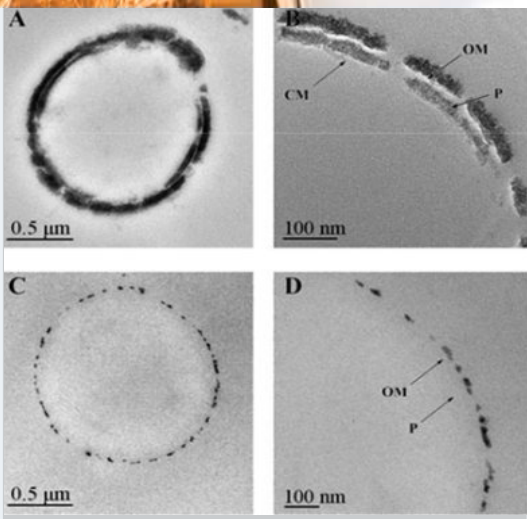
Hydrologic and geophysical characterization of the well field began in late August and continued through the fall. Scientists have started the first injection experiment, followed by a series of science experiments to study the fundamental workings of the local groundwater system.

The entire subsurface surrounding the wells will be comprehensively characterized to enable a complete accounting of the subsurface processes that contribute to the persistent groundwater contamination.

Enabling microbial research – Most of the monitoring wells in the IFRC well plot are about 60 feet deep. However, one well is 160 feet deep and penetrates all sediments above basalt. This well and core materials retrieved from it will allow PNNL's Dr. Allan Konopka and collaborators to identify microbes that are present in the subsurface and understand their contributions to uranium mobility.

Sponsor: DOE's Office of Biological & Environmental Research

Work by PNNL at the Integrated Field Research Challenge Site promises to provide one of the most comprehensive evaluations of the complex 300 Area subsurface along the river in more than 40 years.



To halt toxic technetium before it reaches the Columbia River, scientists are investigating microbes and their ability to transform technetium into a highly immobile form.

SHEWANELLA ONEIDENSIS Cytochromes Convert Contaminant

In the first study of its kind, researchers at Pacific Northwest National Laboratory investigated the mechanisms the bacterium *Shewanella oneidensis* uses to change the highly mobile radionuclide contaminant pertechnetate to a less soluble form. Experts think migration of significant quantities of pertechnetate in the subsurface is an issue for the Columbia River, which borders the Hanford Site. Changing pertechnetate to a less soluble form could greatly decrease its mobility.

The scientists found, using instrumentation at EMSL, that proteins on the microbes' surface that are known for electron transfer also play a crucial role in forming and localizing the reduced technetium nanoparticles. These are known as outer membrane c-type cytochromes. This finding demonstrates that *Shewanella* can use either organic matter or hydrogen as a source of electrons for pertechnetate reduction. The results of this work provide an important insight into the biomolecular mechanisms of electron transfer by *Shewanella* to pertechnetate.

Marshall MJ, AE Plymale, DW Kennedy, L Shi, Z Wang, SB Reed, AC Dohnalkova, CJ Simonson, C Liu, DA Saffarini, MF Romine, JM Zachara, AS Beliaev, and JK Fredrickson. 2008. "Hydrogenase- and Outer Membrane c-Type Cytochrome-facilitated Reduction of Technetium(VII) by *Shewanella oneidensis* MR-1." *Environmental Microbiology* 10(1):125-136.

Sponsors: DOE's Environmental Remediation Sciences Program; EMSL Scientific Grand Challenge; DOE's Genomics: GTL Program

Chemical & Materials Sciences

Multidisciplinary teams at PNNL have used careful characterization techniques and state-of-the-art instrumentation to provide insights into spintronics oxides, catalysts, and other materials.

CAREFUL CHARACTERIZATION Is Key

EXPERIMENTS can be difficult to interpret, especially in the area of semiconductor spintronics, which avoids many limitations of today's computer chips by carrying data via the spin of an electron rather than the charge. To make spintronics a reality, materials that are intrinsically magnetic at room temperature are needed. A highly controversial and heavily studied material for spintronics is cobalt-doped zinc oxide.

A team from Pacific Northwest National Laboratory synthesized and analyzed crystalline films of the material using sophisticated instruments at EMSL. They found that the material is not intrinsically magnetic, but rather that the magnetism comes from trace amounts of cobalt metal that form near the film's surface.

Kaspar TC, T Droubay, SM Heald, MH Engelhard, P Nachimuthu, and SA Chambers. 2008. "Hidden Ferromagnetic Secondary Phases in Cobalt-doped ZnO Epitaxial Thin Films." *Physical Review Letters B* 77:201303(R).

Sponsor: DOE's Office of Basic Energy Sciences

ROCK: Electrons Run Through It

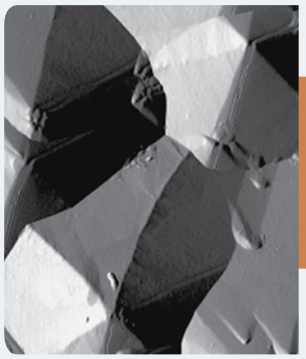
If the Flintstones had electricity, their wires might have been made of rock. New results published in *Science* show that a chunk of hematite can conduct electrons under certain chemical conditions. In addition, the current causes some mineral surfaces to build up while others degrade. These results, made possible by EMSL resources, with iron oxide could be important for water quality, soil evolution, and environmental cleanup.

"Considering iron as an important nutrient, the finding could help us understand how soils evolve from nutrient rich to nutrient poor," says lead investigator Dr. Kevin Rosso, a chemist at Pacific Northwest National Laboratory. "And it has implications for other common minerals such as pyrite and manganese oxides—even particles in the atmosphere."

Scientists have long known that electrons can travel through some iron oxides when a voltage is applied, but they have assumed that electrons stemming from chemical reactions alone won't move spontaneously through the mineral's bulk. That long-standing assumption has caused chemists to treat different faces of a hunk of mineral as independent entities that don't "communicate" with each other. The new results suggest otherwise.

Yanina SV and KM Rosso. 2008. "Linked Reactivity at Mineral-Water Interfaces through Bulk Crystal Conduction." *Science* 320(5873):218-222.

Sponsor: DOE's Office of Basic Energy Sciences



Researchers discovered that iron building up into pyramids on one face of an iron (III) oxide crystal sends electrons to another face, which slowly dissolves.

CAGING INDUSTRIAL Carbon Dioxide

Help Wanted: Hard working, selective material capable of quickly capturing carbon dioxide from busy exhaust stream. Must enjoy long hours and high stress. Apply at your local chemical plant.

Industries that use coal as a feedstock for manufacturing plastics, fertilizers, and other chemicals need such materials, and scientists at Pacific Northwest National Laboratory are working to oblige. Using computer simulations, researchers showed the crystal p-tert-butylcalix[4]-arene easily pulls in carbon dioxide. Their study, featured on the front cover of the March 3, 2008, issue of *Chemical Physics Letters*, shows the material easily holds several carbon dioxide molecules in each cavity.

The calixarene is composed of hollow cavities. Gaseous molecules, such as carbon dioxide, can slip into these cavities. To explore applying this material, researchers needed to know how carbon dioxide behaves as a guest molecule in p-tert-butylcalix[4]arene.

Simulating molecular behavior – To gain this knowledge, the researchers at PNNL began by designing computer simulations of carbon dioxide molecules interacting with p-tert-butylcalix[4]arene. The team set up the simulation for temperatures from 100K to 400K, which is slightly above the temperature at which water boils. Based on the molecules behavior during the simulation, the researchers calculated the rattling motion, or Einstein frequency, of the gas molecules.

The Einstein frequency told the researchers if the motion of the carbon dioxide was influenced by the rising temperature. If heat influences the motion, carbon dioxide could escape from the crystalline structure when the material is heated, a behavior that would need to be accounted for in potential applications.

Next, the team determined if the material could absorb carbon dioxide or if additional energy, which often increases the expense of the process, would be needed to coax the process along. The calculation, known as Gibbs free energy, showed it is easy for p-tert-butylcalix[4]arene to absorb carbon dioxide.

Daschbach JL, PK Thallapally, BP McGrail, and LX Dang. 2008. "Dynamics and Free Energies of CH_4 and CO_2 in the Molecular Solid of the p-tert-butylcalix[4]arene." *Chemical Physics Letters* 453(4-6):123-128. This research was featured on the front cover of the journal.

Sponsor: DOE's Office of Basic Energy Sciences

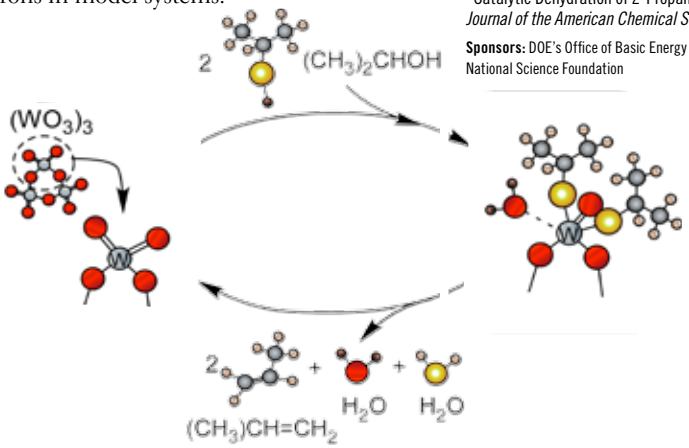
A MOLECULAR Makeover

Because catalysts reduce the amount of energy needed for reactions such as transforming alcohol into other molecules, the use of catalysts can save large amounts of power, potentially lowering industrial costs. So, researchers at Pacific Northwest National Laboratory's Institute for Interfacial Catalysis and the University of Texas at Austin are studying the behavior of the atoms and electrons in model systems.

In 2008 at EMSL, the researchers focused on trimming an alcohol into a smaller, more desirable molecule. The team figured out the steps that occur when a catalyst helps split an alcohol, generating water and a carbon-based molecule known as an alkene. Tungsten trioxide was selected to fill the role of model catalyst, and propanol, the alcohol. Using the catalyst cut—in half—the energy required to drive the reaction.

Kim YK, R Rousseau, BD Kay, JM White, and Z Dohnálek. 2008. "Catalytic Dehydration of 2-Propanol on $(WO_3)_3$ Clusters on TiO_2(110)." *Journal of the American Chemical Society* 130(15):5059-5061.

Sponsors: DOE's Office of Basic Energy Sciences; Robert A. Welch Foundation; National Science Foundation



USING NEGATIVITY to Get Attached

Electrons spur the chemical reaction between an acid and a base, according to the results published in *Science*. A team of experimental and theoretical chemists from three research institutions supported by computer programs at EMSL used a simple acid and base, hydrogen chloride and ammonia, to investigate how the two react to form the product ammonium chloride without help from their surroundings. The result revealed that supplying or removing an extra electron—not one already residing in the molecules—can make the reaction go from acid and base to neutral molecule or back again.

"The dream of chemists is to control chemical reactions," says coauthor Dr. Greg Schenter of Pacific Northwest National Laboratory. Adds coauthor Dr. Maciej Gutowski, formerly of Pacific Northwest National Laboratory and now at the Heriot-Watt University in Edinburgh, UK, "We want the reaction to happen when we want it to happen, and to go along a certain chemical pathway."

"We may be able to use this to get hydrogen out of the solid state, like in hydrogen storage materials," says Schenter. If so, that might lead to economic, safe, and practical hydrogen-fueled automobiles. The fundamental result could help illuminate biological reactions as well, such as when radiation damages DNA within cells, says coauthor Kit Bowen of Johns Hopkins University.

Eustis SN, D Radisic, KH Bowen, RA Bachorz, M Haranczyk, GK Schenter, and M Gutowski. 2008. "Electron-Driven Acid-Base Chemistry: Proton Transfer from Hydrogen Chloride to Ammonia." *Science* 319:936.

Sponsors: National Science Foundation; DOE's Offices of Basic Energy Sciences and Biological & Environmental Research

HALTING METHANE Squanderlust

The pipes that rise from oil fields, topped with burning flames of natural gas, waste fossil fuels and dump carbon dioxide into the air. In new work, Pacific Northwest National Laboratory researchers and their collaborators, using EMSL resources, identified the structure of a catalytic material that can turn methane into a safe and easy-to-transport liquid. The insight lays the foundation for converting excess methane into useful fuels and chemicals.

Why it matters – "There's a big interest in doing something with this 'stranded' methane other than flaring it off," said Dr. Chuck Peden of Pacific Northwest National Laboratory's Institute for Interfacial Catalysis. "An important thing researchers have struggled with is determining the structure of the active catalyst."

That catalyst—molybdenum oxide sitting on a zeolite mineral—converts methane gas into the more tractable liquid benzene. But, the process is not yet commercially viable. Scientists don't understand enough about the molecular details to improve the catalyst. Now, researchers at Pacific Northwest National Laboratory and the Chinese Academy of Sciences' Dalian Institute of Chemical Physics have worked out some of the details that will help researchers develop an efficient catalyst.

Working with China – This work resulted in the first publication to come out of the International Consortium for Clean Energy, a collaboration between Pacific Northwest National Laboratory, the Dalian Institute of Chemical Physics, and China's Institute of Coal Chemistry.

Zheng H, D Ma, X Bao, JZ Hu, JH Kwak, Y Wang, and CHF Peden. 2008. "Direct Observation of the Active Center for Methane Dehydroaromatization Using an Ultra-High Field ^{95}Mo NMR Spectroscopy." *Journal of the American Chemical Society* 130(12):3722-3723.

Sponsors: Natural Science Foundation of China; DOE's Office of Basic Energy Sciences

Computational Sciences & Mathematics

To trap or treat contaminants in groundwater, researchers developed a computational model that provides a more realistic view of how the contaminants are mixing.

NEW MATHEMATICAL Model Provides Better Data on Subsurface Mixing

NEW DISCOVERIES and development of advanced multi-scale mathematical modeling methods are helping to solve DOE's groundwater remediation issue. To trap or treat strontium or other contaminants in the soil, researchers need to know how the contaminated water behaves in the complex subsurface. So, researchers from Pacific Northwest National Laboratory, University of California at San Diego, and Idaho National Laboratory developed a computational model that provides a more realistic view of how the contaminants are mixing. The new model treats the different types of mixing, advective and diffusive, separately. Classical advection-dispersion models lump the two mixing types together, overestimating key parameters. This new model and the improved understanding it brings is critical for remediating contaminated sites, such as the plutonium production site in southeastern Washington State.

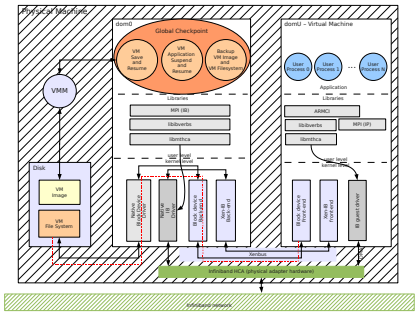
Tartakovsky AM, DM Tartakovsky, and P Meakin. 2008. "Stochastic Langevin Model for Flow and Transport in Porous Media." *Physical Review Letters* 101:044502.

Sponsor: DOE's Advanced Scientific Computing Research and Environmental Management Science Programs

COLLABORATION FOCUSES on Fault Tolerance for Supercomputers

Pacific Northwest National Laboratory is leading a collaboration with Ohio State University and Oak Ridge National Laboratory to make supercomputers more tolerant of faults. In supercomputers built with thousands of components, the failure of a single component, such as a processor or a hard disk, can require a scientist to re-run the entire calculation, an expensive proposition in terms of time and money.

To combat these costs, the collaborators are taking a two-pronged approach on this 3-year project. First, they have developed a virtual machine-based technique to perform periodic checkpoints of the state while the application is running. In the event of a fault, the computation is restarted from the most recent checkpoint, losing only hours of time, not weeks. Most importantly, this approach does not require any change to the application itself.



The team designed the architecture of a virtualization-based fault-tolerance mechanism.

Also, they are designing a model that organizes the computation as a set of tasks. Each task modifies the regions of global data defined in the task description. In the event of a failure, only the failed node is restarted from a checkpoint. The task descriptions are used to identify the updates to data stored in the failed node since the last checkpoint. The relevant tasks are re-executed; the updates are stored in the restarted node, bringing it up to date. The remaining processes are not restarted from the previous checkpoint and, other than cooperating to identify tasks to be re-executed, continue executing. Unlike the checkpoint-based approach, the work lost due to a fault is only proportional to the number of faults encountered.

The team plans to test these two approaches on supercomputers at DOE's EMSL.

Scarpazza DP, P Mullaney, O Villa, F Petrini, V Tipparaju, DML Brown Jr, and J Nieplocha. 2007. "Transparent System-level Migration of PGAS Applications using Xen on Infiniband." In *Proceedings IEEE Cluster 2007*, pp 74-83. Austin, Texas.

Tipparaju V, M Krishnan, F Petrini, J Nieplocha, and BJ Palmer. 2007. "Towards Fault Resilient Global Arrays." *In Parallel Computing: Architectures, Algorithms and Applications Proceedings*, pp. 347-354, Amsterdam, The Netherlands.

Sponsor: DOE's Advanced Scientific Computing Research

DATA INTENSIVE Computing for Complex Biological Systems

Super Plant! Mighty Microbe! While these are silly names fit for cartoon characters, plants and microbes could play vital roles in providing low-cost fuel and cleaning up industrial waste. However, to help these biological systems fill these roles requires a deep understanding of their behavior, right down to their DNA. And, this is where a key problem starts. Many of today's computer programs have a hard time keeping up with the massive data created by analyzing biological systems.

Tackling this problem is BioPilot, a joint project between Pacific Northwest National Laboratory and Oak Ridge National Laboratory that relied on EMSL resources. The BioPilot researchers are providing the computer tools necessary for analysis, including predictive modeling and simulation.

Visualizing protein clusters lets users interactively browse complex relationships between organisms.

For example, BioPilot's researchers built ScalaBLAST. This sophisticated "sequence alignment tool" divides the work of analyzing biological data into manageable fragments that can be run concurrently on massively parallel computers. Without it, the analyses would run no faster on the supercomputer than on a personal computer. ScalaBLAST means large problems can be solved in hours, rather than weeks.

A summary of the BioPilot project and the software developed, including ScalaBLAST, are available at https://www.biopilot.org.

Sponsor: DOE Advanced Scientific Computing Research

RESEARCHERS Look to Make Supercomputers Energy Efficient

Data centers are the aluminum smelters of the 21st century, notes Pacific Northwest National Laboratory Dr. Andrés Márquez, director of the Energy Smart Data Center project at EMSL. Large data centers and supercomputers are being built near dams and other power sources because the centers require so much power. For example, new extreme-scale supercomputers can use as much energy as about 20,000 homes.

To design computing centers that are more energy efficient, researchers at Pacific Northwest National Laboratory and their collaborators are first determining how much energy is used for powering the banks of processors, cooling the computers, and operating the facility.

A valuable tool in obtaining these metrics is a custom software known as FRED, built by scientists at Pacific Northwest National Laboratory. This software measures parameters such as temperatures and power usage. With

FRED, scientists gather metrics on new energy-saving cooling systems and other technologies. Pacific Northwest National Laboratory and The Green Grid are using FRED and other tools to measure productivity; that is, power used versus time needed to get your answer.

With the metrics they and others have gathered, Pacific Northwest National Laboratory researchers are helping to develop fair and efficient industrial or regulatory energy standards for data centers.

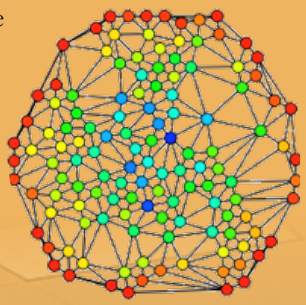
Sponsor: DOE's National Nuclear Security Administration

SUPERCOMPUTER SEEKS Software for Data Intensive Computing

Researchers at a multi-institutional center are developing specialized software to aid multithreaded supercomputers in solving problems ranging from power grid stability to complex biological networks. Multithreaded supercomputers access data differently than traditional parallel systems, which can significantly improve performance for certain applications. But, old software won't run on the multithreaded hardware any more than a PC program will run on a Macintosh®. So, the Center for Adaptive Supercomputing Software, a joint project between Pacific Northwest National Laboratory, Cray, Inc., the Georgia Institute of Technology, and Sandia National Laboratories, is developing innovative software for advanced supercomputers.

Cray machines are built with so-called "multithreaded processors" that enable overlapping of data transfers with processing. The Center is focusing on applications for the multithreaded Cray XMT.

For example, the researchers have applied the Cray XMT to the cyber security domain involving large sets of network traffic data. Analysis was performed to detect anomalies in snippets of Internet communication between computers to locate and characterize network attacks, and to help predict and mitigate future attacks.



Complex social networks can be visualized and analyzed on the Cray XMT system.

Sponsor: Department of Defense

SCIENTIFIC APPLICATION Partnership—Enhances Analysis of Global Cloud-Resolving Models

In collaboration with the developers of the open-source NetCDF Operators and using EMSL resources, researchers at Pacific Northwest National Laboratory added capabilities for processing geodesic grid data and optimized performance to support manipulating data sets consisting of many files of tens to hundreds of gigabytes in size. The new tools enhance the ability to analyze data generated by the Global Cloud-Resolving Model.

The GCRM portrays the entire globe on a fine enough scale (2-4 km) to accurately show cloud behavior. The behavior of clouds is widely agreed to be a major source of uncertainty in existing models.

Researchers will use the model's results to increase the accuracy of climate models that can be run more efficiently at coarser resolutions to simulate longer periods of time. To reach this scale, the model uses a geodesic grid. In this grid, each cell on the globe is roughly equal in size while having the same number of neighbors.

The Community Access to GCRM Data and Analyses project has enhanced the popular NetCDF Operators data manipulation software to support data that is generated on the geodesic grid. Working with the NetCDF Operators team, Pacific Northwest National Laboratory researchers identified a major performance bottleneck. Breaking this bottleneck improved the performance by a factor of up to 500 times for certain operations.

Sponsor: DOE's Advanced Scientific Computing Research

Awards & Honors

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CONTRIBUTIONS to Nobel Peace Prize for Climate Change Awareness

MORE THAN 20 SCIENTISTS from Pacific Northwest National Laboratory contributed to the Nobel Peace Prize awarded to Al Gore and the Intergovernmental Panel on Climate Change. Through their involvement in the IPCC, the following researchers are shaping how the world views climate change: **Antoinette Brenkert, William Chandler, Leon Clarke, James Dooley, Sylvia Edgerton, James Edmonds, Meredydd Evans, Steve Ghan, Tony Janetos, Nels Laulainen, Ruby Leung, Elizabeth Malone, Richard Moss, Hugh Pitcher, Steve Rayner, Kenneth Richards, Norman Rosenberg, Paul Runci, Michael J. Scott, and Steven Smith.**

These people served as convening authors, lead authors, review editors, and expert reviewers on IPCC reports. Seminal research from Pacific Northwest National Laboratory is cited throughout the reports. Also, these scientists contributed intellectual frameworks that influenced IPCC assessments and the broader climate change community in areas as diverse as integrated assessment, technology's role in mitigation, carbon dioxide capture and storage, and social science contributions in addressing climate change challenges.

In a press release following the award announcement, IPCC chairman Rajendra Pachauri stated, "This is an honour that goes to all the scientists and authors who have contributed to the work of the IPCC."

JULIA LASKIN Received Major Early Career Awards

Dr. Julia Laskin accepted DOE's Office of Science and the Presidential Early Career Award for Scientists and Engineers and the Biemann Medal, the highest honor granted to a young scientist by the American Society for Mass Spectrometry. These awards recognize her contributions to understanding the activation, fragmentation, and deposition of large molecules when they collide with surfaces. Her research directly advances DOE's goals to develop biomaterials and biological processes for clean energy production, as well as to create biologically inspired systems, novel catalysts, and biosensors.

BRUCE KAY Accepted National Science Advisory Committee Seat

As part of the 25-member Basic Energy Sciences Advisory Committee, Dr. Bruce D. Kay provides recommendations to DOE's Office of Science on research and facility priorities. In addition, he advises on the appropriate balance among scientific disciplines and collaboration among research institutes and industries.

Kay was selected for his internationally recognized leadership in the chemical sciences. A Fellow of the American Physical Society, AVS, and the American Association for the Advancement of Science, Kay has written more than 120 journal articles and technical reports and given nearly 200 invited lectures around the world.

BILL WEBER Named Materials Research Society Fellow

Dr. Bill Weber was selected as an inaugural Fellow in the Materials Research Society. This is the first year, since being founded in 1973, that the society has honored notable members for their contributions to advancing materials research. Weber received this honor for his "seminal contributions, leadership, mentoring and innovative research on defects, defect properties, ion-solid interactions, radiation effects and models of radiation damage processes in glasses and ceramics."

"Career-wise, I almost grew up with the MRS," said Weber with a smile, "and to be selected the first time they had fellows was a significant recognition."

MOE KHALEEL Elected ASME Fellow

Dr. Moe Khaleel was selected as a Fellow of the ASME. Khaleel was recognized for his exceptional engineering achievements and contributions to the engineering profession. He serves as the national coordinator for modeling activities associated with solid oxide fuel cells for the Solid Energy Conversion Alliance, and is a member of the Industry Advisory Board of Edison Welding Institute. He has published more than 100 technical articles and won the Federal Laboratory Consortium for Excellence in Technology Transfer of superplastic forming of aluminum and the ASME International McGrattan Literature Award.

CÉSAR IZAURRALDE
Elected Soil Science Fellow

Dr. César Izaurralde received the highest honor bestowed by the Soil Science Society of America; he was named a Fellow by the society. The society is dedicated to the conservation and wise use of natural resources to produce crops while maintaining and improving the environment. Izaurralde was selected because of his outstanding achievements in leadership, professional service, and research in sustainable agriculture, climate change impacts and adaptation, and climate change mitigation through soil carbon sequestration and reduced soil emissions of nitrous oxide.

MICHEL DUPUIS
Elected Physics Society Fellow

Dr. Michel Dupuis was selected as a Fellow in the American Physical Society. The APS is a leading voice for physics, including chemical physics, in both the U.S. and international scientific communities. Dupuis received this honor for his outstanding contributions to the development of electronic structure methods and computer codes for simulating molecular properties and reactivity.

SEVEN JOINED
Ranks of AAAS Fellow

Seven members of the Fundamental & Computational Sciences Directorate were elected Fellows of the American Association for the Advancement of Science. They were recognized at the AAAS national meeting in Boston in February 2008:

Dr. James Edmonds– *"distinguished contributions to the field of climate change economics, particularly modeling and analyzing interactions of energy, the economy, technology, carbon cycle, and climate."*

Dr. Richard Kouzes– *"distinguished contributions to defining the technical basis and implementation of nuclear radiation detection systems for applications to homeland security, nuclear structure and neutrino physics."*

Dr. David Koppenaal– *"pioneering development of advanced techniques for analytical atomic/isotopic mass spectrometry and for distinguished scientific leadership."*

Dr. Richard Moss– *"leadership in national and international assessments of climate change and development of the nation's long-term plan for integrated research to address this problem."*

Dr. Jun Liu– *"distinguished contributions to the development, understanding and commercialization of self-assembled functional nanoporous materials, and to the development of environmentally friendly solution approaches for oriented nanostructures."*

Dr. Lai-Sheng Wang– *"distinguished and innovative contributions to the field of atomic clusters and for pioneering work on gaseous multiply-charged anions."*

Dr. Tony Janetos– *"distinguished contributions in ecology and biology of particular relevance to environmental policy."*

The LAST WORD

In these pages you saw some of the most significant accomplishments in the biological, chemical, computational, environmental, and materials sciences by **Fundamental & Computational Sciences Directorate** scientists in fiscal year 2008. I am proud of their potential to transform our ability to understand or control chemical, physical, and biological processes and to impact the most important challenges in energy, national and homeland security, and environmental sustainability.

Please don't hesitate to contact me or one of the individuals listed at right for more information or if you are interested in collaborating with us.

Douglas Ray, Ph.D.
Associate Laboratory Director
Fundamental & Computational Sciences Directorate
Pacific Northwest National Laboratory

About the Cover: *In 2008, Dr. Alla Zelenyuk operated SPLAT II, the Single Particle Laser Ablation Time-of-Flight mass spectrometer, to measure the characteristics of tiny aerosol particles in the atmosphere that contribute to climate change.*

About Pacific Northwest National Laboratory

Pacific Northwest National Laboratory is a Department of Energy Office of Science national laboratory where interdisciplinary teams advance science and technology and deliver solutions to America's most intractable problems in energy, national security and the environment.

PNNL employs 4,200 staff, has a $850 million annual budget, and has been managed by Ohio-based Battelle since the lab's inception in 1965.

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