Pacific Northwest
NATIONAL LABORATORY

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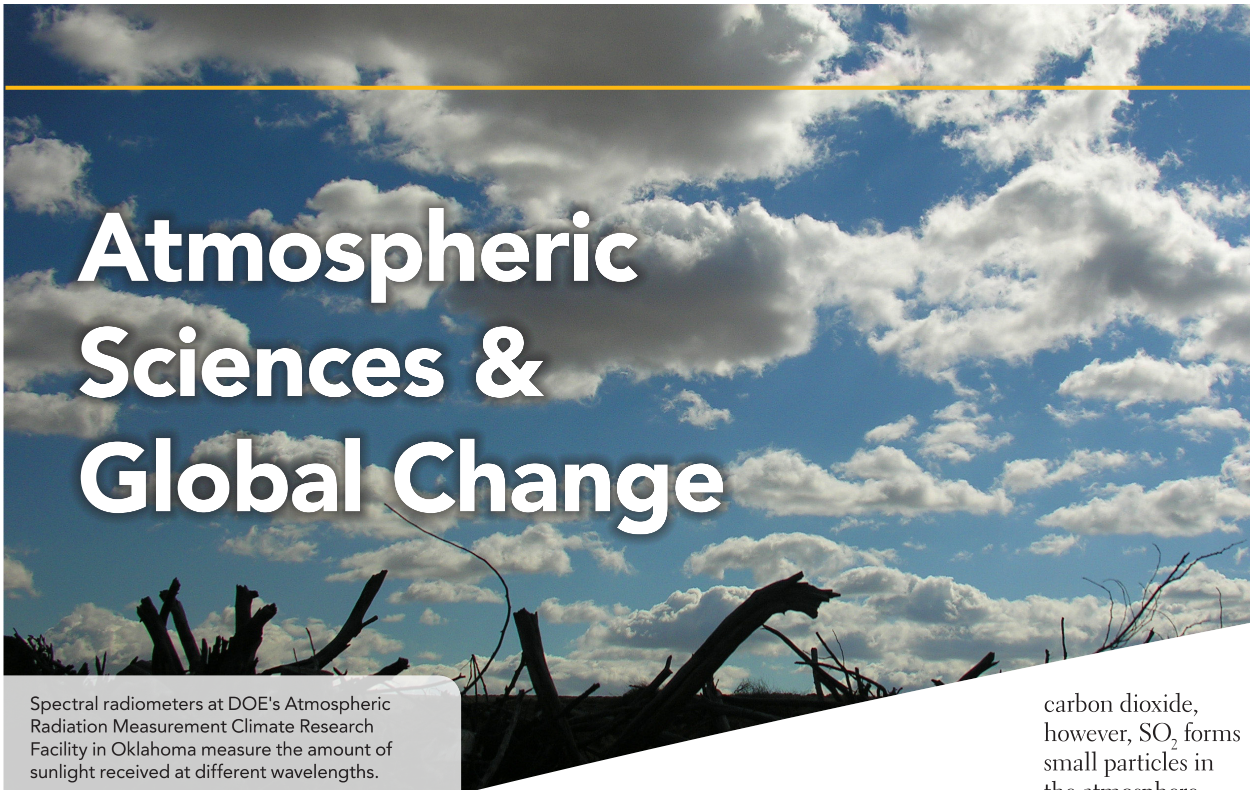
2011 KEY ACCOMPLISHMENTS

Fundamental & Computational Sciences Directorate



Atmospheric Sciences & Global Change

Spectral radiometers at DOE's Atmospheric Radiation Measurement Climate Research Facility in Oklahoma measure the amount of sunlight received at different wavelengths.

Clouds and the COLOR OF SUNLIGHT

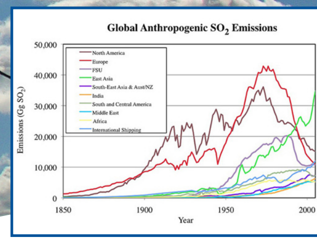
Clouds have a significant influence on the amount of sunlight reaching the Earth's surface and hence on the planet's energy balance. Atmospheric scientists from Pacific Northwest National Laboratory discovered that the amount of sunlight scattered by clouds varies more strongly by wavelength, or the "color" of light, than previously thought. Aerosols, those tiny particles of dust or pollution found in both clouds and clear air, are likely responsible for these variations. This research will help scientists improve how they portray clouds in climate models, which in turn will increase their ability to accurately model and predict climate change.

Kassianov EI, J Barnard, LK Berg, CN Long, and C Flynn. 2011. "Shortwave Spectral Radiative Forcing of Cumulus Clouds from Surface Observations." *Geophysical Research Letters* **38**:L07801. DOI: 10.1029/2010GL046282.

Sponsor: Department of Energy Office of Biological and Environmental Research

Worldwide SULFUR EMISSIONS Rose Between 2000-2005

After declining for a decade, worldwide sulfur dioxide (SO_2) emissions started rising again in 2000. An analysis by researchers at the Joint Global Change Research Institute, a partnership between Pacific Northwest National Laboratory and the University of Maryland, attribute this increase to a rise in international shipping and a growing Chinese economy. SO_2, like carbon dioxide, is released when fossil fuels are burned. Unlike carbon dioxide, however, SO_2 forms small particles in the atmosphere that reflect sunlight back to space, offsetting some, but not all, heating associated with greenhouse gases. SO_2 and related compounds also lead to acid rain and can negatively impact human health. An accurate record of SO_2 emissions will help researchers track and predict future changes in climate as well as impacts on human health and the environment.



Manmade sulfur dioxide emissions by country show a decline by the historically large emitters, Europe and the U.S., over the past several decades but a recent increase by China and other emerging economies.

Smith SJ, J van Aardenne, Z Klimont, RJ Andres, A Volke, and S Delgado Arias. 2011. "Anthropogenic Sulfur Dioxide Emissions: 1850-2005." *Atmospheric Chemistry and Physics* **11**(3):1101-1116. DOI: 10.5194/acp-11-1101-2011.

Sponsors: Department of Energy Office of Biological and Environmental Research and other agencies

Human Influence on 21ST CENTURY CLIMATE

The least costly way to manage the heat-trapping effect of greenhouse gases in the atmosphere is to pursue every available option to reduce emissions. That's the conclusion of scientists at Pacific Northwest National Laboratory and the Joint Global Change Institute in a scenario provided to the Intergovernmental Panel on Climate Change. The researchers point to a future with greater reliance on nuclear and renewable energy, new technologies that capture and store carbon dioxide, and changes in agricultural and forestry practices. Their study also shows that the longer it takes to reduce greenhouse gas emissions, the more difficult and expensive it will be.

To reach these conclusions, scientists modeled greenhouse gas emissions from energy use, agriculture, and other human activities through the year 2100. They estimated the cost of reducing emissions both overall and from different sources.

PNNL scientists have shown that society's lowest cost option to reduce the heat-trapping effect of greenhouse gases is to use every available means to reduce emissions, including greater reliance on nuclear and renewable energy-generated electricity and expanding forests to naturally absorb and store carbon.

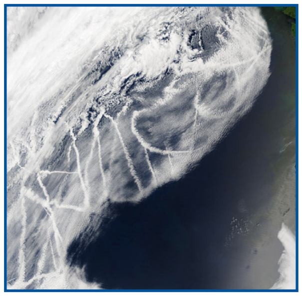
PNNL's scenario, one of four being used by the IPCC, limits the heat-trapping effect of greenhouse gases in the atmosphere to levels only 65 percent of what they could reach by the end of the century if no emissions controls are implemented.

Thomson A, K Calvin, S Smith, P Kyle, A Volke, P Patel, S Delgado-Arias, B Bond-Lamberty, M Wise, L Clarke, and J Edmonds. 2011. "RCP 4.5: A Pathway for Stabilization of Radiative Forcing by 2100." *Climatic Change* DOI: **10**.1007/s10584-011-0151-4.

Sponsor: Department of Energy Office of Biological and Environmental Research

BRIGHTENING CLOUDS

What happens when tiny seawater particles are injected into low clouds over the ocean? To answer this question, scientists at Pacific Northwest National Laboratory and the National Oceanic and Atmospheric Administration developed a high-resolution model capable of simulating the microphysical processes within certain marine clouds. This model showed that particle injection can "brighten" these clouds, causing them to reflect more solar radiation back to space, by making the cloud droplets smaller and more numerous. The amount of sunlight reflected depends on several factors, including the distribution of injected particles and ambient levels of water vapor and pollution. The PNNL and NOAA team also found that adding aerosols changes the amount of rain falling from the clouds.

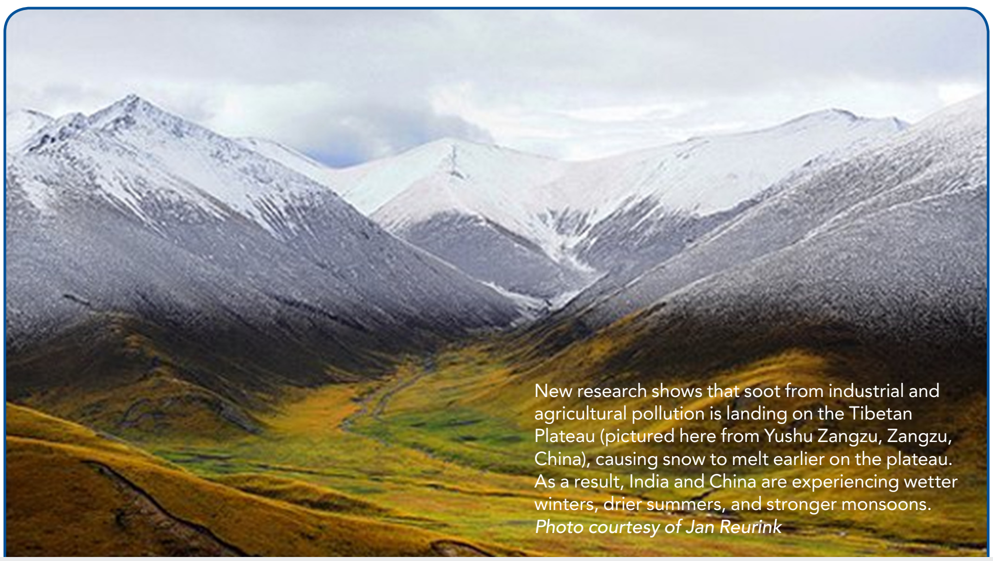


When aerosol particles from ship exhaust enter the lower atmosphere, marine stratocumulus clouds are brightened, leaving "ship tracks" visible in satellite images. *Photo courtesy of Jeff Schmaltz, MODIS Rapid Response Team, NASA/GSFC*

Their results have important implications for proposals to offset some of the impacts of climate change by increasing the amount of sunlight reflected back to space.

Wang H, PJ Rasch, and G Feingold. 2011. "Manipulating Marine Stratocumulus Cloud Amount and Albedo: A Process-Modelling Study of Aerosol-Cloud-Precipitation Interactions in Response to Injection of Cloud Condensation Nuclei." *Atmospheric Chemistry and Physics* **11**, 4237-4249. DOI: 10.5194/acp-11-4237-2011.

Sponsors: University of Calgary's Fund for Innovative Climate and Energy Research, National Oceanic and Atmospheric Administration Climate Goal Program



New research shows that soot from industrial and agricultural pollution is landing on the Tibetan Plateau (pictured here from Yushu Zangzu, Zangzu, China), causing snow to melt earlier on the plateau. As a result, India and China are experiencing wetter winters, drier summers, and stronger monsoons. *Photo courtesy of Jan Reurink*

Polluted Snow **CAUSES EARLY RUNOFF, STRONGER MONSOONS** in Asia

In some cases, soot—the fine, black carbon silt released from stoves, cars, and manufacturing plants—packs more of a climatic punch than greenhouse gases. Researchers at Pacific Northwest National Laboratory, the University of Michigan, and the National Oceanic and Atmospheric Administration found that soot landing on snow on the massive Tibetan Plateau can do more to alter snowmelt and monsoon weather patterns in Asia than carbon dioxide and other greenhouse gases. Soot on snow hastens the plateau's annual snowpack melt each year. The faster melting then prods two of the region's monsoon systems to become stronger over India and China. These changes have important implications for water resources in the region, which is home to more than two billion people.

The team used a series of numerical experiments with a global climate model that simulated the radiative effects of black carbon and dust in snow. They assessed the relative impacts of these changes with those produced by human-induced increases in greenhouse gases and particles in the atmosphere.

Qian Y, MG Flanner, LR Leung, and W Wang. 2011. "Sensitivity Studies on the Impacts of Tibetan Plateau Snowpack Pollution on the Asian Hydrological Cycle and Monsoon Climate." *Atmospheric Chemistry and Physics* **11**:1929-1948. DOI:10.5194/acp-11-1929-2011.

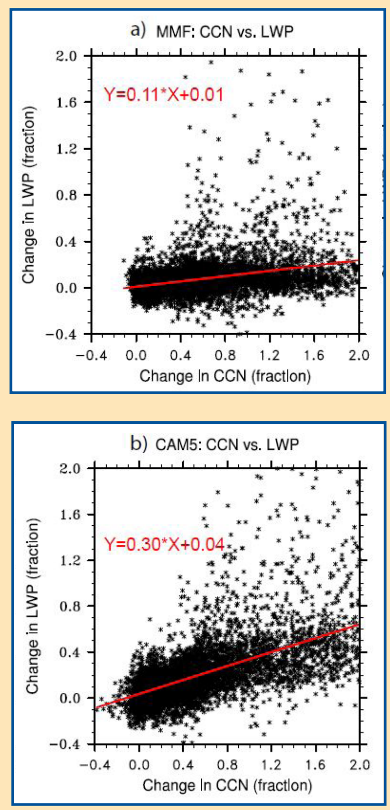
Sponsor: Department of Energy Office of Biological and Environmental Research, under a bilateral agreement with the China Ministry of Science and Technology on regional climate research

CONNECTING THE DOTS on Aerosol Details

Predicting future climate change hangs on understanding aerosols, those tiny particles in the atmosphere. Researchers at Pacific Northwest National Laboratory and the National Center for Atmospheric Research used a new modeling tool to bring the picture of aerosols and their interactions with clouds into sharper focus. This new model can simulate, with unprecedented detail, specific aerosol-cloud interactions and their effects on the Earth's energy budget, one of the toughest climate forecasting problems. The researchers used the model to show that the overall cooling effect of aerosols released by human activities is smaller than previously thought.

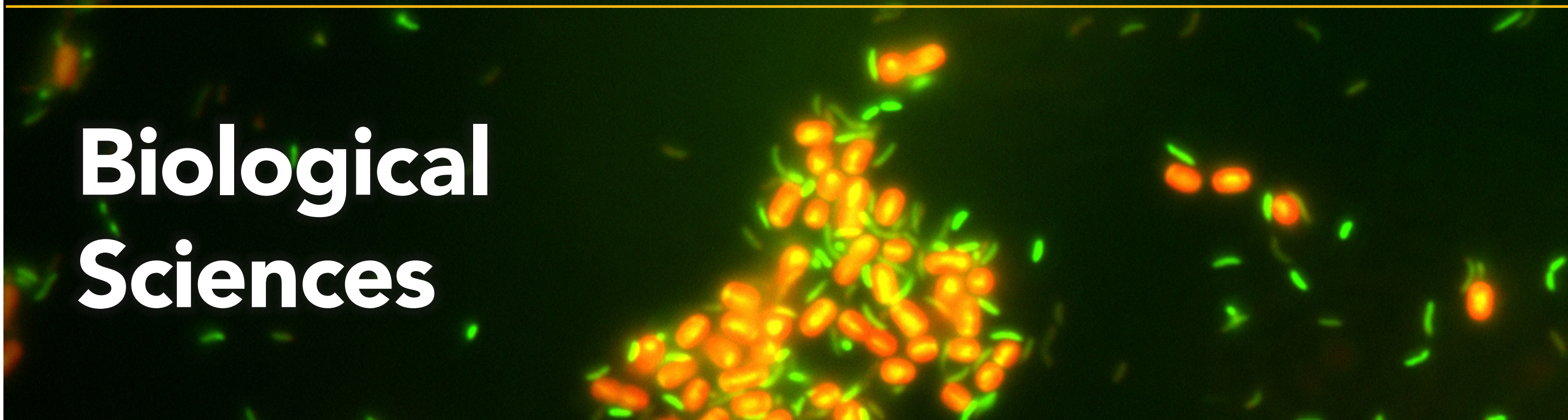
Wang M, S Ghan, M Ovchinnikov, X Liu, R Easter, E Kassianov, Y Qian, and H Morrison. "Aerosol Indirect Effects in a Multi-Scale Aerosol-Climate Model PNNL-MMF." 2011. *Atmospheric Chemistry and Physics* **11**, 5431-5455. DOI: 10.5194/acp-11-5431-2011.

Sponsors: NASA Interdisciplinary Science Program, Department of Energy Office of Biological and Environmental Research



The response of cloud properties to aerosol concentration in the new PNNL-MMF model is only one-third as strong as in current state-of-the-art models. Scatter plots show changes in liquid water path (LWP) versus cloud condensation nuclei (CCN) perturbation in a) MMF (new model), and b) CAM5 (previous model).

Biological Sciences



This co-culture of the bacteria *Synechococcus* sp. PCC 7002 (yellow-orange) and *Shewanella* sp. W18-3-1 (green) are being studied at PNNL to determine if combining them will improve their overall flexibility and efficiency with regard to biomass and potential biofuel production.

ROCK-BREATHING BACTERIA Forms Wires, Dissipates Electricity

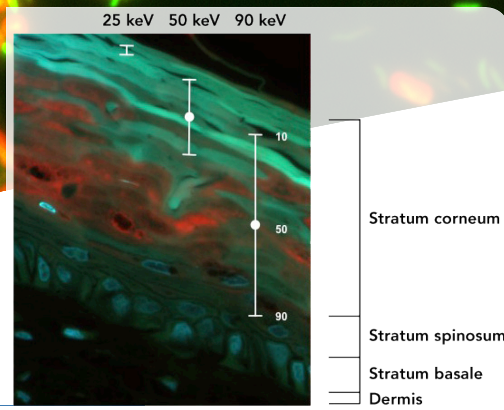
Using bacteria to generate energy is a step closer following a discovery by scientists at the University of East Anglia and Pacific Northwest National Laboratory. Bacteria such as *Shewanella oneidensis* "breathe" metal contaminants, changing the nature of the metal and anchoring it within a mineral. *Shewanella* reaches out with a delicate wire to contact the mineral it is breathing. Breathing creates electricity, and the wire lets the bacteria release excess electricity as it breathes. The research team determined what one of the wire's components looks like, providing insights into how the whole wire might be built.

The discovery means scientists can now start developing ways to "tether" bacteria directly to electrodes, creating efficient microbial fuel cells or "bio-batteries." The advance could also hasten development of microbe-based agents that can clean up oil or uranium pollution, and fuel cells powered by human or animal waste.

Clarke TA, MJ Edwards, AJ Gates, A Hall, GF White, J Bradley, C Reardon, L Shi, AS Beliaev, M Marshall, Z Wang, NJ Watmough, JK Fredrickson, J Zachara, JN Butt, and DJ Richardson. 2011. "Structure of a Bacterial Cell Surface Decaheme Electron Conduit." *Proceedings of the National Academy of Sciences USA* **108**(23):9384-9389. DOI: 10.1073/pnas.1017200108.

Sponsors: UK Biotechnology and Biological Sciences Research Council, Department of Energy Office of Biological and Environmental Research

Modeling RADIATION DEPOSITION IN SKIN



Microscope image of a vertical slice through a skin-tissue model showing range of penetration depths calculated for 25-, 50-, and 90-keV electron beams.

Research involving selective irradiation of a human skin tissue model is improving how scientists determine the effects of low doses of ionizing radiation such as might be received during medical procedures or occupational exposures. Scientists at Washington State University - Tri Cities and Pacific Northwest National Laboratory are modeling electron energy deposition patterns produced by the electron microbeam developed at PNNL to determine its use to study more complex biological systems.

The scientists used a skin tissue model system made of normal human epidermal skin cells and connective tissue cells called fibroblasts. The microbeam can irradiate one cell type and allow a systems biology approach to understand how different cell types interact after irradiation. This will help the development of biologically based models of low dose radiation.

Miller JH, A Suleiman, WB Chrisler, and MB Sowa. 2011. "Simulation of Electron-Beam Irradiation of Skin Tissue Model." *Radiation Research* **175**(1):113-118. doi: 10.1667/RR2339.1.

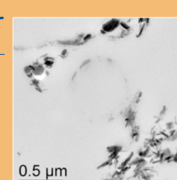
Miller JH, WB Chrisler, X Wang, and MB Sowa. 2011. "Confocal Microscopy for Modeling Electron Microbeam Irradiation of Skin." *Radiation and Environmental Biophysics* **50**(3):365-369 DOI: 10.1007/s00411-011-0371-z.

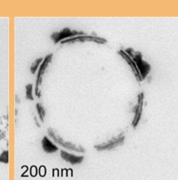
Sponsor: Department of Energy Office of Biological and Environmental Research

DECREASING TECHNETIUM in Groundwater

The long-lasting radionuclide technetium (Tc) goes through the subsurface near former nuclear production and processing sites, moving toward rivers and lakes. But its journey can come to an abrupt end if it hits an area containing high levels of reduced iron generated by microbes. Scientists from Pacific Northwest National Laboratory recently found that microbially generated iron creates significant roadblocks for the pollutant.

They determined that in the presence of commonly occurring iron minerals, indirect Tc reduction by microbially generated ferrous iron may be favored over direct Tc reduction by bacteria, making the technetium as much as 10 times less soluble. This tenfold difference is important, because the Environmental Protection Agency limit for ^{99}Tc in drinking water is extremely low, near the solubility value for the chemically reduced form of Tc, technetium dioxide. Furthermore, the PNNL researchers found that reducing Tc by bacteria generated small-particle technetium colloids that could be highly mobile.





Transmission electron micrograph at left shows ^{99}Tc associated with a *Shewanella putrefaciens* cell along with a fine-grained ^{99}Tc-iron phase and crystallites of magnetite (upper right) and goethite (lower right). At right: in the absence of iron, ^{99}Tc forms deposits on the outside of *Geobacter sulfurreducens* cells.

Plymale AE, JK Fredrickson, JM Zachara, AC Dohnalkova, SM Heald, DA Moore, DW Kennedy, MJ Marshall, C Wang, CT Resch, and P Nachimuthu. 2011. "Competitive Reduction of Pertechnetate ($^{99}TcO_4$-) by Dissimilatory Metal Reducing Bacteria and Biogenic Fe(II)." *Environmental Science & Technology* **45**(3):951-957. DOI: 10.1021/es1027647.

Sponsor: Department of Energy Office of Biological and Environmental Research

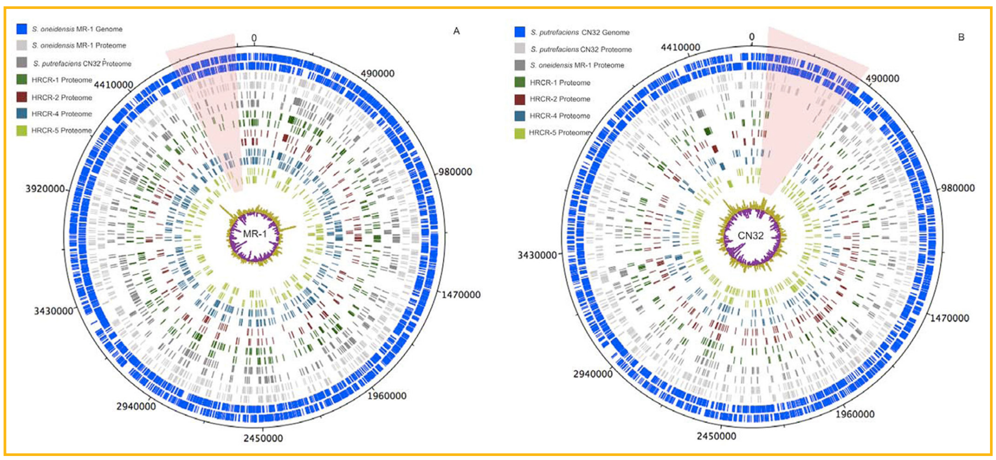
Sequenced Genomes MAKE GOOD NEIGHBORS

The ability to identify the proteins in an organism provides scientists with information important to developing a predictive understanding of biological systems relevant to energy production, environmental remediation, and climate change mitigation. To study an organism's proteomes, a first step often involves using sequenced genomes in conjunction with mass spectrometry for global protein identifications. But what about proteins in an organism not yet sequenced? You could look at its sequenced neighbors, as scientists at Pacific Northwest National Laboratory did. They demonstrated a trans-organism search strategy for determining the extent to which near-neighbor genome sequences can provide global protein identifications in unsequenced organisms isolated from environmental samples.

The scientists searched mass spectra from an unsequenced organism against multiple genome sequences for *Shewanella*, *Deinococcus radiodurans*, and *Salmonella typhimurium*. They identified 300-500 proteins in four uncharacterized bacteria isolated from sediments sampled along the Hanford Reach of the Columbia River and demonstrated an empirical relationship between the numbers of proteins identified.

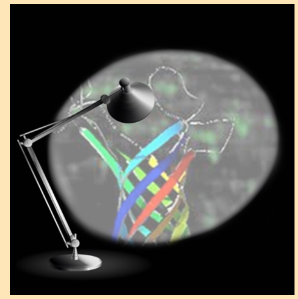
Turse JE, MJ Marshall, JK Fredrickson, MS Lipton, and SJ Callister. 2010. "An Empirical Strategy for Characterizing Bacterial Proteomes Across Species in the Absence of Genomic Sequences." *PLoS ONE* **5**(11):e13968. DOI: 10.1371/journal.pone.0013968.

Sponsors: Department of Energy Office of Biological and Environmental Research, National Institute of Allergy and Infectious Diseases, National Institutes of Health National Center for Research Resources



Two regions of "missing" proteome information from the Hanford Reach isolates are highlighted in the reference genomes of *S. oneidensis* MR-1 (A) and *S. putrefaciens* CN32 (B).

Clustering Key to Lighting Up DARK PROTEOME



A new approach that organizes previously unused mass spectra from proteomics studies gives scientists the ability to use these spectra to gain more information about proteins in a wide range of organisms. Scientists from the University of California, San Diego, and Pacific Northwest National Laboratory created a vast spectral archive from more than a billion mass spectra acquired at PNNL between 2001 and 2009. Typically, unidentified spectra are ignored or discarded, and as a result, a significant fraction of the proteins remain unidentified, constituting an effective "dark proteome" of unknown content.

Spectral archives use all mass spectra—identified or unidentified—as clusters. To shed light on the dark proteome, the scientists not only showed the feasibility of constructing large archives and their basic utility for run-of-the-mill peptide identification, they developed new applications now possible because a diverse collection of datasets can be analyzed as a whole.

Frank AM, ME Monroe, AR Shah, JJ Carver, N Bandeira, RJ Moore, GA Anderson, RD Smith, and PA Pevzner. 2011. "Spectral Archives: Extending Spectral Libraries to Analyze Both Identified and Unidentified Spectra." *Nature Methods* **8**(7):587-591. DOI:10.1038/nmeth.1609.

Sponsors: National Institutes of Health National Center for Research Resources, Department of Energy Office of Biological and Environmental Research

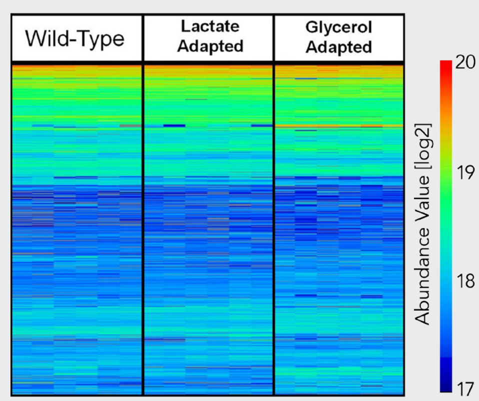
HOW FAST Can Bacteria Grow?

Researchers from the University of California, San Diego led a team from Pacific Northwest National Laboratory, the University of Heidelberg, and the German Cancer Research Center to study how *E. coli* changed and evolved from one environment to another in a laboratory setting. The team then compared proteomics, genomic, and metabolic data from the study with a computational model for bacterial growth. High-performance liquid chromatography coupled to mass spectrometry provided data on how the bacteria changed their protein profile as they grew and reproduced in different mediums. The scientists found that the data and model were correlated to a surprising degree, validating the model's ability to predict the growth of *E. coli* bacteria under specific conditions.

Being able to model the growth of *E. coli* will help scientists begin to develop reliable metabolic models for other more complex organisms. The work will also provide key insights about how to best integrate different complex datasets to more accurately predict how organisms respond to their environment at the molecular level.

Lewis NE, KK Hixson, TM Conrad, JA Lerman, P Charusanti, AD Polpitiya, JN Adkins, G Schramm, SO Purvine, D Lopez-Ferrer, KK Weitz, R Ellis, R König, RD Smith, and BØ Palsson. 2010. "Omic Data from Evolved E. coli Are Consistent with Computed Optimal Growth from Genome-Scale Models." *Molecular Systems Biology* **6**:390. DOI: 10.1038/msb.2010.47.

Sponsors: National Institutes of Health National Center for Research Resources, Department of Energy Office of Biological and Environmental Research



Proteomics data from PNNL allowed scientists to map the abundance of 900 proteins identified in wild-type *E. coli* compared with *E. coli* that had been adapted for growth in the laboratory.

Chemical & Materials Sciences

Images taken by the atomic force microscope of the mineral calcite as it is exposed to and progressively reacts with supercritical carbon dioxide.

ONE TOUGH MICROSCOPE

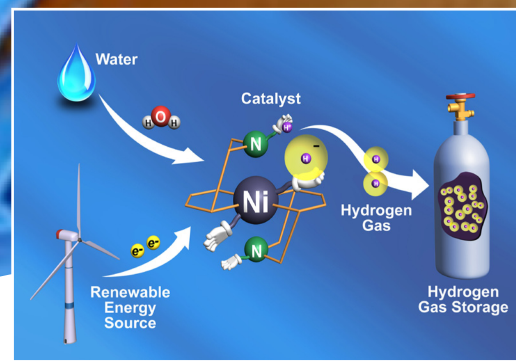
When it comes to seeing how carbon dioxide behaves in a geologic storehouse, most instruments can't take the pressure. But a newly developed atomic force microscope (AFM) created by scientists at Pacific Northwest National Laboratory, Wright State University, and Lawrence Berkeley National Laboratory can handle the pressures the stored greenhouse gas would encounter.

Carbon sequestration will take place in deep rock formations where the temperature and pressure keep the CO_2 in a supercritical fluid state—having properties of a liquid and a gas. Conventional AFMs can't withstand the pressure. So the team designed an apparatus that allows an AFM to handle pressures of 100 atmospheres and temperatures up to ~350 Kelvin, the conditions found a half a mile underground in certain rock formations. With the new tool, scientists can now get sharp pictures and movies of reactions as they happen under conditions found at a carbon sequestration site, providing better understanding of chemical interactions between the supercritical CO_2 and minerals in potential host rocks.

Lea AS, SR Higgins, KG Knauss, and KM Rosso. 2011. "A High-Pressure Atomic Force Microscope for Imaging in Supercritical Carbon Dioxide." *Review of Scientific Instruments* **82**, 043709. DOI: 10.1063/1.3580603.

Sponsor: PNNL Laboratory Directed Research and Development

Catalyst That Makes Hydrogen Gas **BREAKS SPEED RECORD**



The record-breaking catalyst stuffs electrons, the backbone of electricity, seen here as yellow balls or yellow halos, into chemical bonds between hydrogen atoms (H) stolen from water. It uses inexpensive nickel (Ni) to do so.

Looking to nature for their muse, researchers at Pacific Northwest National Laboratory used a common protein to guide design of a material that can make energy-storing hydrogen gas. The synthetic material works 10 times faster than the original protein found in water-dwelling microbes, they report in the August 12 issue of *Science*, clocking in at 100,000 molecules of hydrogen gas every second for every catalyst molecule.

This reaction is just one of a series of reactions to split water and make hydrogen gas, but the result shows that we can learn from nature how to control those reactions to make highly active synthetic catalysts for energy storage, such as in fuel cells. In addition, the natural protein uses inexpensive, abundant metals—such as nickel or iron—which the researchers copied, making a nickel-based catalyst about 100 times faster than the previous record holder. This work was done at the Center for Molecular Electrocatalysis, a DOE Energy Frontier Research Center at PNNL.

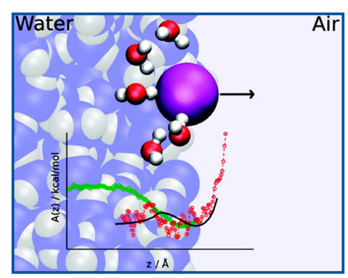
Helm ML, MP Stewart II, RM Bullock, M Rakowski DuBois, and DL DuBois. 2011. "A Synthetic Nickel Electrocatalyst With a Turnover Frequency Above 100,000 s^{-1} for H_2 Production." *Science* **333**(6044):863-866. DOI: 10.1126/science.1205864.

Sponsor: Department of Energy Office of Basic Energy Sciences

The **CHOICES** That Ions Make

From renewable energy sources to pharmaceuticals, iodide ions are a common actor, and now, thanks to scientists at Pacific Northwest National Laboratory, the ions' behavior can be better predicted. By considering electrons' subtler choices about where to reside, the scientists showed the negatively charged iodine ions congregate at the air-water interface. However, they gather at a lower concentration than previously predicted.

The scientists obtained answers about the iodide ion's choices using the laws of quantum mechanics in conjunction with Newton's laws of motion to describe the evolution of aqueous electrolytes, or salty water. These calculations required the use of leadership-class computers through the Department of Energy's INCITE (Innovative and Novel Computational Impact on Theory and Experiment) award. Previous studies relied on empirical potentials, which are simpler mathematical models of molecular motion that do not explicitly consider quantum mechanics. Understanding the nature of ions where air and water meet and at similar interfaces could change how we conduct basic energy research, climate studies, and biological investigations. This research sheds new light on the effects of ions in the vicinity of hydrophobic environments.



Powerful computers and experiments provide insights into the behavior of ions near air and water interfaces.

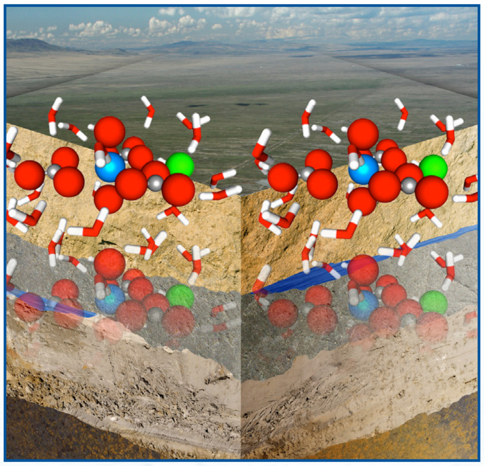
Baer MD and CJ Mundy. 2011. "Toward an Understanding of the Specific Ion Effect Using Density Functional Theory." *Journal of Physical Chemistry Letters* **2**, 1088-1093. DOI: 10.1021/jz200333b.

Sponsors: Department of Energy Office of Basic Energy Sciences and Advanced Scientific Computing Research

New Approach to **CALCULATING URANIUM DIFFUSION** Challenges Traditional Equations

Uranium may move much slower in groundwater than previously believed, according to scientists at Pacific Northwest National Laboratory. Knowing how uranium diffuses in water is critical to predicting its movement and removing it. But previous estimates may have significantly overestimated the radionuclide's ability to move with the groundwater.

Traditional equations used to model chemical diffusion in groundwater were built at the macroscopic level. But only at the molecular level can scientists investigate uranium's diffusion process. The scientists used molecular dynamics techniques and EMSL's Chinook supercomputer to calculate diffusion trajectories of uranium-containing species based on equations describing the way atoms interact. Their results differed by as much as 40 percent from traditional diffusion equation results, showing that uranium may move much slower in groundwater than originally thought.



Diffusion coefficients calculated using EMSL's supercomputer show that uranium-containing species may move slower in groundwater than originally thought.

Kerisit S and C Liu. 2010. "Molecular Simulation of the Diffusion of Uranyl Carbonate Species in Aqueous Solution." *Geochimica et Cosmochimica Acta* **74**:4937-4952. DOI: 10.1016/j.gca.2010.06.007.

Sponsor: Department of Energy Office of Biological and Environmental Research

The **MOLECULE** Movers

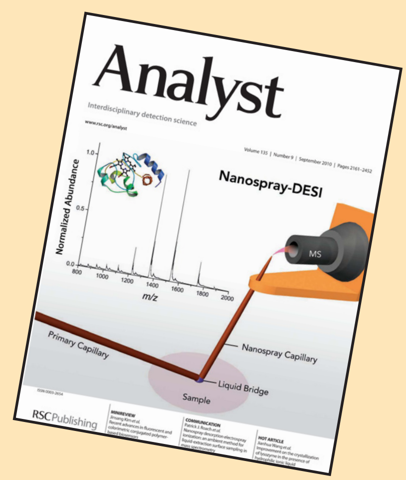
Like the best movers in town, nanoDESI—or Nanospray Desorption Electrospray Ionization—quickly transports delicate chemicals and proteins to their destination in one piece. Created at Pacific Northwest National Laboratory, nanoDESI picks up molecules from substrates using a liquid bridge and transfers them to a mass spectrometer for analysis. Because this technique is very sensitive, scientists obtain detailed data using nanogram-sized samples.

Scientists can use smaller samples of rare bacterial proteins or air pollutants than required for more traditional approaches, skip the sample preparation process, and still get precise data. The team will use this technique to analyze a broad range of environmental and biological samples such as oil samples and *Shewanella oneidensis*, a common microbe of interest for cleaning up contaminated nuclear weapons sites.

Roach PJ, J Laskin, and A Laskin. 2010. "Nanospray Desorption Electrospray Ionization: An Ambient Method for Liquid-Extraction Surface Sampling in Mass Spectrometry." *Analyst* **135**(9):2233-2236. DOI: 10.1039/C0AN00312C.

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

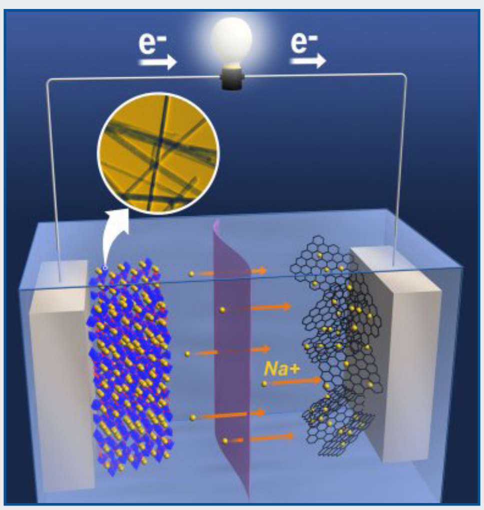
PNNL scientists developed nanoDESI, a fast, user-friendly method for surface sampling in mass spectrometry. It was featured on the September 2010 cover of *Analyst*. Image reproduced by permission of Pacific Northwest National Laboratory and the Royal Society of Chemistry.



The Heat Is On for **RECHARGEABLE BATTERIES**

By adding the right amount of heat to nanomaterials, scientists from Pacific Northwest National Laboratory and China's Wuhan University have improved the electrical capacity and recharging lifetime of sodium ion rechargeable batteries—a cheaper, safer alternative to lithium ion batteries for storing solar and wind energy sources on the electrical grid. Electrodes in lithium batteries are made of manganese oxide, the atoms of which form holes and tunnels that lithium ions go through when batteries are being charged or in use. The free movement of the ions allows the battery to hold electricity or release it in a current. But sodium ions are 70 percent bigger than lithium ions and don't fit or travel as well.

The scientists mixed manganese oxide nanomaterials and treated them with high temperatures to make bigger holes in the electrodes that would enable them to accept sodium ions. Treating the manganese oxide at 750 degrees Celsius created the best crystals through which the ions could flow.

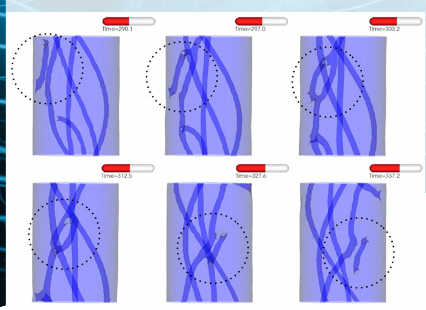


The crystalline, uniform nanostructure of heat-treated manganese oxide provides pathways in which sodium ions can flow, improving the performance of the manganese oxide electrodes.

Cao Y, L Xiao, W Wang, D Choi, Z Nie, J Yu, LV Saraf, Z Yang, and Jun Liu. 2011. "Reversible Sodium Ion Insertion in Single Crystalline Manganese Oxide Nanowires with Long Cycle Life." *Advanced Materials* **23**(38): 3155-3160. DOI: 10.1002/adma.201100904.

Sponsors: Department of Energy Office of Basic Energy Sciences, Office of Electricity Delivery and Energy Reliability

Computational Sciences & Mathematics



Fermionic vortex crossings and exchanges are shown as time progresses in an excited system of cold atoms in an elongated trap. The process is reminiscent of DNA recombination and indicative of the onset of quantum turbulence. The dynamics of quantum turbulence in Fermi systems may provide insight into the pinning and de-pinning vortex mechanisms in neutron stars, for example.

Modeling the Bizarre: QUANTUM SUPERFLUIDS

Superfluidity is a quantum mechanical phenomenon in systems composed of a very large number of microscopic particles that can be observed with the naked eye. Remarkable features of such systems include fluids that creep up the sides of a container and overflow with no external influence. When a superfluid is rotated or swirled, it develops cylinder-like vortices. A team from Pacific Northwest National Laboratory, University of Washington, and China's Key State Laboratory of Magnetic Resonance, Atomic and Molecular Physics has described how these vortices form and evolve microscopically at very low temperatures in fermionic gas systems. They also described the vortices as they cross and reconnect.

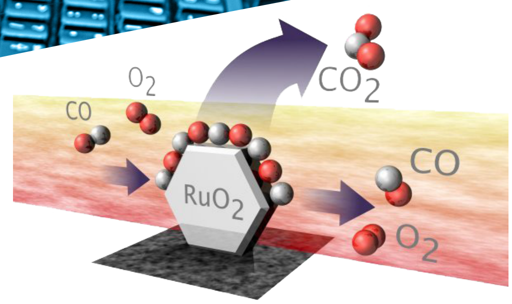
Their simulations show that the system frequently remains superfluid even when stirred at supercritical speeds, in contrast to a decades-old hypothesis that predicts the system would lose its superfluid properties under these circumstances. The methods developed will open new avenues of research both in nuclear physics and astrophysics, as well as in condensed-matter and related fields.

Bulgac A, YL Luo, P Magierski, KJ Roche, and Y Yu. 2011. "Real-Time Dynamics of Quantized Vortices in a Unitary Fermi Superfluid." *Science* **332**(6035):1288-1291. DOI: 10.1126/science.1201968.

Sponsor: Department of Energy Advanced Scientific Computing Research and Office of Nuclear Physics

ACCOUNTING FOR SCALE in Catalysis

Depicting a catalyst's behavior in the real world is now much easier, thanks to scientists in the Institute for Integrated Catalysis at Pacific Northwest National Laboratory. They used complex calculations to describe the surface temperature of a reaction based on the catalyst's thickness, the heat transferred in the reaction, and the reactant's transport. Carbon monoxide oxidation on a ruthenium dioxide (RuO_2) catalyst was the example used because of its importance in industrial reactions. These multi-scale simulations can predict limitations imposed by environmental variables in real-world situations, improving catalysts for many important practical applications, such as oil refining, pharmaceutical manufacturing, and energy production and storage.



The thickness of the RuO_2 catalyst, along with heat and mass transfer, affect the speed with which carbon monoxide is converted to carbon dioxide.

Mei D and G Lin. 2011. "Effects of Heat and Mass Transfer on the Kinetics of CO Oxidation over RuO_2(1 1 0) Catalyst." *Catalysis Today* **165**(1):56-63. DOI: 10.1016/j.cattod.2010.11.041.

Sponsors: Department of Energy Advanced Scientific Computing Research, PNNL Laboratory Directed Research and Development

Improving QUANTUM MECHANICAL MODELING

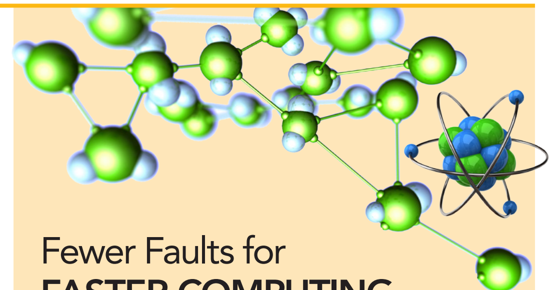
Pacific Northwest National Laboratory researchers led a team that developed a scalable parallel algorithm that overcomes inefficiencies associated with calculating the exact exchange interaction from the Hartree-Fock method, a key computational physics theory, and improves implementation of specific functionals in density functional theory (DFT)—a quantum mechanical modeling method. DFT is used to calculate the properties of solid-state and molecular systems, and it predicts structures, properties, and reactivities for a wide variety of systems important to solar, hydrogen storage, catalytic, nuclear, and environmental remediation technologies. But it frequently gives inaccurate predictions.

The researchers developed parallel algorithms to distribute data and replicated data to overcome bottlenecks associated with calculating the exact exchange term. These algorithms were implemented in a module in PNNL's NWChem high-performance chemistry software package that is used to calculate surfaces and condensed phase systems. The developments were then used to successfully perform hybrid-DFT calculations on several surface and condensed phase systems.

The algorithms scaled up to 25,000 CPUs for a modest problem and can be applied to a wide variety of plane wave programs. Recently they were demonstrated to scale to 100,000 CPUs on the Hopper computer system at the National Energy Research Scientific Computing Center. This work was featured on the cover of the *Journal of Computational Chemistry*.

Bylaska EJ, KL Tsemekhman, SB Baden, JH Weare, and H Jonsson. 2011. "Parallel Implementation of γ-Point Pseudopotential Plane-Wave DFT with Exact Exchange." *Journal of Computational Chemistry* **32**(1):54-69. DOI: 10.1002/jcc.21598.

Sponsor: Department of Energy Advanced Scientific Computing Research and Office of Basic Energy Sciences



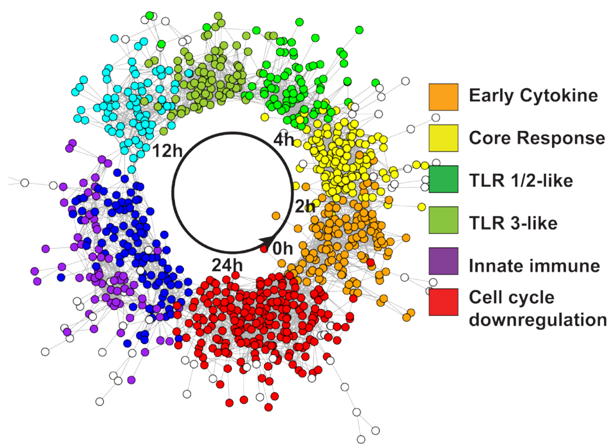
DEFENDING AGAINST DISEASE

Macrophages, tiny cells that provide the immune system with a primary line of defense against pathogens, reveal much about themselves when challenged, according to scientists at Pacific Northwest National Laboratory. They identified a common mechanism underlying macrophage response by presenting the cells with three different insults, viral and bacterial components, silica nanoparticles, and *Salmonella*, to determine patterns and control points within defense response networks. Such knowledge can be used to develop therapeutic treatments for infectious diseases.

The scientists used computational network inference, pathway analysis, and a predictive modeling approach that infers dependencies. Among their findings: a core response module of genes that responded to all three stimuli, the first comparison of macrophage responses to nanoparticles and pathogen exposure, and the first report of applying this approach to data from a vertebrate.

McDermott JE, M Archuleta, BD Thrall, JN Adkins, and KM Waters. 2011. "Controlling the Response: Predictive Modeling of a Highly Central, Pathogen-Targeted Core Response Module in Macrophage Activation." *PLoS One* **6**(2):e14673.

Sponsors: National Institute for Allergy and Infectious Diseases, National Institute of Environmental Health Sciences, PNNL Laboratory Directed Research and Development



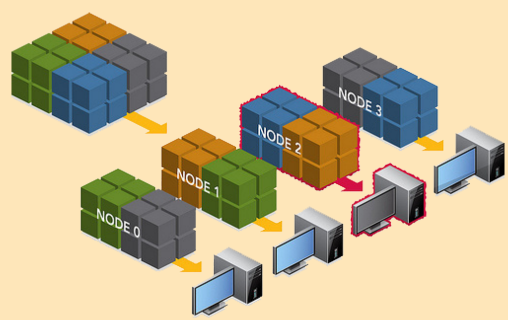
Co-expression network of macrophage response to nanoparticle exposure shows time progression through functional modules identified by color (see legend).

Fewer Faults for FASTER COMPUTING

Computational chemistry challenges are now being addressed with a new, efficient, fault-tolerant method. Researchers at Pacific Northwest National Laboratory designed and implemented a version of the coupled-cluster method, a numerical technique for describing many-body systems such as atoms and molecules, for high-performance computational chemistry. Their method addresses the computational chemistry challenge of reduced mean time to repair between failures, which is currently days and is projected to be hours for upcoming extreme-scale supercomputers. The team extended the Global Arrays toolkit, a library that provides an efficient and portable "shared-memory" programming interface for distributed-memory computers. Such advances in supercomputing will enhance the ability to address climate change and energy solutions using top-end computing platforms.

van Dam HJJ, A Vishnu, and WA de Jong. 2011. "Designing a Scalable Fault Tolerance Model for High-Performance Computational Chemistry: A Case Study with Coupled Cluster Perturbative Triples." *Journal of Chemical Theory and Computation* **7**:66-75. DOI: 10.1021/ct100439u.

Sponsor: PNNL Laboratory Directed Research and Development

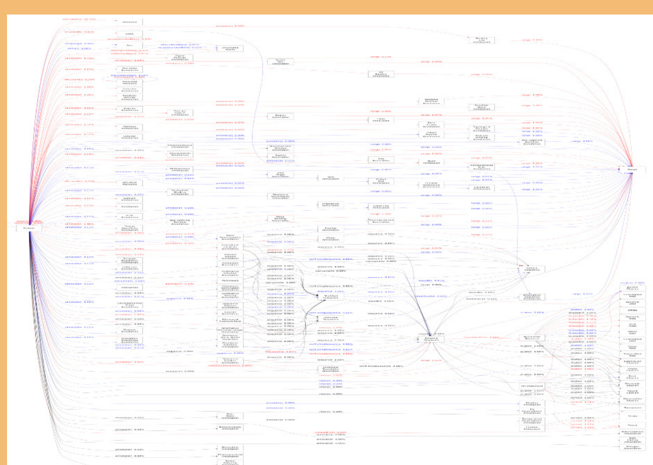


Redundant data distribution of an array showing that a node failure will leave at least one copy of the data available for continued execution.

Team places second in "BILLION TRIPLE CHALLENGE"

Researchers from Pacific Northwest National Laboratory, Sandia National Laboratories, and Cray, Inc., won 2nd place in the "Billion Triple Challenge" for implementing novel high-performance computing applications that can perform semantic factoring of massive semantic graph databases (SGDs).

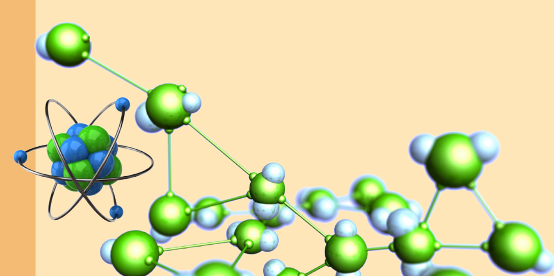
This international competition is focused on demonstrating capability and innovation for dealing with SGDs. The team showed the ability to perform semantic factoring—the process of analyzing categories of information into a collection of related groups—of giga-scale-sized datasets using the large multithreaded architecture of the Cray XMT platform, conventional clusters, and large data stores. The team then used their applications to analyze these datasets for the Challenge.



Massive amounts of data can be analyzed using a novel hybrid system for semantic factoring in graph databases. Each line represents a frequent relationship type between entities in the dataset.

Joslyn C, R Adolf, S al-Saffar, J Feo, E Goodman, D Haglin, G Mackey, and D Mizell. 2010. "High Performance Semantic Factoring of Giga-Scale Semantic Graph Databases." Semantic Web Challenge Billion Triple Challenge.

Sponsor: PNNL's Center for Adaptive Supercomputing Software-Multithreaded Architectures



Awards & Honors

Two Receive EARLY CAREER GRANTS

Matthew Marshall and Alexandre Tartakovsky received the Department of Energy's Early Career Research Award to advance their research involving microbial biofilms and computer modeling. The award supports exceptional researchers during their early career years. Each will receive grants totaling $2.5 million over 5 years.

Matthew Marshall

Alexandre Tartakovsky

Mass Spec Technology Wins R&D 100 AWARD

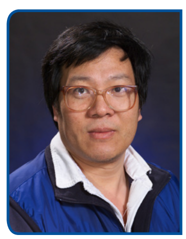
David Koppenaal is lead developer of a breakthrough technology for mass spectrometry detectors that won a 2011 R&D 100 Award from *R&D Magazine* as one of the 100 top technology products. The Array Detection Technology for mass spectrometry simultaneously monitors and detects wide mass ranges, allowing a test sample to be analyzed in a single run, saving time, increasing efficiency, and simplifying the analysis process. Applications include nonproliferation monitoring, forensics, environmental monitoring, and industrial hygiene.

LIEM X. DANG and GREGORY A. KIMMEL American Physical Society Fellows

Dang was honored for developing and applying molecular dynamics simulation methods and reliable polarizable potential models for studying processes in solution and at liquid interfaces.

Kimmel was recognized for his seminal contributions to understanding the structure and electron-stimulated reactivity of interfacial water.

CHONGXUAN LIU Geological Society Fellow



Liu was selected for his outstanding contributions in microscopic reactive transport in porous media and applying geosciences to understand and solve environmental problems.

JIM K. FREDRICKSON and MOE KHALEEL Elected to State Academy of Sciences

Fredrickson and Khaleel were elected to the Washington State Academy of Sciences for outstanding scientific achievement. They will review and assess initiatives and provide state policymakers with scientific counsel.

Fredrickson's research focuses on belowground microbes and their role in moving metals and radioactive contaminants in the subsurface. Khaleel's research focuses on computational engineering and fuel cell technology.

JOHANNES A. LERCHER Robert Burwell Lecturer for Catalysis Society

This honor from the North American Catalysis Society recognizes outstanding contributions in catalysis research. Lercher will present talks at catalysis clubs and societies for the next 2 years.

RICHARD H. MOSS Chair of National Research Council Committee

Moss was appointed Chair of the Committee on the Human Dimensions of Global Change of the National Academy of Sciences' National Research Council based on his leadership and experience working on global change scenarios, characterization and communication of uncertainty, and adaptation to climate change.

RICHARD D. SMITH Scientist of the Year

Smith was named Scientist of the Year by *R&D Magazine* for his pioneering work in effectively combining the development of new technology with its application to biological systems to gain new insights.

WILLIAM F. MORGAN International Commission on Radiation Protection

Morgan was elected to the Main Commission of the International Commission on Radiological Protection (ICRP) and named Chair of the ICRP's committee on Radiation Effects. He has an international reputation as a leading researcher in radiation biology and the long-term biological effects of radiation exposure.

MOE KHALEEL

Fellow of American Society of Civil Engineers

Khaleel was selected for his distinguished contributions to the field of computational engineering sciences, particularly computational multi-physics modeling of complex systems.

L. RUBY LEUNG and JAMES A. EDMONDS

Serving on NRC Study Committee

The National Research Council's "A National Strategy for Advancing Climate Modeling" study committee was selected by the National Academy of Sciences to develop a strategy for improving the nation's ability to accurately simulate climate and related Earth system changes.

Leung is internationally recognized for her research on modeling regional climate change and the hydrologic cycle.

Edmonds is a pioneer in the field of integrated assessment of climate change and the examination of interactions among energy, technology, policy, and the environment.

ORESTE VILLA and ANTONINO TUMEO

Win Computational Research Center for Lab

The work of Villa and Tumeo enabled Pacific Northwest National Laboratory to be named a 2011 NVIDIA CUDA Research Center, one of 35 CUDA Research Centers and CUDA Teaching Centers in 14 countries, further advancing the growth of parallel computing across the world.

KATHY A. HIBBARD

Chair of American Geophysical Union Fall Meeting Program Committee

Hibbard is chairing the Program Committee for the 2011 AGU Fall Meeting, the largest worldwide conference in the geophysical sciences. She is recognized for her expertise in understanding and modeling terrestrial biogeochemical cycles, ecological systems, and interactions between human activities and natural systems.

2011 AAAS FELLOWS

Five scientists were named fellows of the American Association for the Advancement of Science for their exceptional efforts to advance science and apply it to real-world problems. They were honored at the annual meeting in Washington, D.C. in February.

LIEM DANG

For outstanding efforts to develop and use computer models to study how molecules interact at liquid interfaces and help explain how pollutants react in the atmosphere and how toxic metals are transported.

CÉSAR IZAURRALDE

For exceptional efforts to advance science and apply it to real-world problems. His research is critical to how soil, water, and plants are affected by human actions and climate change. He develops and improves computer models that examine climate change in agricultural systems and biogeochemical cycles in soil.

ALLAN KONOPKA

For distinguished contributions to microbial ecology, with particular emphasis on the roles of physiological adaptations to environmental perturbations and the relationship between microbial community structure and its function.

BILL MORGAN

For outstanding contributions toward understanding the biological effects of ionizing radiation and distinguished service to the radiation protection community.

GREG SCHENTER

For development of mathematical models to advance how scientists simulate molecular behavior and help build better batteries and alternative fuels.

ALLA N. ZELENYUK

Invited Speaker at National Academies Workshop

Zelenyuk was selected to speak at the workshop "Challenges in Characterizing Small Particles" October 25 in Washington, D.C., because of her reputation in developing and applying instruments to study processes governing nanoparticle chemistry and microphysics.

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 2011. 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 2011, PNNL welcomed a new director, Johannes Lercher, to the Institute for Integrated Catalysis, the largest non-industrial catalysis research and development effort in the United States. The Institute will advance catalysis science to help the nation secure a strong, clean energy future.

You can find out even more about our research, staff, and capabilities on our website at **http://www.pnnl.gov/science/**. Please don't hesitate to contact me or one of the division directors 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 Pacific Northwest National Laboratory

Pacific Northwest National Laboratory is a Department of Energy Office of Science national laboratory where interdisciplinary teams advance scientific frontiers and deliver solutions to America's most intractable problems in energy, the environment, and national security. PNNL employs 5,000 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.

For more information about the Fundamental & Computational Sciences Directorate, contact:

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▶ www.pnnl.gov/science

About the Cover: *Scientists at Pacific Northwest National Laboratory have embedded a high-resolution cloud and aerosol model within each grid cell of a global climate model for a new way to account for the effects of small pollution particles. PNNL is at the forefront of global and regional modeling of climate and related human and environmental systems, especially the development and testing of new methods for incorporating multi-scale microphysical, environmental, and socio-economic factors for more accurate climate predictions.*

Pacific Northwest NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY

PNNL-SA-82929 | October 2011

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