Pacific Northwest
NATIONAL LABORATORY

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FY 2010

KEY ACCOMPLISHMENTS

Fundamental & Computational Sciences Directorate

Atmospheric Sciences & Global Change

Scientists found a connection between the size of dust particles in clouds and the possibility of precipitation. This finding will improve the accuracy of climate prediction models.

Clouds + Mineral Dust = **RAIN**

A critical link between the size of dust particles in clouds and their likelihood to produce rain was found by a team of atmospheric scientists, including Xiaohong Liu of Pacific Northwest National Laboratory. The number of dust particles larger than 0.5 μm in diameter had a close correlation with the number of ice nuclei, which are known to form seeds for rain droplets in clouds. This relationship allowed the team to develop a more accurate parameterization to predict ice nuclei numbers in clouds, reducing uncertainty by a factor of 100.

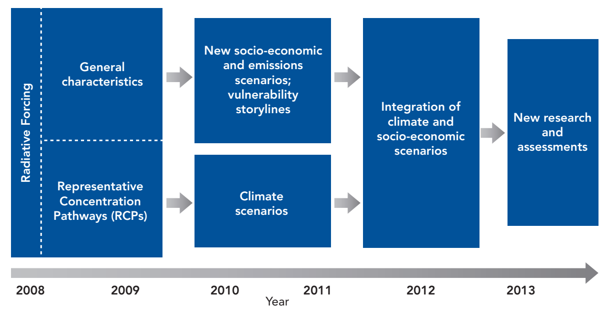
Results from this study provide a more accurate picture of how ice nuclei form and at what temperature, increasing the accuracy of climate models. Past predictions were based on an assumption of 10 times more ice nuclei present in clouds. This breakthrough follows a 14-year investigation drawing on field studies from the Amazon Rainforest in Brazil to the Arctic Circle.

DeMott PJ, AJ Prenni, X Liu, SM Kreidenweis, MD Petters, CH Twohy, MS Richardson, T Eidhammer, and DC Rogers. 2010. "Predicting Global Atmospheric Ice Nuclei Distributions and Their Impacts on Climate." *Proceedings of the National Academy of Sciences of the United States of America* **107**(25), 11217-11222. DOI: 10.1073/pnas.0910818107.

Sponsors: Department of Energy, Office of Biological & Environmental Research; Atmospheric System Research Grant; NASA's Modeling and Analysis Program; and National Science Foundation

FUTURE CLIMATE SCENARIOS: Getting a Better Look at the Big Picture

An international team of climate scientists, including Pacific Northwest National Laboratory's Richard Moss, Jae Edmonds, Kathy Hibbard, Steve Smith, and Allison Thomson, designed an approach to modeling the earth's climate future. The approach more tightly links analyses of greenhouse gas emissions, climate projections, impacts of climate change, and human decisions, such as increasing energy efficiency. The new approach will influence the next international scientific assessment by the Intergovernmental Panel on Climate Change and provide a framework for individual scientific studies.



Until now, scenarios were developed and applied in a linear causal chain. The alternative "parallel" approach integrates the models to study interactions of human and natural influences on climate.

Using this approach, climate model and socioeconomic data will be available more rapidly to those modeling the potential impacts of climate change. Researchers will be better able to diagnose how different models treat feedbacks that could further amplify climate change.

Moss RH, JA Edmonds, K Hibbard, M Manning, SK Rose, DP van Vuuren, TR Carter, S Emori, M Kainuma, T Kram, G Meehl, J Mitchell, N Nakicenovic, K Riahi, SJ Smith, RJ Stouffer, A Thomson, J Weyant, and TJ Wilbanks. 2010. "The Next Generation of Scenarios for Climate Change Research and Assessment." *Nature* **463**, 747-756.

Sponsors: Department of Energy Office of Science and many other funding agencies

Even **SOIL** Feels the **HEAT**

As the earth grows warmer, plants and microbes in the soil release more carbon dioxide, according to scientists at Pacific Northwest National Laboratory. "There's a big pulse of carbon dioxide coming off of the surface of the soil everywhere in the world," said ecologist Ben Bond-Lamberty of PNNL. "We weren't sure if we'd be able to measure it going into this analysis, but we did find a response to temperature."

Bond-Lamberty and Allison Thomson, working at the Joint Global Change Research Institute, made this discovery based on a survey of 439 soil respiration studies published between 1989 and 2008. The analysis of past studies reveals that soil respiration has increased about one-tenth of 1% per year since 1989. Understanding the source and mechanisms of that increased soil respiration can advance our knowledge about global climate change.

Bond-Lamberty B and A Thomson. 2010. "Temperature-Associated Increases in the Global Soil Respiration Record." *Nature* **464**, 579-582.

Sponsors: Pacific Northwest National Laboratory and the Department of Energy, Office of Biological and Environmental Research

Better-than-new Lidar Provides **24/7 ATMOSPHERIC AEROSOL DATA**

Perplexing software and hardware problems with the ground-based Raman lidar were solved by a team of researchers from eight institutions led by Pacific Northwest National Laboratory. Not only did they fix the problem, but the instrument now performs better than it did when it was new. Lidar, similar to radar which calculates distances by bouncing radio waves off of objects, measures how light bounces off aerosols in the sky.

The team upgraded the electronics and other hardware. They also modified the raw data processing algorithm, which resulted in a significant improvement in aerosol data products as well. By calibrating all measurements to consistent standards, the data can help reduce scientific uncertainties in computer models used to simulate climate change.

Schmid B, CJ Flynn, RK Newsom, DD Turner, RA Ferrare, MF Clayton, E Andrews, JA Ogren, RR Johnson, PB Russell, WJ Gore, and R Dominguez. 2009. "Validation of Aerosol Extinction and Water Vapor Profiles from Routine Atmospheric Radiation Measurement Program Climate Research Facility Measurements." *Journal of Geophysical Research* **114**, D22207. DOI:10.1029/2009JD012682.

Sponsors: Department of Energy, Office of Biological and Environmental Research and NASA Radiation Science and Airborne Science Programs

Oh, the Secrets **ICE CRYSTALS** Will Tell!

The campaign: Scientists from Pacific Northwest National Laboratory and other organizations undertook a 5-month mission to squeeze the secrets out of ice crystals in cirrus clouds. A primary objective of the SPARTICUS, or Small Particles in Cirrus, campaign was to determine if the new probes treat ice crystals more gently than previous probes, which shattered the crystals during sampling.

Why it matters: Ice crystals reflect a portion of the solar energy that reaches the earth, and absorb energy emitted by the earth, making cirrus clouds the only cloud type that warms the atmosphere. Accurate information about crystal shape and size will contribute to improving our understanding of the effects of clouds in a warming climate.

Sponsor: Department of Energy ARM Climate Research Facility

In Search of **HAZE**

A team of Pacific Northwest National Laboratory scientists led an intensive month-long field study to examine the effects of carbonaceous aerosols, often seen as haze, on climate. The Carbonaceous Aerosols and Radiative Effects Study–or CARES–field campaign examined the evolution and radiative effects of aerosol particles emitted from sources such as exhaust fumes, wildfires, and agricultural burning sources. PNNL's leadership included Rahul Zaveri as lead scientist, Beat Schmid handling the aircraft operations, and Will Shaw running the ground site operations. The research team is evaluating data gained from the study to improve climate modeling as part of PNNL's "measurements-to-models" integrated approach to climate research.

Data generated by CARES will help create a better understanding of how urban and natural atmospheric particles impact climate. CARES data will help scientists model the effects of aerosols and particles for improved future research and enhanced computer models of global climate change.

Zaveri R. 2010. "CARES: Carbonaceous Aerosol and Radiative Effects Study Science Plan." Available at http://campaign.arm.gov/cares/.

Sponsors: Department of Energy, Biological & Environmental Research and the Environmental Molecular Sciences Laboratory

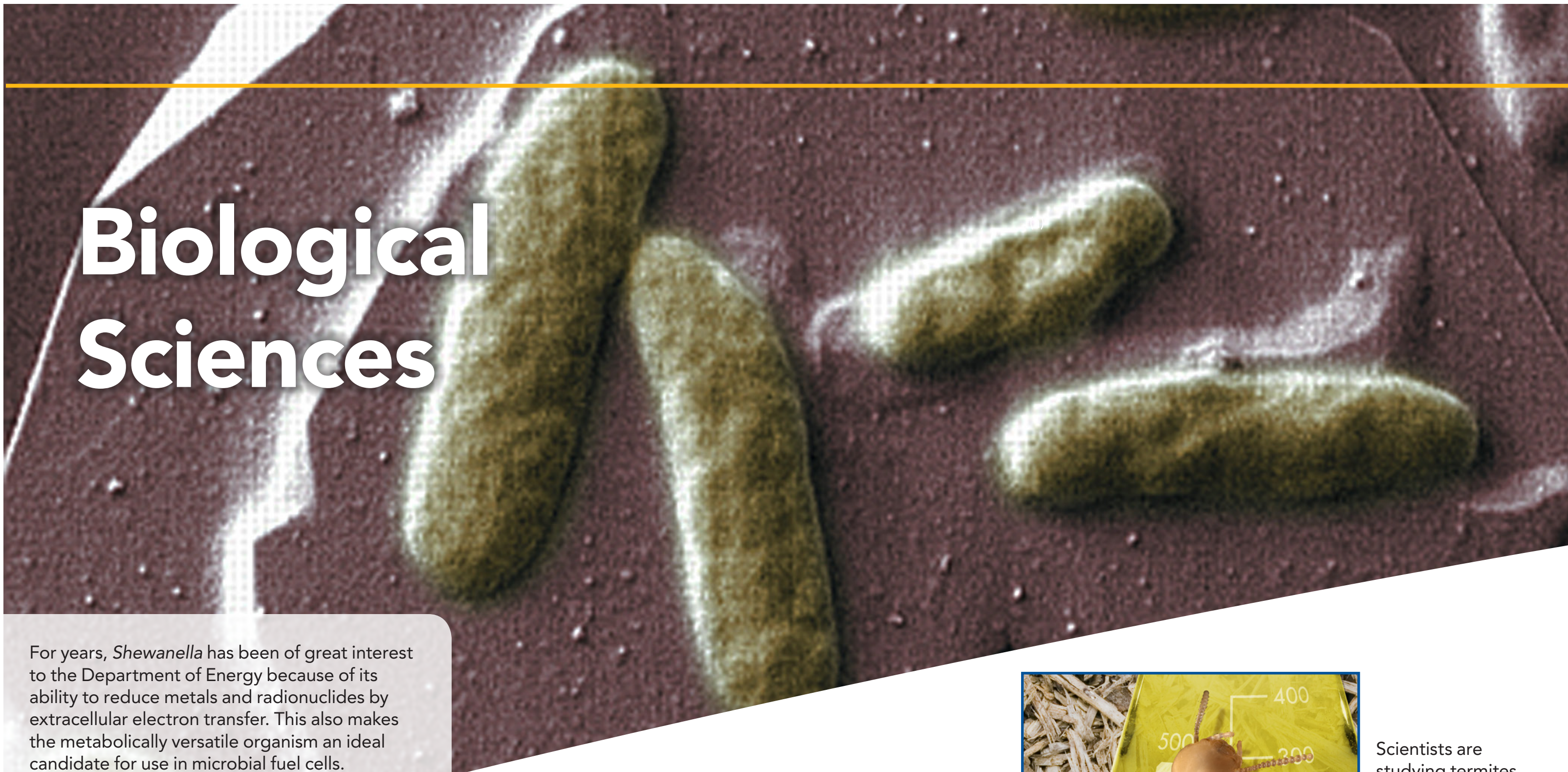
Accurate data is the cornerstone of predictions about climate change. Much of the uncertainty in climate projections is due to the complexity of clouds, aerosols, and cloud-aerosol interactions. Improving the accuracy of lidar data improves the accuracy of projections.

Rahul Zaveri, lead scientist for CARES, stands next to the G-1 Aircraft. The aircraft is equipped with a new ultra-high sensitivity aerosol spectrometer, which measures atmospheric aerosol particles.

CHIEF SCIENTIST ADDRESSES CONGRESS on Geoengineering

Phil Rasch testified on climate change geoengineering to the U.S. House of Representatives Committee on Science and Technology in Washington, D.C., on February 4, 2010. He was asked to address the Subcommittee on Energy and Environment on Solar Radiation Management during a hearing entitled "Geoengineering II: The Scientific Basis and Engineering Challenges."

In his testimony, Rasch advocated conducting scientific research to understand approaches and implications of geoengineering, particularly as they relate to a deeper understanding of the dynamic processes and interactions of aerosols and cloud systems.



Biological Sciences

For years, *Shewanella* has been of great interest to the Department of Energy because of its ability to reduce metals and radionuclides by extracellular electron transfer. This also makes the metabolically versatile organism an ideal candidate for use in microbial fuel cells.

MICROBE'S METABOLIC POTENTIAL

Knowing an organism's metabolism can provide insights into how it uses its resources. These insights can then enable tweaking the metabolism to enhance the microbe's use of these resources in beneficial ways, such as to reduce contamination in soil or to produce biofuels.

Collaborators from Pacific Northwest National Laboratory, Burnham Institute for Medical Research, University of Wisconsin-Madison, and Dartmouth College used computational and high-throughput experimental approaches to reconstruct the metabolic network of *Shewanella oneidensis*. This has enabled the team to develop a predictive understanding of the microbe's metabolism.

Pinchuk GE, EA Hill, OV Geydebrekht, J De Ingeniis, X Zhang, A Osterman, JH Scott, SB Reed, MF Romine, A Konopka, AS Beliaev, JK Fredrickson, and JL Reed. 2010. "Constraint-Based Model of *Shewanella oneidensis* MR-1 Metabolism: A Tool for Data Analysis and Hypothesis Generation." *PLoS Computational Biology* **6**(6):e100082. DOI:10.1371/journal.pcbi.1000822.

Sukovich DJ, JL Seffernick, JE Richman, KA Hunt, JA Gralnick, and LP Wackett. 2010. "Structure, Function, and Insights into the Biosynthesis of a Head-to-Head Hydrocarbon in *Shewanella oneidensis* Strain MR-1." *Applied Environmental Microbiology* **76**(12):3842-3849. DOI:10.1128/AEM.00433-10.

Sponsor: Department of Energy, Office of Biological and Environmental Research, Genomic Science Program

It Takes "Guts" to Explore the **NEXT PROTEOMICS FRONTIER**

In the quest to find new sources of biofuel, researchers are studying one of the most efficient bioreactors on earth: the termite. The same insect that causes distress to homeowners also provides scientists with a fascinating area of study: the symbiotic microbial community that enables the termite to digest wood cellulose.

Researchers at Pacific Northwest National Laboratory analyzed the metaproteome—all proteins—of the bacterial community that lives in the hindgut paunch segment of the wood-feeding "higher" termite (*Nasutitermes*). Their goal was to define the contribution and sources of enzymes from the community to the insect.

Scientists are studying termites to understand how the microbial communities that reside in their gut could help turn wood into fuel.

Initially, they believed this information would lead to identifying new and novel cellulases, which in turn could provide raw materials for the synthesis of ethanol. While such insights remain elusive, the team gained insights into the necessary associations of this symbiotic system, advancing understanding of the microbial community function in the termite gut and pointing to important interactions in the degradation of wood products.

Burnum KE, SJ Callister, CD Nicora, SO Purvine, P Hugenholtz, F Warnecke, RH Scheffrahn, RD Smith, and MS Lipton. 2010. "Proteome Insights into the Symbiotic Relationship between a Captive Colony of *Nasutitermes corniger* and Its Hindgut Microbiome." *The ISME Journal.* DOI:10.1038/ismej.2010.97.

Sponsor: Department of Energy, Office of Biological and Environmental Research, Genomic Science Program

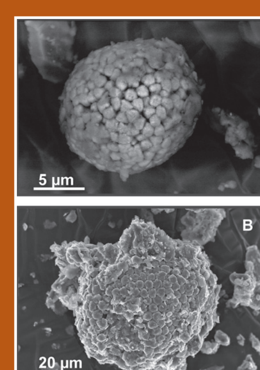
UNIQUE URANIUM SOURCE in Naturally Bioreduced Sediment

Framboidal pyrites or fool's gold in silty sediment where microbes reside may initially sequester subsurface uranium and then serve as a long-term source under the right conditions, according to a study by Pacific Northwest National Laboratory and Argonne National Laboratory. The study provides the first-ever evidence of a useful pyrite mineral formation within the sample.

At sites around the country, including former nuclear weapons sites, uranium has contaminated sediments and groundwater. Understanding how and when uranium migrates may aid in creating remediation approaches.

Qafoku N, RK Kukkadapu, JP McKinley, BW Arey, SD Kelly, CM Wang, CT Resch, and PE Long. 2009. "Uranium in Framboidal Pyrite from a Naturally Bioreduced Alluvial Sediment." *Environmental Science & Technology* **43**(22): 8528-8534. DOI:10.1021/es9017333.

Sponsors: Department of Energy, Office of Biological and Environmental Research, Subsurface Biogeochemical Research



Naturally bioreduced sediments reveal insights into the long-term persistence of uranium in groundwater.

Scientists Show How Bacteria Move **ELECTRONS ACROSS A MEMBRANE**

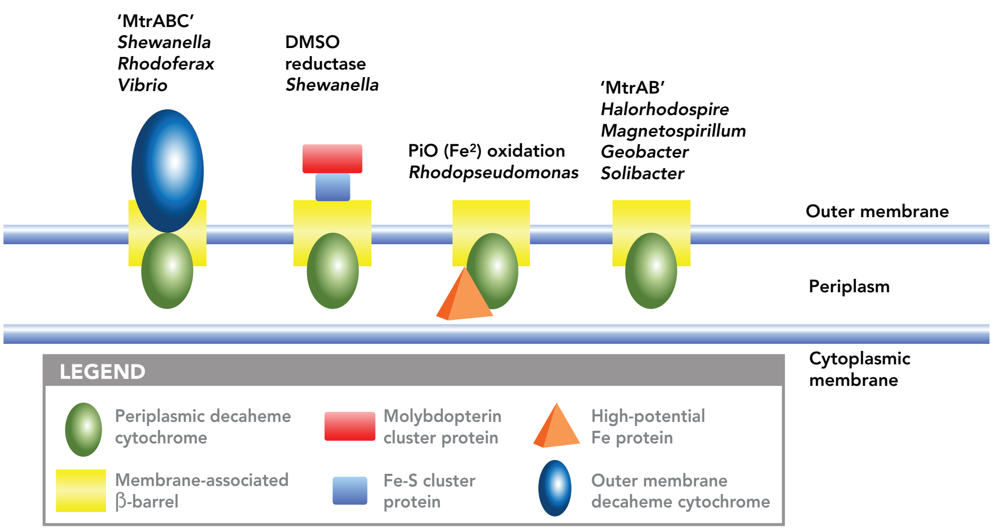
For the first time, scientists demonstrated how some bacteria can transfer electrons across a membrane to the cell exterior, allowing them to "breathe" metals. The scientists from the University of East Anglia, Pacific Northwest National Laboratory, and Pennsylvania State University showed that these iron-respiring bacteria link the cycling of iron and carbon in subsurface and surface sediments and can catalyze the immobilization of subsurface contaminants, such as uranium.

The researchers described the protein complex—and its electrochemical properties—from *Shewanella oneidensis*, a bacterium renowned for its diverse metabolism and ability to immobilize certain radioactive contaminants. This research demonstrated a novel outer membrane-spanning electron transfer system that enables the proteins MtrA (inward facing) and MtrC (outward facing) to embed sufficiently within a third transmembrane protein, MtrB, to allow electron transfer to take place between them.

"This is an exciting advance in our understanding of bacterial processes in the earth's subsurfaces," said David Richardson of UEA's School of Biological Sciences, who is leading this research effort.

Hartshorne RS, CL Reardon, DE Ross, J Nuester, TA Clarke, AJ Gates, PC Mills, JK Fredrickson, JM Zachara, L Shi, AS Beliaev, MJ Marshall, M Tien, SL Brantley, JN Butt, and D Richardson. 2009. "Characterization of an Electron Conduit Between Bacteria and the Extracellular Environment." *Proceedings of the National Academy of Sciences of the United States of America* **106**(52):22169-22174.

Sponsors: Environmental Molecular Sciences Laboratory Biogeochemistry Grand Challenge and Department of Energy, Office of Biological and Environmental Research, Climate and Environmental Sciences Division



For the first time, scientists demonstrated how *Shewanella oneidensis* move electrons across a membrane to the cell's exterior, allowing the microbes to "breathe" metals.

PROTEOMIC PROFILING of Low-Dose Radiation Effects on Human Skin Cells

In the most comprehensive analysis of its type published to date, scientists at Pacific Northwest National Laboratory found that exposing human skin fibroblasts to low doses of ionizing radiation regulates phosphorylation of proteins involved in a wide range of biological processes. In short, the body can sense low doses of radiation and activate the cell signaling pathways needed to respond to any induced cellular damage.

While a number of the affected proteins have been implicated in various human diseases including cancer, further studies are needed to determine if these changes result in increased disease risk or whether they are part of normal cellular defense mechanisms that kick in to prevent disease from occurring.

Yang F, KM Waters, JH Miller, MA Gritsenko, R Zhao, X Du, EA Livesay, SO Purvine, ME Monroe, DG Camp II, RD Smith, and DL Stenoien. 2010. "Phosphoproteomic Profiling of Human Skin Fibroblast Cells Reveals Pathways and Proteins Affected by Low Doses of Ionizing Radiation." *PLoS ONE* (Accepted).

Sponsor: Department of Energy, Office of Biological and Environmental Research, Low Dose Radiation Research Program

Thousands of **NEW PROTEINS DISCOVERED** in Spinal Fluid

Using integrated proteomics resources, a team of researchers from Pacific Northwest National Laboratory, University of Medicine and Dentistry of New Jersey, and Uppsala University, Sweden identified 2,630 proteins in the clear fluid that protects the brain and spinal cord. This discovery nearly triples the number of proteins known to exist in spinal fluid. Slightly more than half of the proteins were not found in blood.

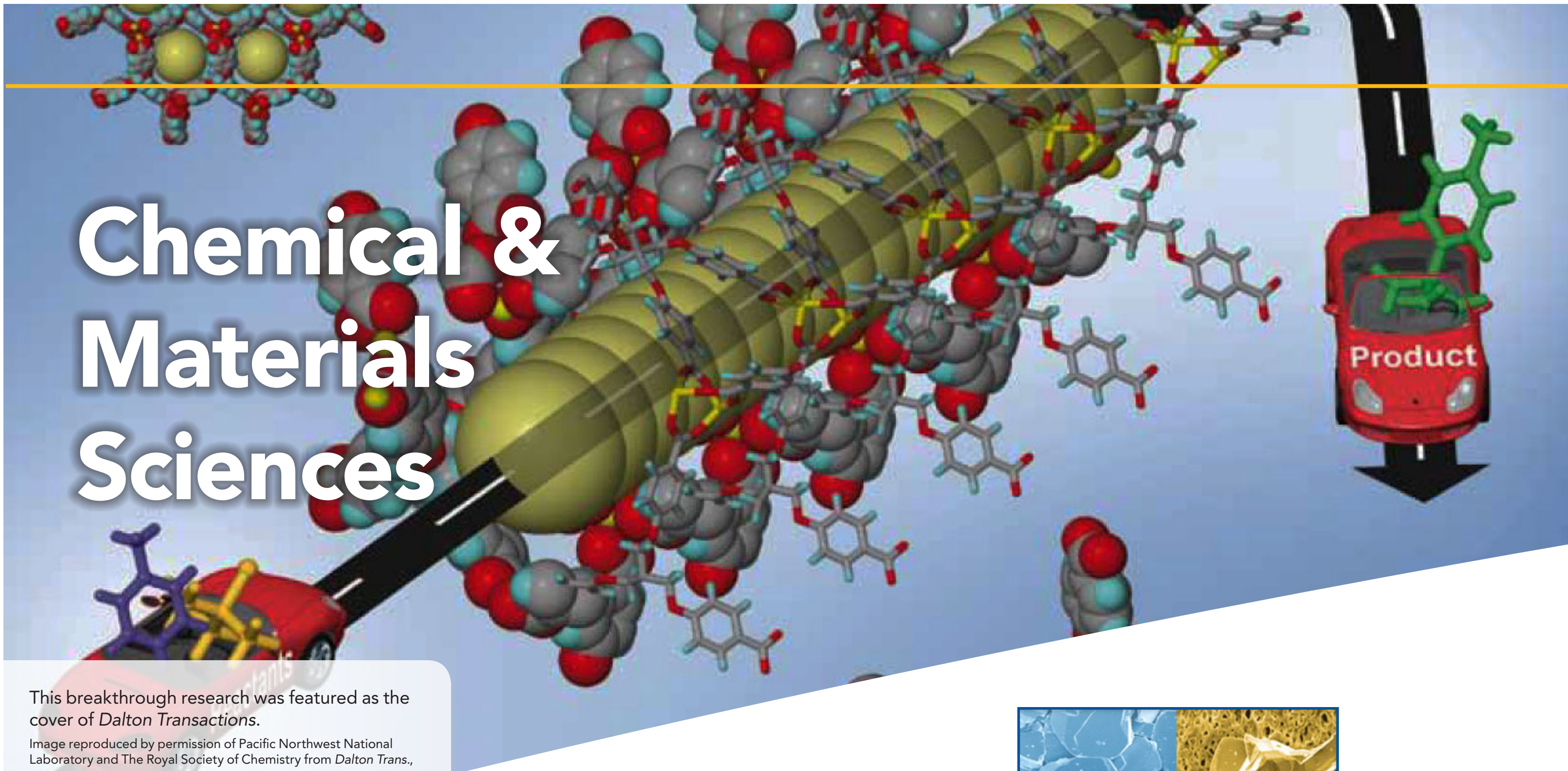
The research establishes a reference that may help researchers and clinicians determine the root causes of Alzheimer's, Parkinson's and other neurological conditions. And, it could improve the chances of devising faster, more efficient diagnostic tests and treatments for diseases with neurological and psychiatric features. While the work is the most comprehensive characterization of normal spinal fluid to date, it is only the beginning. Quickly and precisely determining the proteins in different samples opens doors to fundamentally understanding human health.

Schutzer SE, T Liu, BH Natelson, TE Angel, AA Schepmoes, SO Purvine, KK Hixson, MS Lipton, DG Camp II, PK Coyle, RD Smith, and J Bergquist. 2010. "Establishing the Proteome of Normal Human Cerebrospinal Fluid." *PLoS ONE* 5(6):e10980. DOI: 10.1371/journal.pone.0010980.

Sponsors:The National Institutes of Health, the National Center for Research Resources, the Swedish Research Council, and Uppsala Berzelii Technology Center for Neurodiagnostics.

A U.S. and Swedish team identified 2,630 proteins in the clear fluid that protects the brain and spinal cord. This research establishes healthy benchmark to aid in understanding neurological disorders.

Chemical & Materials Sciences



This breakthrough research was featured as the cover of *Dalton Transactions*.

Image reproduced by permission of Pacific Northwest National Laboratory and The Royal Society of Chemistry from *Dalton Trans.*, 2010, 39, 1692-1694, DOI: 10.1039/b921118g.

New Class of Catalyst Sports **SHAPE SELECTIVITY**

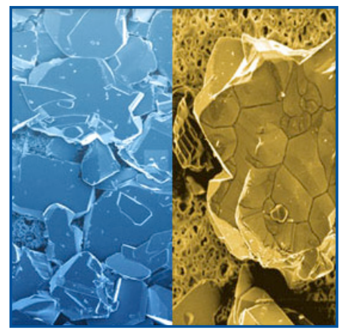
Scientists at Pacific Northwest National Laboratory synthesized and studied a new class of catalytic materials called crystalline metal-organic frameworks, which have high surface area and thermal stability. The researchers found that these materials display a unique three-dimensional structure that is highly selective and reactive, with performance that is up to 50% better than commercial materials in the tested reactions. The catalyst's high shape selectivity—the ability to select certain molecules in the reaction based on structure—points to energy, environmental, and other applications.

Thallapally PK, CA Fernandez, RK Motkuri, SK Nune, J Liu, and CHF Peden. 2010. "Micro and Mesoporous Metal-Organic Frameworks for Catalysis Applications." *Dalton Transactions* **39**(7):1692-1694.

Sponsors: Department of Energy, Office of Basic Energy Sciences and PNNL Laboratory-Directed Research and Development Program

Unlocking **SUBSURFACE** Secrets

In answering fundamental questions about subsurface behavior, scientists at Pacific Northwest National Laboratory and their collaborators clarified previously contradictory work on hematite (Fe_2O_3). They connected separate studies and proved that hematite growth involves electron and atom exchange facilitated by moving electrons supplied by Fe(II) through the mineral's bulk. In a separate study, scientists discovered that pentavalent uranium, an unstable form previously isolated only under certain conditions in the laboratory, can persist in the subsurface. This occurs because pentavalent uranium was found to be stabilized on certain iron-containing minerals.



Scanning electron micrographs of hematite before (blue) and after (gold) pyramidal hematite overgrowths.

Rosso KM, S Yanina, CA Gorski, P Larese-Casanova, and M Scherer. 2009. "Connecting Observations of Hematite (α-Fe_2O_3) Growth Catalyzed by Fe(II)." *Environmental Science & Technology* **44**(1):61-67.

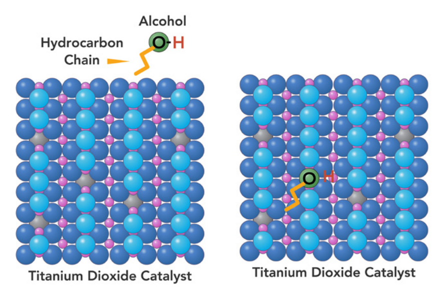
Ilton, ES, JF Boily, EC Buck, FN Skomurski, KM Rosso, CL Cahill, JR Bargar, and AR Felmy. 2009. "Influence of Dynamical Conditions on the Reduction of U(VI) at the Magnetite-Solution Interface." *Environmental Science & Technology* **44**(1):170-176.

Sponsors: Department of Energy, Office of Basic Energy Sciences (both papers) and Offices of Biological and Environmental Research (uranium); National Science Foundation (iron)

Finding the **PERFECT SPOT** to Rest

Carbon chains are particular about where they want to land on a titanium dioxide catalyst, according to a study from Pacific Northwest National Laboratory and the University of Texas at Austin. The catalyst's surface is ridges of oxygen atoms that run parallel to valleys of titanium atoms. Influenced by a weak attraction to the titanium, the hydrocarbon chain settles into the valleys.

The location of the hydrocarbon chain determines, in part, how well the model catalyst titanium dioxide will perform. Understanding where the carbon chain is and why it selects that location is vital data for those seeking to modify catalyzed reactions; for example, making the reactions faster or more selective.



Scientists added alcohol molecules to the surface of the titanium dioxide catalyst. The alcohol's oxygen atom sheds its hydrogen atom and slides into a vacant oxygen spot on the catalyst's surface. Influenced by a weak attraction to the titanium, the hydrocarbon chain settles into the valleys on the surface of the titanium dioxide.

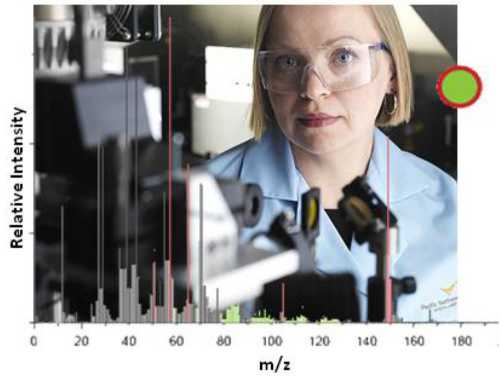
Zhang Z, R Rousseau, J Gong, BD Kay, and Z Dohnálek. 2009. "Imaging Hindered Rotations of Alkoxy Species on TiO_2(110)." *Journal of the American Chemical Society* **131**(49):17926-17932. DOI: 10.1021/ja907431s.

Sponsor: Department of Energy, Office of Basic Energy Sciences

Scientists Characterize Poorly Understood, **CLIMATE-INFLUENCING ATMOSPHERIC PARTICLES**

Two very different forms of climate-influencing particles do not behave as expected, according to scientists at Pacific Northwest National Laboratory and Imre Consulting. The team's measurements using SPLAT II show that when the particles mix, they create new, layered particles, not the expected mixtures. The team also found that one form adsorbs onto the other, creating bigger particles that do not behave as predicted in climate models. This study led to an invited paper in a special issue of *Proceedings of the National Academy of Science*.

Whether created by nature or humankind, tiny particles in the atmosphere influence the planet's climate. In particular, scientists are concerned with primary and secondary organic aerosols. Abundant in the atmosphere, these particles are derived from fossil fuels and other sources. Scientists aim to model the effect of these particles and other factors to predict the effect of remediation strategies on climate. Studies like this one are essential to understand the processes that determine the numbers and properties of particles, leading to more accurate models and predictions.



Using SPLAT II, researchers generate mass spectra and then analyze them to identify the morphology of different particle types.

Vaden TD, C Song, RA Zaveri, D Imre, and A Zelenyuk. 2010. "Morphology of Mixed Primary and Secondary Organic Particles and the Adsorption of Spectator Organic Gases during Aerosol Formation." *Proceedings of the National Academy of Sciences* **107**(15):6658-6663. DOI: 10.1073/pnas.0911206107.

Sponsors: Department of Energy, Offices of Basic Energy Sciences and Biological and Environmental Research

Simulation, Calculations Show Hydroxide **IONS ORIENTATION IN WATER**

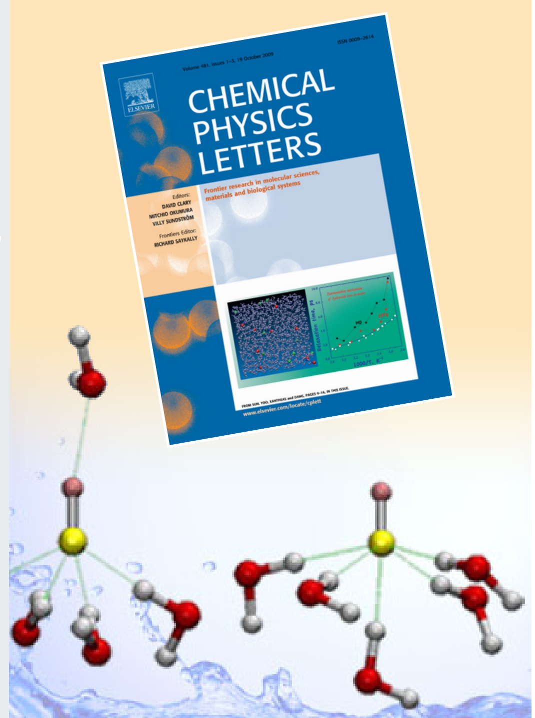
Whole water molecules form complex shapes around hydroxide ions, simple negatively charged particles, according to a study by scientists at Pacific Northwest National Laboratory. The shapes are the result of hydrogen bonds between the ions and the molecules. This research answers the question, debated in scientific circles for more than 70 years, of how hydroxide ions are oriented in water. The work was done using NWChem.

Knowing how hydroxide ions are arranged in water could aid scientists in fine-tuning current industrial processes, such as manufacturing biodiesel ormaking processes more efficient or less wasteful. Further, it could assist in developing future industrial processes, such as turning poplar trees and other vegetation into automotive fuel.

Sun X, S Yoo, SS Xantheas, and LX Dang. 2009. "The Reorientation Mechanism of Hydroxide Ions in Water: A Molecular Dynamics Study." *Chemical Physics Letters* **481**(2009):9-16.

Sponsor: Department of Energy, Office of Basic Energy Sciences

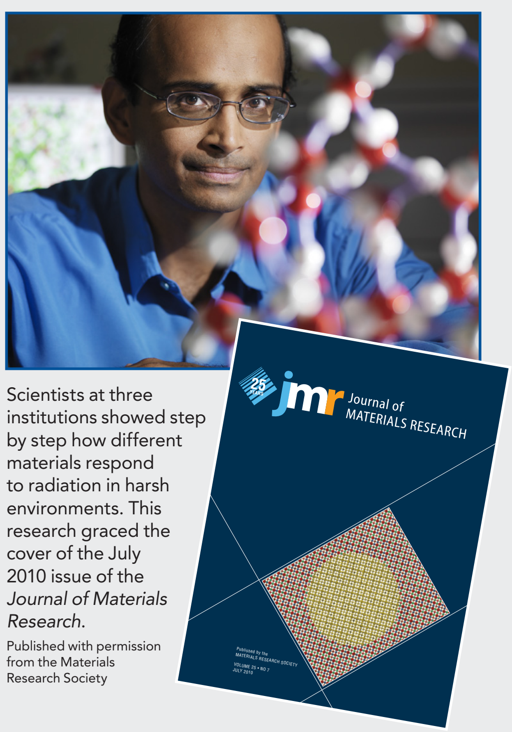
This work graced the cover of the October 19, 2009, issue of *Chemical Physics Letters*.



When Ions **ATTACK**

In extreme environments, some materials quickly recover from being hit by energetic ions, while other materials are permanently scarred, according to scientists at Pacific Northwest National Laboratory, the University of Michigan, and the Interdisciplinary Research Centre Ions Lasers in France. The article, which integrated independent experiments and simulations, showed step by step how the materials respond.

Communication satellites, nuclear waste disposal, and other technologies need resilient materials that can withstand radiation in environments characterized by extreme heat, cold, or stress. To determine how materials will behave and design better alternatives, researchers need the rare insights into the atomic-level behavior this study provides. In addition, this research has geological applications. Minerals are often dated based on the tracks left by the heavy swift ions. A better understanding of how these tracks evolve can lead to more accurate dating information.

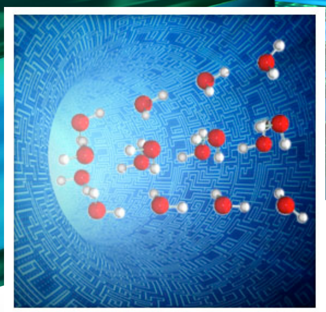


Scientists at three institutions showed step by step how different materials respond to radiation in harsh environments. This research graced the cover of the July 2010 issue of the *Journal of Materials Research*.

Zhang J, M Lang, RC Ewing, R Devanathan, WJ Weber, and M Toulemonde. 2010. "Nanoscale Phase Transitions Under Extreme Conditions Within an Ion Track." *Journal of Materials Research* **25**(7):1334-1351.

Sponsors: Department of Energy, Office of Basic Energy Sciences and German Science Foundation DFG

Computational Sciences & Mathematics



SCALING Goes eXtreme

The scalability of high-level excited-state coupled-cluster approaches and parallel-in-time algorithms was demonstrated—reaching a staggering 34,000 Core Processing Units—by researchers at Pacific Northwest National Laboratory. The team is targeting the software that can describe the behavior of molecules in excited states, as well as simulate their dynamics.

To effectively attack scientific problems in energy, the environment, and national security, state-of-the-art algorithms need to be developed that can run effectively on emerging computer systems capable of performing more than a quadrillion operations per second (known as a petaflop). The development of advanced algorithms that will perform on these petascale—and on soon-to-be exascale—computer architectures will make it feasible to perform massive modeling and simulation calculations on these types of computers.

Kowalski K, S Krishnamoorthy, O Villa, J Hammond, and N Govind, 2010. "Active-Space Completely-Renormalized Equation-of-Motion Coupled-Cluster Formalism: Excited-State Studies of Green Fluorescent Protein, Free-Base Porphyrin, and Oligoporphyrin Dimer." *Journal of Chemical Physics* **132**:154103. DOI: 10.1063/1.3385315.

Sponsor: Pacific Northwest National Laboratory eXtreme Scale Computing Initiative

QUIETING Your Data

Noisy or irrelevant data can distract scientists and consume expensive storage space and computing time, especially when studying ultra-large, dynamic, incomplete climate data sets to predict how regulations will influence the global climate. Scientist at Pacific Northwest National Laboratory, along with a host of collaborators, created a new approach that can discern between noise and nonlinear events. This new data-reduction approach, called Stochastic Proper Orthogonal Decomposition (SPOD), quantifies the uncertainty and extracts the useful information from the large-scale noisy data sets. This approach helps scientists to calibrate climate models using SPOD-filtered, large-scale noisy climate data, which results in more accurate prediction of climate change. The collaborators in this research project are Courant Institute, New York University, Brown University, and Louisiana State University.

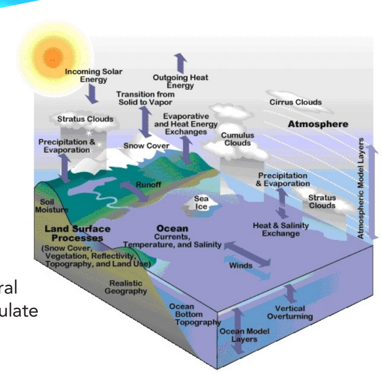


Diagram of data inputs of all natural processes to simulate earth's complex climate system.

Sponsor: Department of Energy, Office of Advanced Scientific Computing Research

SCIENTIFIC PROCESS AUTOMATION TECHNOLOGY Makes Journal Cover

Written by Terence Critchlow at Pacific Northwest National Laboratory, the cover article in the September/October 2009 issue of *Scientific Computing* describes the Scientific Process Automation (SPA) component of the Scientific Discovery through Advanced Computing Scientific Data Management Center. The center is focused on improving scientists' ability to interact with their data in three key areas:

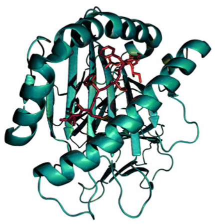
- reading and writing data through storage-efficient access
- analysis of large data sets to find features of interest using data mining and analysis
- automation of the overall simulation and analysis process through SPA.

The article describes the scientific workflow infrastructure developed through the SPA thrust area that is significantly improving scientists' ability to effectively use computational resources and analyze their data. This technology has been successfully applied in computational science domains including fusion, astrophysics, biology, climate modeling, groundwater, and combustion.

Critchlow T. 2009. "Scientific Process Automation Improves Data Interaction." *Scientific Computing* **26**(5):6-9.

Sponsor: Department of Energy, Scientific Discovery through Advanced Computing Program

HIERARCHICAL, MULTI-OBJECTIVE OPTIMIZATION of Microbial Community Proteomics Systems



A new high-performance computing model developed by researchers at Pacific Northwest National Laboratory significantly increases sensitivity and specificity in identifying peptides and proteins that occur within microbial communities. The analysis of hundreds of thousands of spectra using this novel approach resulted in a 125% increase in the number of identifiable spectra compared to standard data analysis methods.

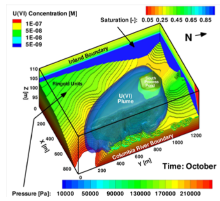
Investigating how these peptides are involved in critical biological processes will lead to a better understanding of how to solve major national challenges in carbon sequestration, bioremediation, and bioenergy. The process uses mathematical models to implement and leverage scientific principles from various domain sciences.

Cannon WR. 2010. Metaproteomics: Phylogenomic-based identification of microbes from MS/MS environmental samples and unprecedented assignment of peptides and proteins using spectral libraries. Presented by William R. Cannon at the Annual Meeting of the American Society for Mass Spectrometry, Salt Lake City, UT, on May 22, 2010.

Sponsors: Department of Energy, Advanced Scientific Computing Research, Scientific Discovery through Advanced Computing Program and Biological and Environmental Research

PFLOTRAN: Advanced Computing MODELING for a CLEANER ENVIRONMENT

Findings from the PFLOTRAN (petascale reactive multiphase flow and multicomponent transport) code are strengthening scientists' ability to more accurately predict groundwater contaminant movement.



Simulated uranium plume at the Hanford 300 Area in the October 2009 time frame.

PFLOTRAN simulated the migration of contaminants in groundwater and estimated the release of uranium to the Columbia River. For a conceptual model depicting current conditions near Hanford's South Processing Pond, PFLOTRAN estimated that uranium leaches into the river at a rate of 25 kg/year. The estimate is similar to estimates based on field studies (i.e., 20-50 kg/year). Modeling with PFLOTRAN is helping to inform and guide future cleanup decisions.

Lichtner, PC and GE Hammond. 2010. "Placing the Hanford 300 Area IFRC Site in Perspective: Plume Scale Modeling of Uranium Attenuation and Its Flux to the Columbia River." 5th Annual DOE SBR PI Meeting, March 29-31, 2010, Washington D.C.

Sponsors: Department of Energy, Offices of Biological & Environmental Research and Advanced Scientific Computing Research, DOE SciDAC-2 program. Supercomputing resources were provided by the DOE Office of Science Innovative and Novel Computational Impact on Theory and Experiment program with allocations on NCCS Jaguar at Oak Ridge National Laboratory.

Computational Science Programming Model CROSSES THE PETAFLOP BARRIER

The Global Arrays computational programming model can perform at the petascale level, according to researchers at Pacific Northwest National Laboratory and Oak Ridge National Laboratory. The demonstration was performed at 1.4 petaflops—or 1.4 quadrillion numerical operations per second—using over 200,000 processors. This represents about 50% of the processors' peak theoretical capacity. Developed at PNNL, Global Arrays is one of only two parallel programming models that have achieved this level of performance.

Global Arrays enables researchers to more efficiently access global data, run bigger models, and simulate larger systems, resulting in a better understanding of the data and processes being evaluated.

The Global Arrays technology was used in a computational chemistry simulation that was presented during the annual International Conference on High-Performance Computing, Networking, Storage and Analysis. The simulation provided more accurate data pertaining to the molecular-level properties of water and its behavior at interfaces. The paper describing the simulation was a finalist for the Gordon Bell prize that recognizes outstanding achievement in high-performance computing applications.

Apra E, RJ Harrison, W de Jong, AP Rendell, V Tipparaju, and SS Xantheas. 2009. "Liquid Water: Obtaining the Right Answer for the Right Reasons." *Supercomputing '09, Proceedings of the Conference on High Performance Computing Networking, Storage and Analysis*. Portland, Oregon, SESSION: Gordon Bell finalists, Article No.: 66. ISBN:978-1-60558-744-8.

Part of this work was performed using PNNL's NWChem computational chemistry package.

Sponsors: Department of Energy, Basic Energy Sciences and Advanced Scientific Computing Research as part of the Scientific Discovery through Advanced Computing Program, and the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory

Making HASH with the CRAY XMT

"Hashing strategies" are methods for slicing and dicing data to assign it to locations within a computer. Now, scientists at Pacific Northwest National Laboratory and Sandia National Laboratories have improved hashing strategies for multithreaded machines. They adapted two of the most commonly used variations of hashing strategies to run efficiently on the Cray XMT. As a result, they decreased computing time for the same problem from 536 to 77 seconds. The new strategies can be scaled efficiently from 2 to 128 processors.

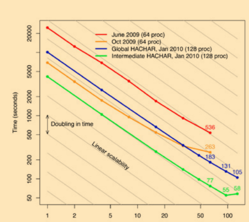
Hashing strategies speed up computing tasks by assigning an identifier to a certain piece of data so it can be found quickly. An identifier will always be placed into a particular location – or bucket – in the computer's memory. When multiple identifiers need to be stored in the same bucket, a collision occurs. Even though collisions are almost inevitable, hashing strategies must still compute accurately.

Hashing strategies for the Cray XMT are challenging to adapt because of its multithreaded architecture. Unlike massively parallel machines, which typically use around 64 computing threads per cluster node at one time, the Cray XMT could use 16,000 computing threads all accessing its 1 terabyte of shared memory. If all 16,000 threads want to use the same information at the same time, the computer slows down. The researchers adapted the "linear probing" and "hashing with chaining" strategies to minimize memory contention during data processing in the multithreaded environment.

Advances in multithreaded computing could improve analyses of irregular, data-intensive applications in a variety of scientific domains.

Goodman EL, DJ Haglin, C Scherrer, D Chavarría-Miranda, JA Mogill, and JT Feo. 2010. "Hashing Strategies for the Cray XMT." In *IEEE International Symposium on Parallel & Distributed Processing, Workshops and Phd Forum* (IPDPSW 2010), pp. 1-8. Institute of Electrical and Electronics Engineers, Piscataway, NJ. doi:10.1109/IPDPSW.2010.5470688

Sponsor: This work was funded under the Center for Adaptive Supercomputing Software – Multithreaded Architecture (CASS-MT) at the Department of Energy's Pacific Northwest National Laboratory.



By adapting hashing strategies for a multithreaded environment, researchers decreased the CRAY XMT compute time from 536 seconds to 77 seconds in solving a problem using the same number of processors.

Awards & Honors

Three Receive EARLY CAREER GRANTS

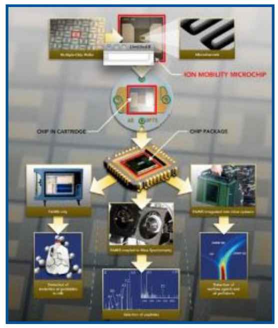
Three members of the Fundamental & Computational Sciences Directorate received the Department of Energy's Early Career Research Award. The award bolsters the scientific workforce by supporting exceptional researchers during their early career years, when many scientists do their most formative work:

William Gustafson – enhance climate model capabilities to enable scientists to perform long-term global cloud studies in high resolution using improved computer architectures. This will require merging two modeling cultures, one that uses coarse model resolutions integrated over long time periods, and another that uses high-resolution models for detailed process studies over shorter periods.

Wei-Jun Qian – develop a suite of quantitative proteomics technologies to gain understanding of the spatial and temporal regulation of cellular functions in environmental eukaryotes—complex organisms—such as *Aspergillus niger*, a fungus that plays an important role in biofuel production and global carbon cycling.

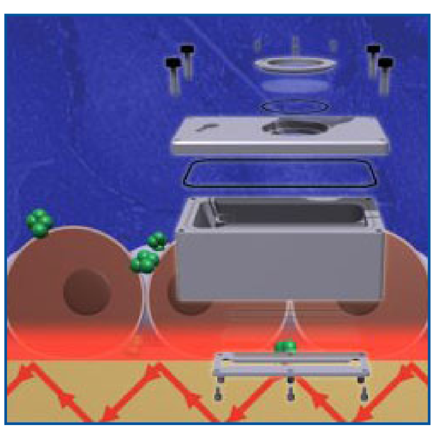
Wendy Shaw – design effective, inexpensive catalysts that will ultimately enable the efficient use of renewable energy by mimicking the outer coordination sphere of natural enzymes that facilitate efficient transformation between fuels and energy. While today's industrial catalysts rely on platinum, which is rare and expensive, natural catalysts use nickel or iron, which are inexpensive and abundant.

Biological Technologies Win R&D 100 AWARDS



Congratulations to Alexandre Shvartsburg, Keqi Tang, Richard Smith, Tom Weber, and Colette Sacksteder for winning 2010 R&D 100 Awards from *R&D Magazine* for two of the top high-technology products of the year. Shvartsburg, Tang, and Smith are developers, with Owlstone Nanotech, of the Ion Mobility Spectrometer on a Microchip. This miniaturized device accelerates the speed of analyses by >100 times using ion mobility separations, enabling capabilities for rapidly and confidently monitoring a broad range of chemicals at very low concentrations.

Sacksteder and Weber were on the development team for IncubATR™—the Live-Cell Monitor along with lead developer SK Sundaram and Brian Riley, also at PNNL. Developed in cooperation with Simplex Scientific LLC, the IncubATR™ works with existing spectroscopy devices to pioneer real-time, *in-situ* screening of live-cell responses to stimuli and removing the limitations posed by traditional live-cell testing methods.



BRUCE D. KAY, American Chemical Society Fellow

Kay was honored as an American Chemical Society Fellow. This award reflects his contributions to the study of chemical reactions that occur on surfaces. In particular, he examines the molecular behavior of amorphous solid water. Better understanding its behavior will help scientists understand the stars, other planets, and the behavior of water here on earth.

L. RUBY LEUNG Named Fellow, Joins Advisory Committee

Based on her outstanding contributions and leadership in regional climate modeling, Leung was elected a Fellow of the American Meteorological Society, an award that is given to only two-tenths of one percent of AMS members each year. Leung also was appointed to the Biological and Environmental Research Advisory Committee. As a member, she provides advice on complex issues related to developing and implementing the biological and environmental research program.

GREG SCHENTER, American Physical Society Fellow

Schenter was named a Fellow of the American Physical Society. Schenter earned this honor for his contributions in chemical physics. His work on calculating molecular and atomic behavior and his work in nucleation theory has appeared in top journals, with nearly half of his publications in top five journals.

TERENCE CRITCHLOW
Selected for National Academy of Engineers Symposium

Critchlow was chosen to participate in the National Academy of Engineering's 16th Annual U.S. Frontiers of Engineering symposium. The event brings together the country's outstanding young engineers from industry, academia, and government to discuss pioneering technical and leading-edge research in various engineering fields and industry sectors.

GUANG LIN Recognized for Uncertainty Research

Lin received a 2010 Advanced Scientific Computing Research Leadership Computing Challenge award, which presents computational resources for high-risk, high-payoff simulations in areas directly related to the Department of Energy's missions. His project focuses on extracting and reducing data from massive volumes of information to quantify and reduce the uncertainty in climate models.

Also, Lin was invited to serve on the editorial board for the *International Journal for Uncertainty Quantification*. The publication features information in the areas of analysis, modeling, design, and control of complex systems in the presence of uncertainty in physical and biological sciences.

JIM DOOLEY Recognized for International Greenhouse Gas Control

Dooley was invited to provide his insights at a major meeting of the White House Interagency Task Force on Carbon Capture and Storage. The event gave the public the chance to provide input on what actions the government should take to accelerate the commercial deployment of carbon dioxide capture and storage projects to reduce greenhouse gas emissions to the atmosphere.

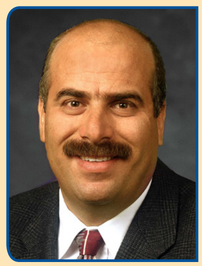
Dooley, along with PNNL colleagues Robert Dahowski and Casie Davidson and other collaborators also received an award from the Carbon Sequestration Leadership Forum, an international climate change initiative focused on developing carbon capture and sequestration technologies.

Five Joined Ranks of **AAAS FELLOW**

Five 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 San Diego in February 2010.

SCOTT CHAMBERS

Distinguished contributions in understanding the electronic and magnetic properties of crystalline films, and their ability to transform electricity from chemicals responding to light. These films could be used to make microelectronic devices, convert energy, and make energy by splitting water. They're also studied for the field of spintronics, where scientists are trying to harness the magnetic properties of electrons.



MOE KHALEEL

Distinguished work in computational engineering, including computational models for solid oxide fuel cells and advanced lightweight materials. He develops methods and computational tools that allow scientists and engineers to build and test fuels cells and their material components.

YUEHE LIN

Outstanding contributions to nanotechnology. He's developing chemical and biological sensors made with nanoparticles, graphene, and carbon nanotubes. These sensors can detect important molecules in biological systems, explosives, and pesticides and could deliver drugs to fight diseases like cancer, among other uses.

PHIL RASCH

Outstanding contributions to climate modeling, which is used to understand the environment and ongoing climate change. He develops and improves atmospheric circulation models, some of which simulate the movement of water vapor, sulfate, and aerosols.

SOTIRIS XANTHEAS

Distinguished contributions to highly accurate electronic structure calculations on aqueous molecular clusters, results that are widely used in the physical chemistry community. He combines data gathered in the lab with computer theories to refine scientists' understanding of aqueous systems and water.

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, the environment, and national security. PNNL employs 4,900 staff, has an annual budget of nearly $1.1 billion, and has been managed by Ohio-based Battelle since the lab's inception in 1965.

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▶ www.pnl.gov/science

The LAST WORD

In these pages you saw some of the noteworthy achievements in the biological, chemical, computational, environmental, and materials sciences by Fundamental & Computational Sciences Directorate scientists in fiscal year 2010. I am proud of their potential to transform our understanding and control of chemical, physical, and biological processes and to unravel the most important challenges in energy, national security, and environmental sustainability.

In FY 2010, PNNL enhanced its computing infrastructure by expanding its Cray XMT, adding a data transfer node, and improving connectivity to ESnet. These and other internal investments are leading to new discoveries and a more effective computing environment.

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

About the Cover: *This scanning electron micrograph shows bacterial cells that accumulated on titanomagnetite minerals upon exposure to groundwater at the Hanford Site. Titanomagnetite minerals are naturally occurring metal oxides comprising one type of iron source in the mineralogy of Hanford sediments. They are potentially important to microbiological activity and contaminant transport in the subsurface. Data from this controlled experiment is providing a better understanding of energy and materials transfer in the subsurface. The image is false colored.*

PNNL-SA-76361 | November 2010

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