Pacific Northwest
NATIONAL LABORATORY

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PACIFIC NORTHWEST NATIONAL LABORATORY

2015 Key Accomplishments

IN PNNL'S SCIENCE MISSION

U.S. DEPARTMENT OF
ENERGY

DISCOVERY *in Action*

This year has brought many exciting changes to the science mission at Pacific Northwest National Laboratory. The laboratory appointed a new director, Steve Ashby, who made the bold decision to create an additional directorate devoted to science. Thus, PNNL now has two complementary science directorates—the Earth and Biological Sciences Directorate and the Physical and Computational Sciences Directorate. This change strengthens and elevates the impact and visibility of our science mission generally, and for the Department of Energy Office of Science in particular.

The development, effective Oct. 1, 2015, is the capstone to a year of outstanding science progress at PNNL. We're proud of the impact of our science on many of the nation's most important challenges in environmental sustainability, national security, and health, among other areas.

Many of our new findings this year furthered our knowledge of climate science. Researchers ferreted out the mighty role that the ocean's tiniest creates play in the formation of clouds and described the part that microbes play in many facets of our climate. Many of the findings form the basis for ever-better climate models, which are key to understanding climate issues in the future.

Other findings address a range of challenges. PNNL scientists continue to be very active in the search for dark matter, in investigations that shed light on the origins of the universe. We are tackling the biggest challenges in the realm of computing, pioneering the science that underpins a level of computing power barely thought possible just a decade ago. Our work on catalysts, which power so many chemical processes, is critical to energy production.

EMSL delivered top-notch science this past fiscal year while bringing online new capabilities to drive future advances. We kicked off the 12 projects chosen the previous year in the Collaborative Science Initiative with the DOE Joint Genome Institute. We're pleased with the progress the teams have seen, and these projects follow other impactful collaborations between the two user facilities, such as the Archaeal study you'll read about on page 12. We also welcomed the new 21 Tesla Fourier Transform Ion Cyclotron Resonance Mass Spectrometer, which was developed to realize advancements in carbon cycling, microbial biology and atmospheric aerosol characterization. In FY16, we anticipate seeing early fruits of the labor with the 21T.

Thank you for taking the time to learn about some of the scientific progress delivered by PNNL in the past year. If you are interested in collaborating with us, or desire additional information, please don't hesitate to reach out to us or one of the other individuals listed on the back of this brochure.

Allison A. Campbell, Ph.D.
Acting Associate Laboratory Director
Earth and Biological Sciences Directorate

Louis Terminello, Ph.D.
Acting Associate Laboratory Director
Physical and Computational Sciences Directorate

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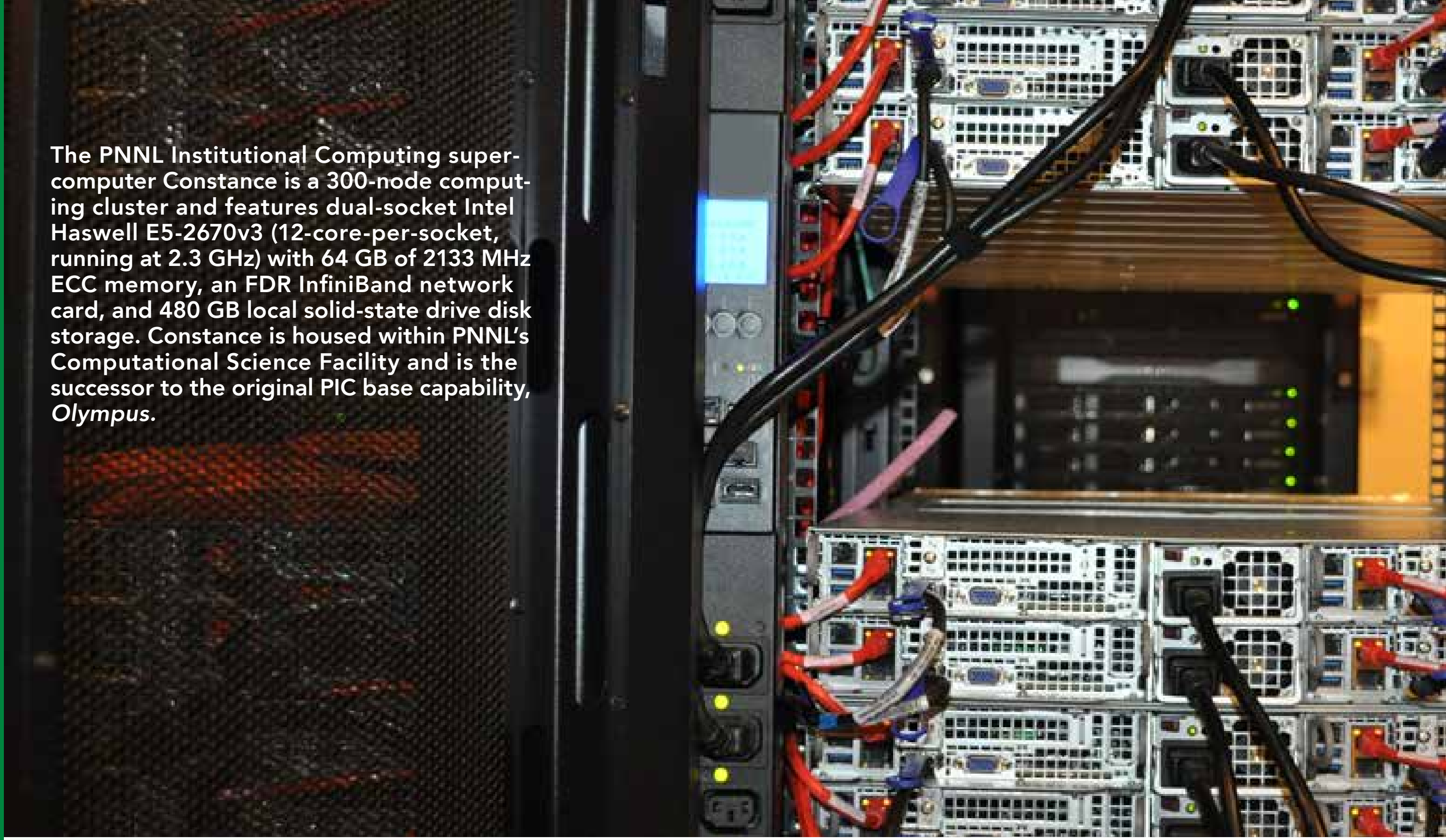
Cover image: The *Arabidopsis* plant's root structure, shown in a cross-section view, is helping to improve understanding of the rhizosphere, or plant root zone. Researchers believe learning more about the rhizosphere will help clarify environmental processes, and perhaps give rise to future climate and environmental solutions. Toward this goal, a rhizosphere research campaign was initiated at EMSL focusing on the plants' management of carbon nutrients and subsequent impacts on the diversity of the rhizosphere. The campaign includes scientists from EMSL, PNNL, DOE's Joint Genome Institute, Brookhaven National Laboratory, the University of Minnesota and the University of Missouri. The work is funded by DOE's Office of Biological and Environmental Research.



The PNNL Institutional Computing supercomputer Constance is a 300-node computing cluster and features dual-socket Intel Haswell E5-2670v3 (12-core-per-socket, running at 2.3 GHz) with 64 GB of 2133 MHz ECC memory, an FDR InfiniBand network card, and 480 GB local solid-state drive disk storage. Constance is housed within PNNL's Computational Science Facility and is the successor to the original PIC base capability, *Olympus.*

The Dynamics of Mixing

Understanding the dynamics of mixing on reaction kinetics at the pore scale can directly influence quality and usability of models that measure reactive transport in carbon dioxide storage, subsurface flow and transport, or mixing-driven biochemical processes in filters and/or living tissues. By considering the reaction front of heterogeneous fluid flows in porous media, whose reaction rates are sharply influenced by compression and diffusion, a collaborative international team of researchers developed a new model for predicting reaction front kinetics in these flows that provides a more complete assessment regarding the effects of many processes—stretching, coalescence, and fluid particle dispersion—on reactive transport dynamics.

"This new method provides a more complete look at the reaction front kinetics—one that accounts for compression, diffusion, and lamellae behaviors—rather than being based solely on geometric analysis. It has great potential for improving reactive transport modeling used in a range of applications."

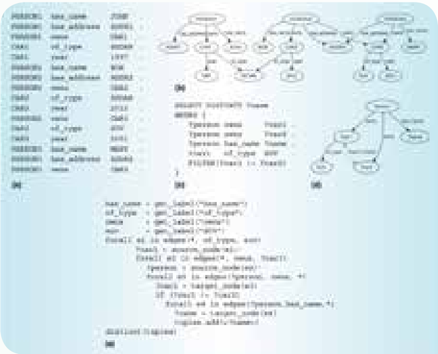
—Dr. Alexandre Tartakovsky, PNNL Associate Division Director, Computational Mathematics

de Anna P, M Dentz, A Tartakovsky, and T Le Borgne. 2014. "The Filamentary Structure of Mixing Fronts and its Control on Reaction Kinetics in Porous Media Flows." *Geophysical Research Letters* 41(13):4586-4593. DOI:10.1002/2014GL060068.

Sponsor: DOE Office of Science, Office of Advanced Scientific Computing Research

A Meaningful Data Miner

As data sets grow increasingly large and heterogeneous, or "too big," their value diminishes if they cannot be mined with precision and purpose. Furthering work involving the Graph Engine for Multithreaded Systems, or GEMS, a multilayer software framework for querying graph databases developed at PNNL, scientists from PNNL and NVIDIA Research used GEMS to customize commodity, distributed-memory high-performance computing clusters and applied graph algorithms to large-scale data sets on clusters. By incorporating GEMS, HPC query solutions, such as parallel processing, are exploited and results are more predictable. When compared with alternate approaches, GEMS provided noticeable speedups, particularly with larger data sets. GEMS represents a promising solution to tackle the "too big" challenge as it already can process data in the scale of 10 billion triples, which is prohibitive for most available systems.



Data mining through graph methods using the GEMS framework on currently available computing components, or commodity clusters, affords more efficient use of space and added performance by exploiting graph parallelism.

Castellana VG, A Morari, J Weaver, A Tumeo, D Haglin, O Villa, and J Feo. 2015. "In-Memory Graph Databases for Web-Scale Data." *Computer* 48(3):24-35. DOI:10.1109/MC.2015.74.

Sponsor: DOE Office of Science, Office of Advanced Scientific Computing Research

Energy Star

To achieve high resiliency and efficiency on future exascale computing systems (capable of a billion billion calculations per second), scientists examined some advanced high-performance computing systems and determined that undervolting, or dynamic voltage scaling to reduce power consumption, that leverages existing mainstream resilience techniques at scale improved system failure rates. The team demonstrated up to 12 percent energy savings over baseline runs (with eight HPC benchmarks) and up to nine percent savings against state-of-the-art dynamic voltage and frequency scaling solutions currently used to lower the operating frequency of hardware. Notably, the results are based on a conservative assumption of the total energy savings because the model applies the peak range of the failure rates.

"Power sources are not unlimited nor are they free, and in a computing system, primary reasons for failures include radiation from the cosmic rays, packaging materials, and temperature fluctuation. These are crucial challenges affecting the push to extreme-scale systems. Our undervolting method does not modify existing hardware or require pre-production machines and has shown positive results toward achieving a cost-efficient energy-savings implementation for the HPC field."

—Dr. Shuaiwen Leon Song, PNNL computational scientist

Tan L, SL Song, P Wu, Z Chen, R Ge, and DJ Kerbyson. 2015. "Investigating the Interplay between Energy Efficiency and Resilience in High Performance Computing." In *2015 IEEE International Parallel & Distributed Processing Symposium (IPDPS 2015)*, pp. 786-796. May 25-29, 2015, Hyderabad, India. Institute of Electrical and Electronics Engineers, Piscataway, New Jersey. DOI:10.1109/IPDPS.2015.108.

Sponsors: DOE Office of Science, Office of Advanced Scientific Computing Research, National Science Foundation

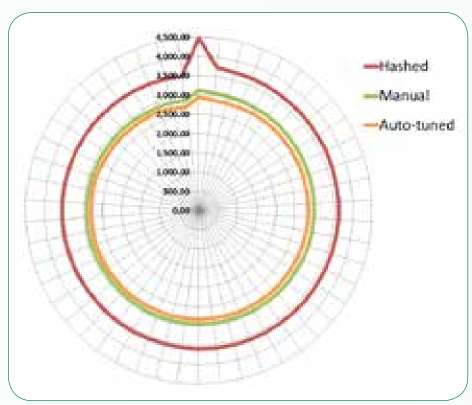
The Speed to Solution

For scientists at PNNL, whose work often crosscuts many domain science sectors, seeking a way to use algorithmic graph theory to enhance data analytics of biological sequences led to a distinct intersection with work being done for high-performance computing applications contending with obstacles related to power constraints and massive data movement.

While working on research involving biological sequencing, an associate professor at Washington State University faced a challenge: because of the sheer scope of data generated from varied technologies, it was essential to find a way to make said data both less redundant and useful. He partnered with PNNL to improve the value of the biological data using mathematical tools, namely graph theory and a clustering operation known as "community detection," used in graph applications to reveal natural divisions that exist in networks without size or element constraints.

An interesting side effect of the research that started with a biology data dilemma is that the underlying data analytics efforts spawned yet another problem to explore: tackling the challenges posed by power constraints and data movement, which currently inhibit HPC applications. In this case, a scalable tool for community detection on the Tilera platform was developed—the first effort of its kind to address graph algorithms using the many-core architecture. These architectures are relevant in addressing the mismatch between ever-growing data sets and constraints in power and energy available to individual platforms and data centers.

Markedly, the case studies presented by these combined works involving algorithm development, parallelization, and testing for the community detection application show how the evolution of specific graph theory methods are a boon to developers seeking to improve application performance.

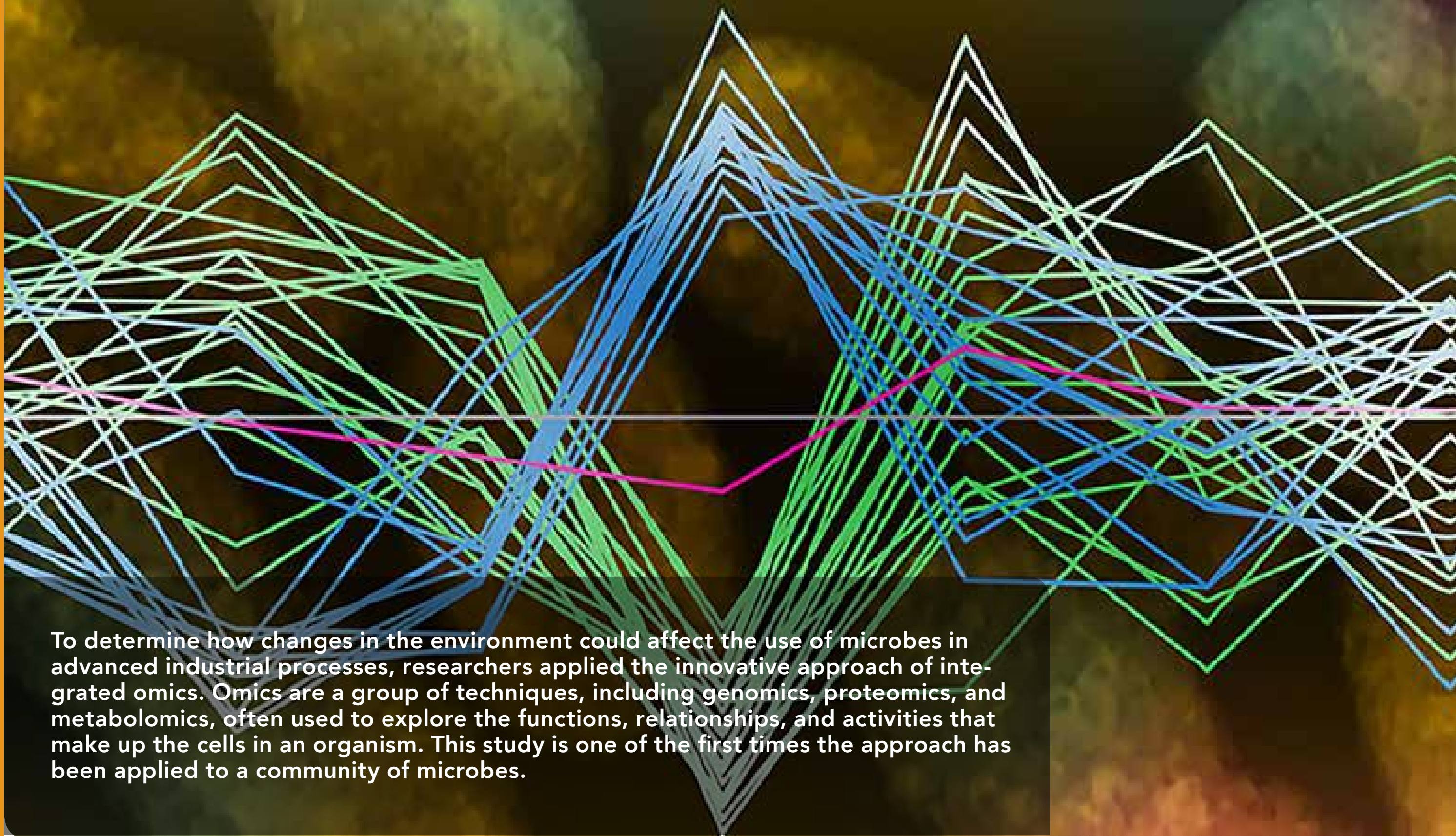


Energy consumption of different implementations for community detection on Tilera platform—the first effort of its kind to address graph algorithms using the many-core architecture. Lower consumption is better.

Lu H, M Halappanavar, and A Kalyanaraman. 2015. "Parallel Heuristics for Scalable Community Detection." *Parallel Computing* 47:19-37. DOI:10.1016/j.parco.2015.03.003.

Chavarría-Miranda D, M Halappanavar, and A Kalyanaraman. 2014. "Scaling Graph Community Detection on the Tilera Many-core Architecture." *21st International Conference on High Performance Computing* (HiPC), pp.1-11. December 17-20, 2014, Goa, India. IEEE Computer Society, Washington, D.C. DOI:10.1109/HiPC.2014.7116708.

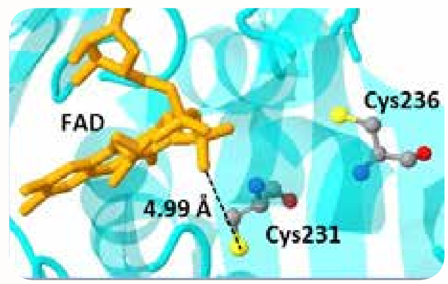
Sponsors: DOE Office of Science, Office of Advanced Scientific Computing Research; the U.S. Department of Defense under the Autotuning for Power, Energy & Resilience (ATPER) project



To determine how changes in the environment could affect the use of microbes in advanced industrial processes, researchers applied the innovative approach of integrated omics. Omics are a group of techniques, including genomics, proteomics, and metabolomics, often used to explore the functions, relationships, and activities that make up the cells in an organism. This study is one of the first times the approach has been applied to a community of microbes.

Mapping Redox Reactions in Cyanobacteria

Chemical reactions involving reduction and oxidation, or redox, play a key role in regulating photosynthesis in plants and metabolism in animals and humans, keeping things running on an even keel. A team of scientists from PNNL and Washington University in St. Louis shed light on the role redox plays in cyanobacteria, tiny organisms with the potential to produce a lot of energy. The team discovered more than 2,100 molecular locations inside a cyanobacterium where an amino acid known as cysteine either switched on or off by redox processes when the cyanobacteria were exposed to light or dark. The work significantly expanded the current repertoire of known redox changes within cyanobacteria.



A research team led by PNNL mapped more than 2,100 sites that may switch redox reactions on and off in cyanobacteria. How these redox switches react in light and darkness will affect cyanobacteria's use in producing biofuels.

Guo J, AY Nguyen, Z Dai, D Su, MJ Gaffrey, RJ Moore, JM Jacobs, ME Monroe, RD Smith, DW Koppenaal, HB Pakrasi, and W Qian. 2014. "Proteome-wide Light/Dark Modulation of Protein Thiol Oxidation in Cyanobacteria Revealed by Quantitative Site-Specific Redox Proteomics." *Molecular & Cellular Proteomics* 13(12):3270-3285. DOI:10.1074/mcp.M114.041160.

User Facility: EMSL
Sponsor: DOE Office of Science, Office of Biological and Environmental Research

"This work provides a quantitative and site-specific analysis across the entire complement of proteins in cyanobacteria, giving us a much clearer picture of the kind of conditions cyanobacteria will need to thrive in industrial settings."

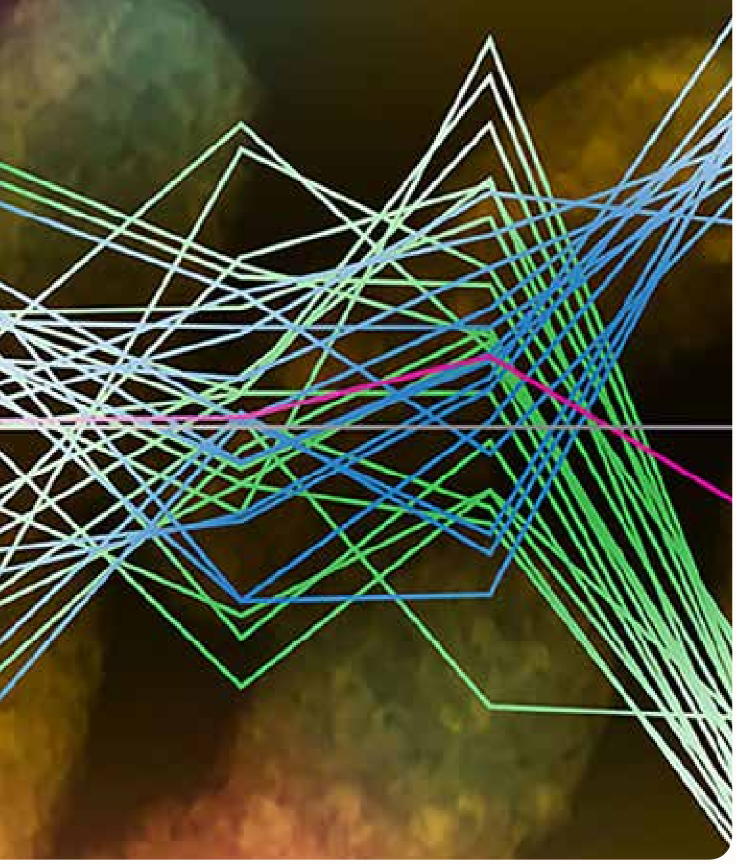
—Dr. Wei-Jun Qian, PNNL bioanalytical chemist

The Best Light for Biofuel

Rapidly growing bacteria that live in the ocean and can manufacture their own food hold promise as host organisms for producing chemicals, biofuels, and medicine. Researchers at PNNL and Pennsylvania State University are closely studying one of these photosynthetic species of fast-growing cyanobacteria, *Synechococcus*, using a photobioreactor custom built by PNNL. The reactor simulates a natural environment for an organism, allowing scientists to vary things like food, water, air, and light. To determine the optimum environment that contributes to record growth and productivity, the team exposed cyanobacteria to orange light, red light, and a combination. They discovered that a combination of the two pigment-specific light sources yielded the highest growth rate overall. Their work could help determine the optimum growing conditions for biofuels. A deeper understanding of the basic biology for this organism is helping us develop solutions for efficient renewable energy production and will ultimately help us develop novel technologies based on microbial communities.

Bernstein HC, A Konopka, MR Melnicki, EA Hill, LA Kucek, S Zhang, G Shen, DA Bryan, and AS Beliaev. 2014. "Effect of Mono- and Dichromatic Light Quality on Growth Rates and Photosynthetic Performance of Synechococcus sp. PCC 7002." *Frontiers in Microbiology* 5:488. DOI:10.3389/fmicb.2014.00488.

Sponsor: DOE Office of Science, Office of Biological and Environmental Research



New Assay Platform Detects Largest Number of Known Biotoxins Simultaneously

The largest panel of biotoxins simultaneously detected was achieved using an assay platform developed by scientists at PNNL. The enzyme-linked immunosorbent assay microarray detected 10 plant and microbial toxins in a diverse range of samples such as blood, saliva, urine, stool, milk, and apple juice. The detected toxins included ricin, botulinum neurotoxins, shiga, and staphylococcal enterotoxin B. Previously, the largest number of toxins to be simultaneously detected was six.

Protein toxins are potential biological threat agents because of their extreme toxicity, widespread availability, and ease of use. Such toxins have been stockpiled for bioweapon use and even used in previous bioterrorism events. To treat exposures, sensitive and specific detection systems are needed to quickly identify multiple biothreat toxins.

"Most assays to detect toxins target one or two toxins at a time, at best. In the event of a bioterrorist attack, it may not be obvious which agent was released, although this knowledge is critical for delivering appropriate medical treatment."

—Dr. Susan Varnum, PNNL cell biologist and biochemist

Jenko K, Y Zhang, Y Kostenko, Y Fan, C Garcia-Rodriguez, J Lou, JD Marks, and SM Varnum. 2014. "Development of an ELISA Microarray Assay for the Sensitive and Simultaneous Detection of Ten Biodefense Toxins." *Analyst* 139(20):5093-5102. DOI:10.1039/c4an01270d.

Sponsor: National Institutes of Health and other funding

Low-Dose Radiation Impacts Skin Sensitivity

PNNL scientists found a skin tissue model showed previously undetectable changes when exposed to low doses of ionizing radiation, suggesting that the skin's stability is altered. This exposure, in turn, could change skin's susceptibility to insults, such as infection. The team exposed tissue samples of normal human surface, or epidermal, skin cells and underlying dermal fibroblasts to low levels of ionizing radiation. They then measured the response of the skin over the next 1 to 72 hours. Using a global omics approach, they identified patterns of perturbed biological pathways that indicated persistent alterations in the cell and tissue stability. This change in stability could change skin's sensitivity after exposure to low-dose radiation. For example, patients receiving even low doses of radiation from medical applications could have altered skin resistance to opportunistic infections or other environmental exposures, in addition to an increased risk of cancer.

Global omics studies at PNNL show impacts of low doses of radiation, such as those from a CT scan, on skin stability.

Tilton SC, TJ Weber, BJM Webb-Robertson, H Shankaran, MB Sowa, DL Stenoien, WF Morgan, and KM Waters. 2015. "Data Integration Reveals Key Homeostatic Mechanisms Following Low Dose Radiation Exposure." *Toxicology and Applied Pharmacology* 285(1):1-11. DOI:10.1016/j.taap.2015.01.019.

User Facility: EMSL
Sponsor: DOE Office of Science, Office of Biological and Environmental Research

Microbial Life in Permafrost Could Lead to Increased Methane Releases

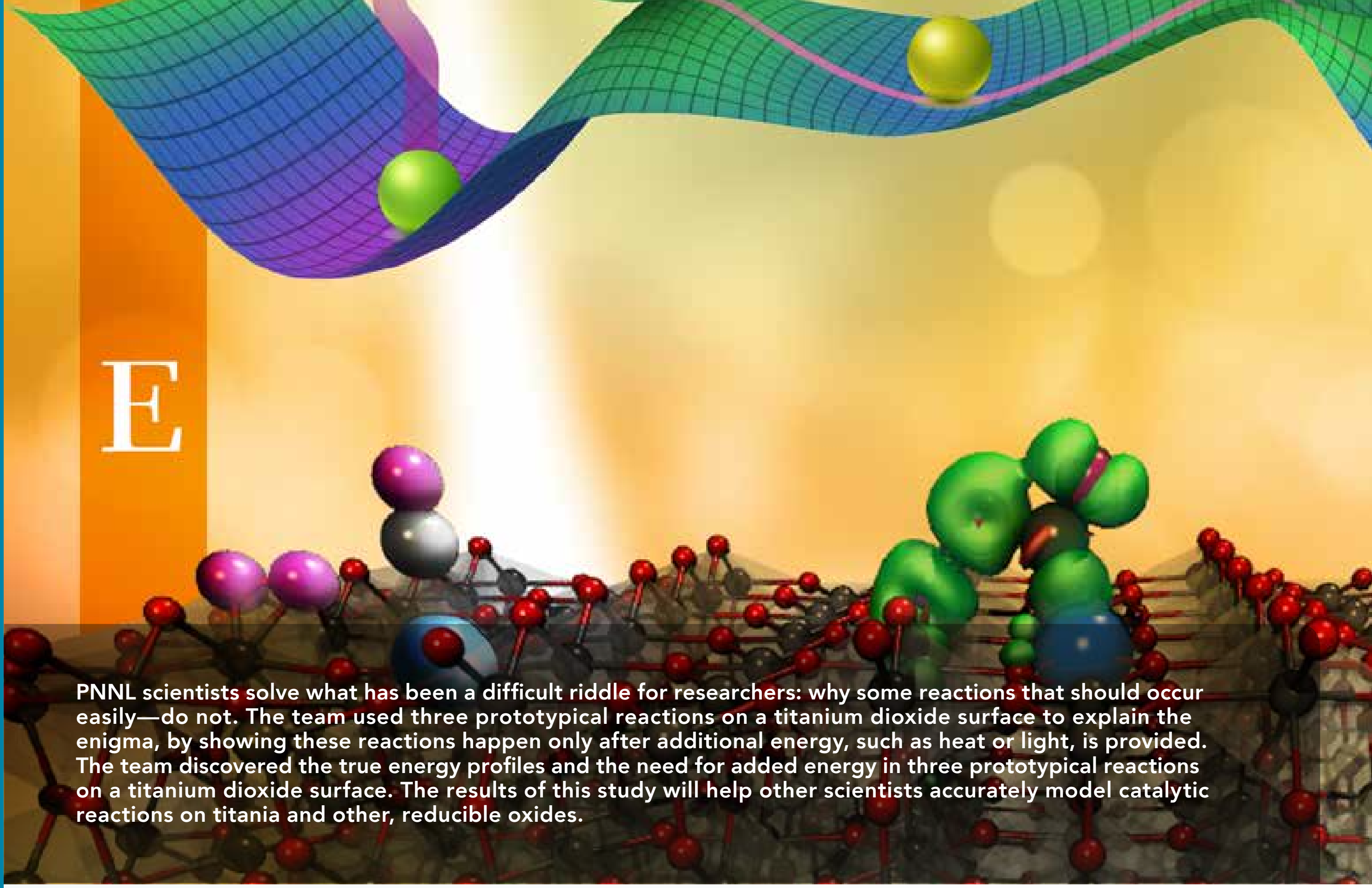
PNNL scientists who looked at microbes in different types of Arctic soil have a new picture of life in permafrost, revealing an entirely new species and hinting that subzero microbes might be active. Their work found an undiscovered diversity of microbes in Arctic soils and was able to describe several completely novel microbes in each type of soil. The activity of the microbes was also notable. Although the permafrost microbes lived at subzero temperatures and had many proteins to protect against freezing, they also wielded proteins that indicated they could move through the soil, use iron for energy, or live on methane. Such information is key to prepare for the release of gigatons of methane, which could set the Earth on a path to irreversible global warming.

"The microbes in permafrost are part of Earth's dark matter. We know so little about them because the majority have never been cultivated and their properties are unknown. This work hints at the life strategies they use when they've been frozen for thousands of years."

—Dr. Janet Jansson, PNNL chief scientist, Biological Sciences

Hultman J, MP Waldrop, R Mackelprang, M David, J McFarland, SJ Blazewicz, JW Harden, M Turetsky, AD McGuire, MB Shah, NC VerBerkmoes, LH Lee, K Mavrommatis, and JK Jansson. 2015. "Multi-omics of Permafrost, Active Layer and Thermokarst Bog Soil Microbiomes." *Nature* 521(7551):208-212. DOI:10.1038/nature14238.

Sponsor: DOE Office of Science, Office of Biological and Environmental Research



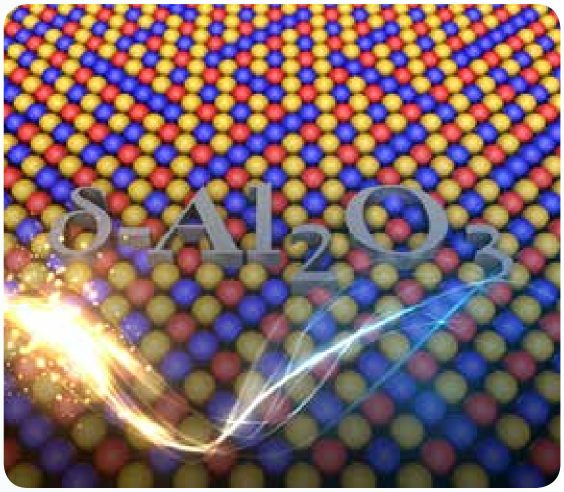
PNNL scientists solve what has been a difficult riddle for researchers: why some reactions that should occur easily—do not. The team used three prototypical reactions on a titanium dioxide surface to explain the enigma, by showing these reactions happen only after additional energy, such as heat or light, is provided. The team discovered the true energy profiles and the need for added energy in three prototypical reactions on a titanium dioxide surface. The results of this study will help other scientists accurately model catalytic reactions on titania and other, reducible oxides.

Weaving a Catalyst

Less waste. More product. Less energy. More speed. These items are on nearly every manufacturer's wish list. One way to check the items off the wish list is to rejigger the structure of the catalyst's support. Such changes require a detailed understanding of the structure. For the first time, scientists at PNNL and FEI Company obtained an atomically resolved view of the alumina support form known as delta alumina. The team showed the oxide is two crystal variants woven together. By taking a different approach to synthesis and chemical imaging, the team obtained detailed information that could, one day, help industrial processes be faster and more efficient.

Kovarik L, M Bowden, A Genc, J Szanyi, CHF Peden, and JH Kwak. 2014. "Structure of δ-Alumina: Toward the Atomic Level Understanding of Transition Alumina Phases." *Journal of Physical Chemistry C* 118(31):18051-18058. DOI:10.1021/jp500051j.

User Facility: EMSL
Sponsors: DOE Office of Science, Office of Basic Energy Sciences, Chemical Imaging Initiative



Using experiments and computational approaches, the team showed delta alumina is two crystal forms woven together.

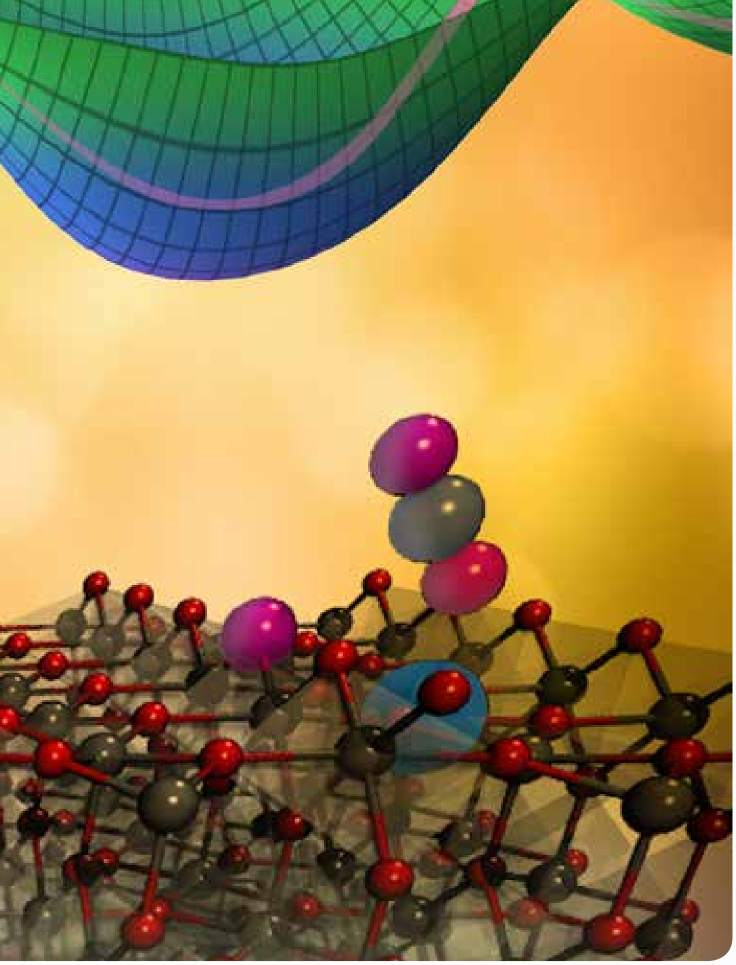
Speeding Up the Epochs

Minerals can require years or mere moments to form. For scientists who want to trap carbon dioxide emissions from coal-fired power plants and turn them into minerals, the amount of time matters. The challenge is that—in the lab—it is difficult to create the full range of conditions the carbon dioxide might experience underground to accurately measure whether carbonate minerals will form. At PNNL, scientists devised a new model using first principles to determine the time it took for mineral formation.

By calculating the thermodynamics from first principles, scientists are providing a way to understand why some minerals form and others do not. This information can be generalized to any material structure with impurities, defects, and a mixed composition.

Chaka AM and AR Felmy. 2014. "Ab Initio Thermodynamic Model for Magnesium Carbonates and Hydrates." *Journal of Physical Chemistry A* 118(35):7469-7488. DOI:10.1021/jp500271n.

User Facility: EMSL
Sponsors: Geosciences Research Program in the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences



Cherry Picking Molecules Based on their Pi Electrons

Specialized windshield glass, everyday plastic water bottles, and countless other products are based on ethylene, a simple two-carbon molecule, which requires an energy-intense separation process to pluck the desired chemical away from nearly identical ethane. To eliminate the extreme cooling required in the separation, an international team including researchers at PNNL designed a material with a porous framework that greatly prefers ethylene. As a bonus, this highly selective sorbent is stable in air and water. In addition, the framework offers a high surface area that speeds sorting. This study describes a promising material that does not require extreme pressures or temperatures and far surpasses current zeolites, a popular class of aluminosilicate catalysts, and any other modified framework reported in the scientific literature.

Li B, Y Zhang, R Krishna, K Yao, Y Han, Z Wu, D Ma, Z Shi, T Pham, B Space, J Liu, PK Thallapally, J Liu, M Chrzanowski, and S Ma. 2014. "Introduction of π-Complexation into Porous Aromatic Framework for Highly Selective Adsorption of Ethylene over Ethane." *Journal of the American Chemical Society* 136(24):8654-8660. DOI:10.1021/ja502119z.

Sponsors: National Science Foundation, DOE Office of Science, Office of Basic Energy Sciences, National Natural Science Foundation of China

Even at High Humidity, Aerosols Stick Around

Models have persistently and significantly underestimated atmospheric secondary organic aerosols, or SOAs, created by emissions from cars, trees, and other sources. Now, scientists at PNNL have provided hard data about viscosity, shape, morphology, volatility, and other fundamental particle properties. For example, the team found these aerosols evaporate very slowly at relatively high humidity, sticking around for days. Adding in the aerosols' true properties will help more accurately represent the real world and understand how SOAs, the most abundant particulates in the atmosphere, affect our climate and air quality.

Wilson J, D Imre, J Beránek, M Shrivastava, and A Zelenyuk. 2015. "Evaporation Kinetics of Laboratory-Generated Secondary Organic Aerosols at Elevated Relative Humidity." *Environmental Science & Technology* 49(1):243-249. DOI:10.1021/es505331d.

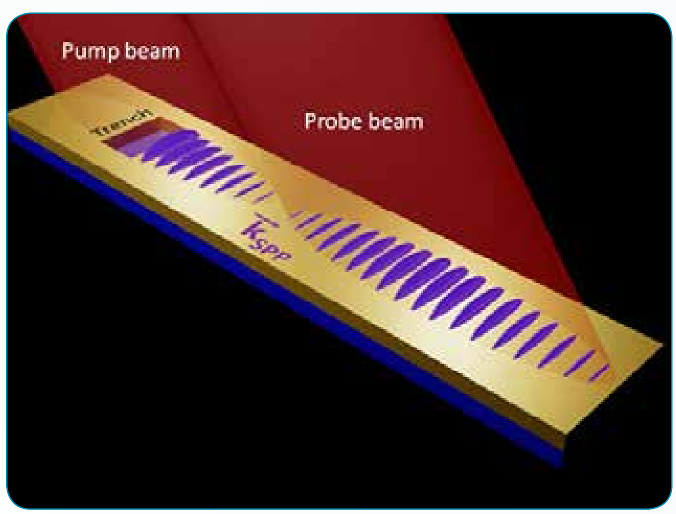
User Facility: EMSL
Sponsors: DOE Office of Science, Office of Basic Energy Sciences and Office of Biological and Environmental Research

Could Computers Reach Light Speed?

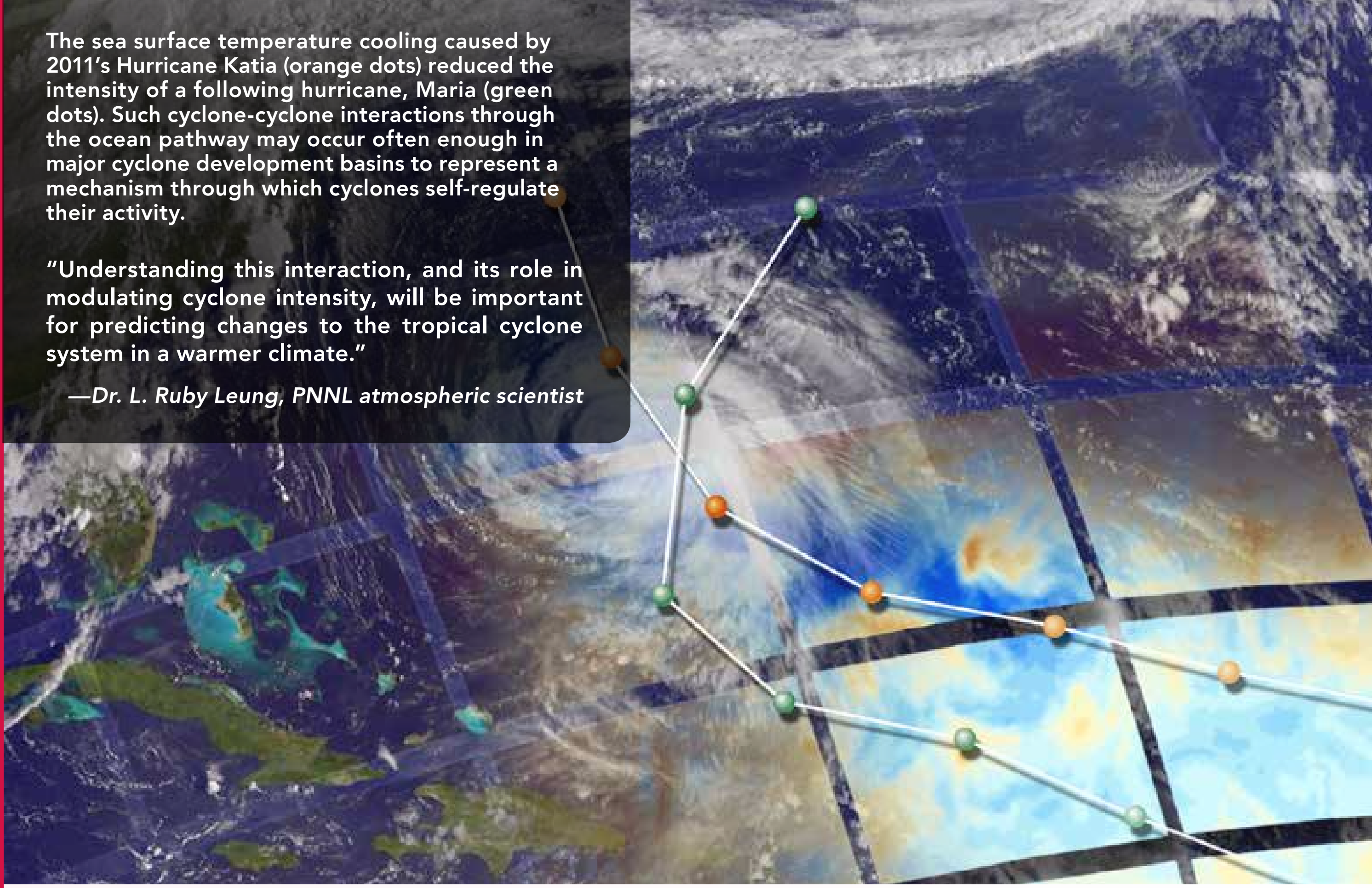
New research at PNNL found trapped light waves go farther than expected, giving insights into designing faster computer circuits and providing new advances in scientific fields. These light waves, called surface plasmons, travel at least 250 microns (or about 1/100th of an inch) across the surface. The team also found that plasmons have a long life and low dissipation, critical information needed to use the waves in computer circuits and other applications.

Gong Y, AG Joly, D Hu, PZ El-Khoury, and W Hess. 2015. "Ultrafast Imaging of Surface Plasmons Propagating on a Gold Surface." *Nano Letters* 15(5):3472-3478. DOI:10.1021/acs.nanolett.5b00803.

User Facility: EMSL
Sponsors: DOE Office of Science, Office of Basic Energy Sciences, PNNL Linus Pauling Fellowship



Specially designed extremely small metal structures can trap light. Once trapped, the light becomes a confined wave that moves from the pump (source) to the probe (detector) almost as fast as light moves through the air. *Copyright 2015: American Chemical Society*



The sea surface temperature cooling caused by 2011's Hurricane Katia (orange dots) reduced the intensity of a following hurricane, Maria (green dots). Such cyclone-cyclone interactions through the ocean pathway may occur often enough in major cyclone development basins to represent a mechanism through which cyclones self-regulate their activity.

"Understanding this interaction, and its role in modulating cyclone intensity, will be important for predicting changes to the tropical cyclone system in a warmer climate."

—Dr. L. Ruby Leung, PNNL atmospheric scientist

Climate Change Speed-Up

Earth's temperature changes are happening faster than historical levels and are starting to speed up. Researchers at PNNL, working at the Joint Global Change Research Institute (JGCRI), found Earth is now entering a period of change that is most likely faster than what's occurred naturally over the last thousand years. The research shows that today's world population will have to live through and adapt to a warming world.

"In the climate model simulations, the world is just now starting to enter into a new place, where rates of temperature change are consistently larger than historical values over 40-year time spans. We need to better understand what the effects of this will be and how to prepare for them."

—Dr. Steven J. Smith, interdisciplinary scientist at JGCRI

Smith SJ, JA Edmonds, CA Hartin, A Mundra, and KV Calvin. 2015. "Near-Term Acceleration in the Rate of Temperature Change." *Nature Climate Change* 5:333-336. DOI:10.1038/nclimate2552.

Sponsor: DOE Office of Science, Office of Biological and Environmental Research

Tracking Down Time Missteps

Pinpointing the culprits responsible for errors in large-scale climate models can take a mathematical magnifier. To identify these transgressors, scientists at PNNL, Sandia National Laboratories, and University of Michigan developed a novel technique that efficiently measures and identifies time-resolution errors in the most complex weather and climate models. This study offers a simple and effective strategy to identify the model components responsible for the missteps.

Wan H, PJ Rasch, MA Taylor, and C Jablonowski. 2015. "Short-Term Time-Step Convergence in a Climate Model." *Journal of Advances in Modeling Earth Systems* 7(1): 215-225. DOI:10.1002/2014MS000368.

Sponsors: Linus Pauling Distinguished Postdoctoral Fellowship under PNNL's Laboratory Directed Research and Development Program, DOE Office of Science, Office of Biological and Environmental Research

Scientists implemented a novel technique to uncover time-resolution errors in complex weather and climate models. Climate modelers will now be able to improve the fidelity and efficiency of climate simulations.

Electricity Needs Water: A State-by-State Assessment

To understand increasing water use by U.S. electric power producers, researchers at PNNL turned to a computational model to estimate the state-by-state need through 2095. They found climate mitigation strategies, such as nuclear power, will increase water consumption while strategies for renewable energy and water-saving technologies will reduce it.

Liu L, M Hejazi, P Patel, P Kyle, E Davies, Y Zhou, L Clarke, and J Edmonds. 2014. "Water Demands for Electricity Generation in the U.S.: Modeling Different Scenarios for the Water-Energy Nexus." *Technological Forecasting and Social Change* 94:318-334. DOI:10.1016/j.techfore.2014.11.004.

Sponsor: DOE Office of Science, Office of Biological and Environmental Research

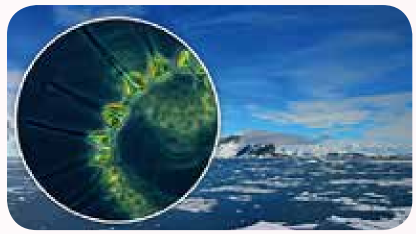
Electrical power generation water consumption was projected through 2095 through three "what if" scenarios. Understanding the consumption and demands for water by the electrical power sector in the future is important as freshwater availability is challenged as a result of climate change.

Sea Critters Rule the Clouds

A study of clouds over the world's remotest ocean shows that ocean life is responsible for up to half the cloud droplets that pop in and out of existence during summer. A team of scientists led by PNNL revealed how tiny natural particles given off by marine organisms—airborne droplets and solid particles called aerosols—nearly double cloud droplet numbers in the summer, which boosts the amount of sunlight reflected back to space. Understanding the amount of energy that clouds over the Southern Ocean reflect might help researchers assess how well climate models are able to capture the effects of these marine particles on clouds.

McCoy DT, SM Burrows, R Wood, DP Grosvenor, SM Elliott, P-L Ma, PJ Rasch, DL Hartmann. 2015. "Natural Aerosols Explain Seasonal and Spatial Patterns of Southern Ocean Cloud Albedo." *Science Advances* 1(6): E1500157. DOI:10.1126/sciadv.1500157.

Sponsor: DOE Office of Science, Office of Biological and Environmental Research



With a strong mix of ocean, wind and marine microorganisms, scientists found that marine life is responsible for half of the summer cloud droplets over the Southern Ocean.

The Microbe Mineral Makeover

Understanding how microbes alter subsurface minerals is key to cleaning up polluted soils—and to growing crops for biofuels. Scientists at PNNL, University of East Anglia, and University College London assessed the state of understanding of a key enzymatic pathway employed by bacteria in these transformations. Their findings suggest geologic sequestration of CO_2 may significantly inhibit sulfate reduction in deep subsurface environments which may help limit harmful subsurface processes such as sulfide-induced corrosion, mineral precipitation, and injection-well blockage. The effect would improve the overall efficiency of CO_2 sequestration.

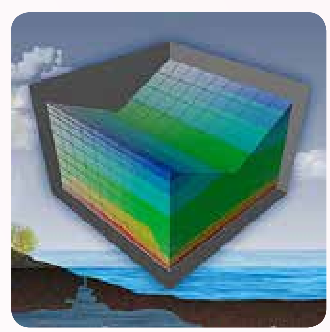
Growing crops for biofuels and cleaning up polluted soils benefit from a deeper understanding of how a specific microbial protein, known as multi-heme cytochromes, reduces iron, manganese, and other subsurface minerals.

Breuer M, KM Rosso, J Blumberger, and JN Butt. 2014. "Multi-haem Cytochromes in Shewanella Oneidensis MR-1: Structures, Functions and Opportunities." *Journal of the Royal Society Interfaces* 12: 20141117. DOI:10.1098/rsif.2014.1117.

Sponsors: DOE Office of Science, Office of Biological and Environmental Research, UK Biotechnology and Biological Sciences Research Council

Simulating Across Scales

Researchers from PNNL and the University of Central Florida developed a unified multiscale model that uses a single set of equations to simultaneously simulate fluid flow in an ecosystem containing both surface water and groundwater. They applied the modeling approach to a field site, where active field monitoring and measuring are ongoing, to understand hydrological and biogeochemical processes. The approach is particularly suitable for simulating water flow in ecosystems with strong surface water and groundwater interactions. It will significantly facilitate modeling hydrological processes in ecosystems where soil or sediment are frequently inundated and drained in response to precipitation, regional hydrological processes, and climate change.



Researchers designed a multiscale model that simulates hydrological processes in an ecosystem with both surface water and groundwater.

Yang X, C Liu, Y Fang, R Hinkle, HY Li, V Bailey, and B Bond-Lamberty. 2015. "Simulations of Ecosystem Hydrological Processes using a Unified Multi-Scale Model." *Ecological Modelling* 296:93-101. DOI:10.1016/j.ecolmodel.2014.10.032.

User Facility: EMSL
Sponsor: DOE Office of Science, Office of Biological and Environmental Research

Installation of the Mini-CLEAN central detector 6800 feet underground at SNOLAB.

Dark Matter: Searching beyond the Standard Model of Particle Physics

It is firmly established that the universe is largely composed of an unknown form of matter, called dark matter, which has never been detected because it neither emits nor absorbs light and is invisible to conventional telescopes. Scientists have deduced its existence only by observing its gravitational effects on visible matter. Understanding the nature of dark matter is one of the highest priorities in modern particle physics. Dark matter is not made up of baryons, the basic constituents of ordinary matter. Observations of structure formation indicate only a small contribution from neutrinos. Dark matter is therefore exotic and one of the very few places where we have direct experimental evidence for physics beyond the Standard Model. Weakly Interacting Massive Particles (WIMPs) are compelling candidates for explaining dark matter that could be directly detected as they scatter from massive, ultra-pure detector targets operating deep beneath the Earth's surface.

Minimizing backgrounds from natural radioactivity (from detector materials, the laboratory, and the cosmos) is critical to finding the postulated, rare nuclear-recoil events expected from WIMPs. Once known backgrounds are removed, technologies that can differentiate WIMP signals from residual backgrounds have a significant advantage. Direct-detection experiments with large enough target masses and control of backgrounds could enable scientists to discover and study these WIMPs. The field requires improvements in sensitivity by as much as two orders of magnitude beyond the best technologies currently available. PNNL scientists are taking a two-pronged approach toward achieving the technological sensitivity needed to detect dark matter directly:

- First, cryogenic germanium detectors lead the field for pursuing "low-mass" WIMPs and the technical challenge will be to demonstrate single charge carrier resolution as a means of background discrimination in order to proceed beyond the state-of-the-art SuperCDMS experiment. PNNL has led the CDMS collaboration efforts to realize its capability as a sensitive probe of low-mass WIMPs.
- Second, a monolithic detector using liquid argon as a target material expected to register flashes of light when hit by WIMPs—dubbed CLEAN for Cryogenic Low Energy Astrophysics with Noble liquids—is likely the only possibility to go beyond the next generation of experiments in detecting "high-mass" WIMPs. PNNL is leading the MiniCLEAN experiment—a prototype to CLEAN that will use about 300 times as much cryogenic liquid to register flashes of light. CLEAN is a unique technology that can, in principle, exchange targets from liquid argon to liquid neon. This capability could be critical in verifying the discovery of a dark matter signal and broadens the scientific portfolio to include precision studies of neutrinos from the sun and supernovae.

PNNL's core capabilities in nuclear and particle physics will continue to enable our scientists to pursue answers to some of the most compelling questions in modern science—among them the search for another compelling dark matter candidate called axions.

Sponsors: PNNL Laboratory Directed Research and Development, DOE Offices of High Energy Physics and Nuclear Physics, U.S.-Japan Collaboration in High Energy Physics

Belle II Project's New Detector for Matter-Antimatter Experiment

The detector for the Belle particle physics experiment is getting an upgrade that will lead to a 50-fold increase in data available for precision rare decay studies, searches for exotic particles, and precise measurements of B and D meson and tau leptons. PNNL is the lead U.S. institution for the upgrade. The U.S. Belle II Project's imaging Time-Of-Propagation (iTOP) detector is the centerpiece of the U.S. contribution to the upgrade.

The iTOP detector is built from extremely precisely ground and polished synthetic fused silica optics and will provide increased background tolerance and improved physics performance for the experiment. When particles produced in electron-positron collisions at the SuperKEKB accelerator traverse iTOP's optics, they produce Cerenkov light in cones around their direction of motion. Cone sizes depend on the particles' velocities.

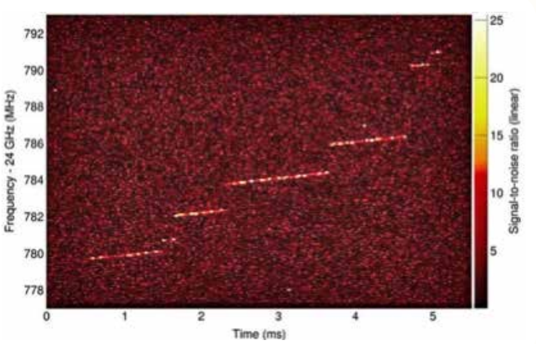
Another detector in the Belle II system is used to measure the momentum of particles by the curvature created as their paths are bent in a 1.5 Tesla magnetic field. Together, these two measurements can be used to determine a particle's mass and type.This system will enable more than 600 high energy physicists from 23 countries who are part of Belle II to differentiate between rare decays of a b (bottom) quark to an s (strange) to the yet rarer decays of a b quark to a d (down) quark. In the previous generation of Belle, the b-to-s transition was the "discovery science" and, in the era of Belle II, it is now the background as we explore ever-rarer phenomena. PNNL scientists have been involved in all aspects of iTOP development, from the optics to the mechanics and now with the assembly of the detector at KEK in Japan.

Constructed iTOP module augmented by external "strong back" to stiffen it until installation. Sixteen such modules will form a cylinder within the Belle II detector. The last module is slated for installation in spring 2016.

PNNL provides high-performance computational capabilities for Belle and Belle II scientists. In the next decade, Belle II is expected to produce one of the world's largest scientific data samples—total data volume of a few hundred petabytes—driving the trans-Pacific network bandwidth requirement. PNNL is developing the distributed data management system and is responsible for the international data network for Belle II. The Belle II computing center at PNNL will store, process and reprocess raw data samples, generate simulation samples, and redistribute data to European collaborators and U.S. institutions.

Project 8: Searching for the Mass of One of the Smallest Particles in the Universe

For the first time ever, scientists from PNNL and five other research institutions measured the cyclotron power radiated by a single electron when trapped in a magnetic field. Not coincidentally, their accomplishment also brings them a step closer to answering some of the most pressing questions about the universe—one of which is determining the weight of a neutrino, one of the smallest subatomic particles in the universe.

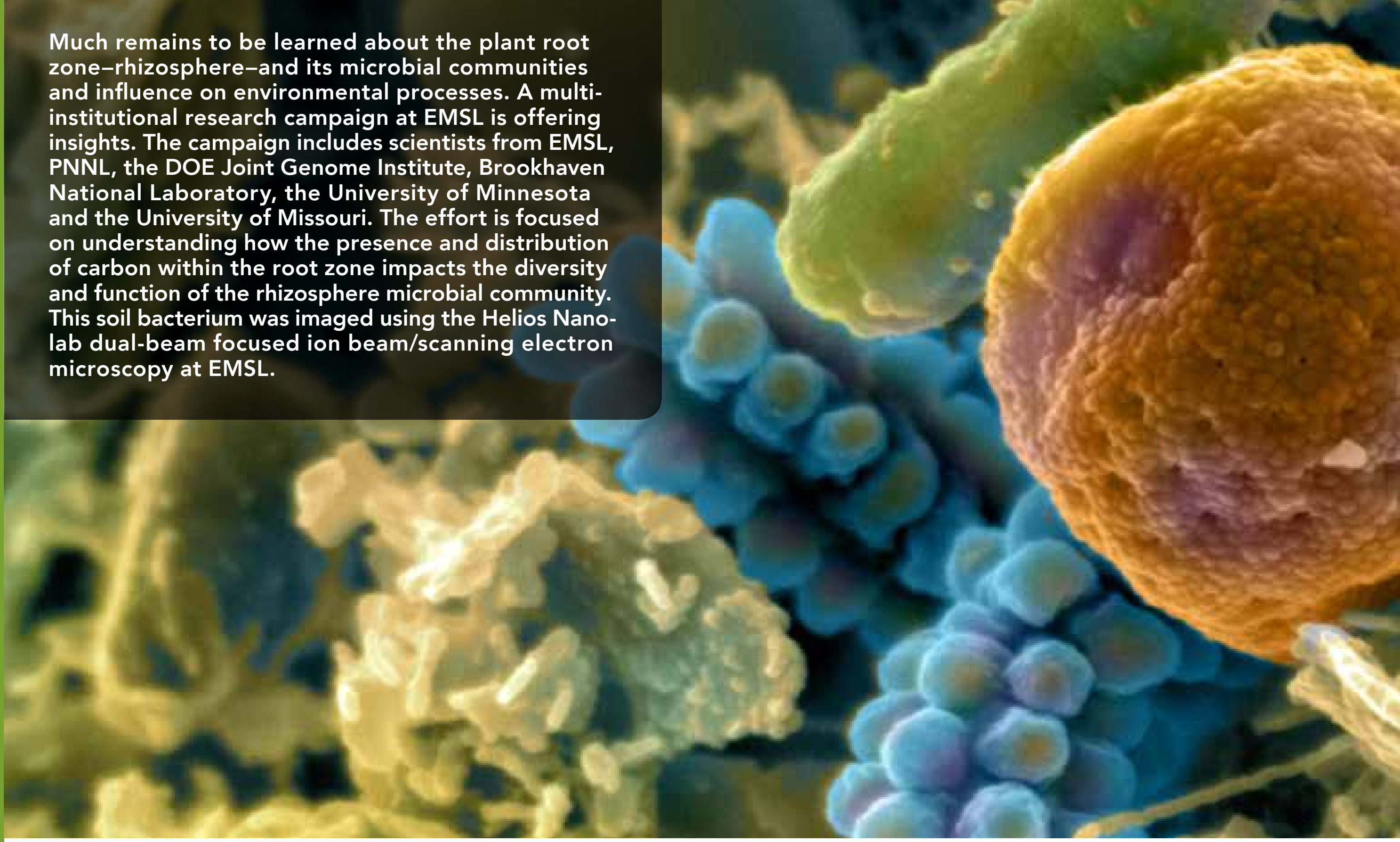


The first electron ever observed by CRES. The frequency of radiated cyclotron power precisely encodes the electron's kinetic energy.

Called Project 8, their work is a joint effort by PNNL, the University of Washington, Massachusetts Institute of Technology, the University of California at Santa Barbara, and Yale University. The group will continue to pursue the goal of quantifying the mass of neutrinos. To do so, the researchers are planning to use a larger version of the technology that enabled them to detect and measure cyclotron radiation from individual electrons. Called CRES (cyclotron radiation emission spectroscopy), the new technology worked well to enable the team to measure the energy of electrons from radioactive krypton gas, but they plan to use tritium gas to discover the mass of the elusive neutrino.

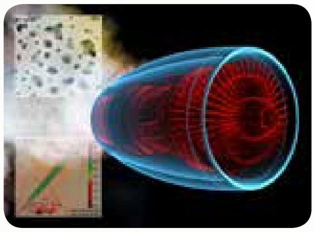
A larger version of the new CRES instrument will provide greater sensitivity for the neutrino experiment, enabling the scientists to measure tritium beta decay electrons with unprecedented precision, gathering information contained in the kinematics of the highest energy tritium beta-decay electrons. When a tritium atom (a hydrogen atom carrying two neutrons) beta decays to helium-3, the scientists can add up the energies of the remaining helium-3 atom and an electron and compare that total to the energy of an intact tritium atom. The difference would be the energy of the neutrino. Plugging that energy value into Einstein's famous equation, $E= mc^2$, they could then calculate the mass of the missing neutrino.

The question of neutrino mass is decades old. Answering it will help shed light on a number of the most compelling unknowns in modern science, questions such as how the universe originated and evolved to what it is today and how the fundamental forces in nature are unified. There is a possibility that the tiny neutrino is unique among known subatomic particles in that it may be its own antiparticle. If so, there could be a connection between the weight of the neutrino and the highest energy scales where scientists theorize that the fundamental forces in the universe would be merged into a single force. If Project 8 is successful in determining neutrino mass, future avenues of research could benefit greatly from that information.



Much remains to be learned about the plant root zone–rhizosphere–and its microbial communities and influence on environmental processes. A multi-institutional research campaign at EMSL is offering insights. The campaign includes scientists from EMSL, PNNL, the DOE Joint Genome Institute, Brookhaven National Laboratory, the University of Minnesota and the University of Missouri. The effort is focused on understanding how the presence and distribution of carbon within the root zone impacts the diversity and function of the rhizosphere microbial community. This soil bacterium was imaged using the Helios Nanolab dual-beam focused ion beam/scanning electron microscopy at EMSL.

Soot Study Improves Climate Models



Studying soot particles from a burning jet fuel surrogate leads to a better understanding of the chemical nature of soot particles, which could lead to improved climate models and cleaner aviation engines.

Soot is produced from incomplete combustion of hydrocarbon fuels. Because soot is an anthropogenic contaminant in the environment and an important contributor to climate change, it is necessary to understand how it forms. A recent study addressed this question by examining the chemical composition of soot particles sampled from a diffusion flame burning a jet fuel surrogate. This research reveals significant variations in the morphology and chemical composition of soot particles as they develop in the flame, indicating molecular processes of soot formation in diffusion flames may be more complex than previously thought.

Research findings suggest fundamental models of soot formation are not completely accurate. By providing a more complete understanding of the chemical nature of soot particles, this research could ultimately lead to improved climate-model representations of anthropogenic soot's chemical and physical properties, greater insight into the role of soot in cloud formation and cleaner aviation engines through more accurate soot models.

Cain J, A Laskin, MR Kholghy, MJ Thomson, and H Wang. 2014. "Molecular Characterization of Organic Content of Soot Along the Centerline of a Coflow Diffusion Flame." *Physical Chemistry Chemical Physics* 16:25862-75. DOI:10.1039/C4CP03330B.

Sponsors: DOE Office of Science, Offices of Biological and Environmental Research and Basic Energy Sciences, PNNL Laboratory Directed Research and Development

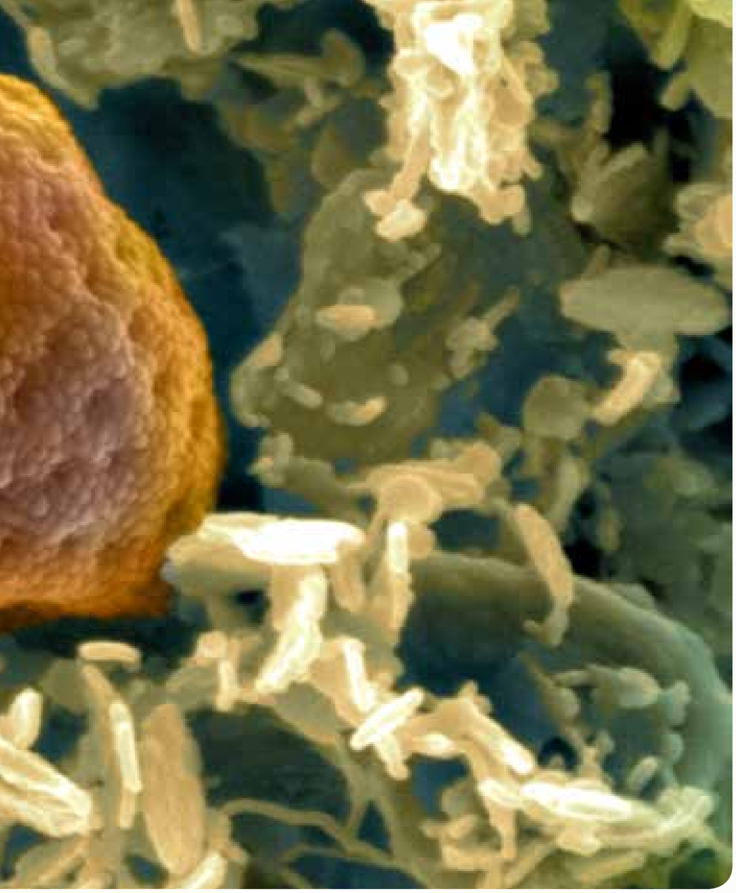
Archaea Genomes Reveal Role in Global Carbon Cycle

Archaea, a domain of single-celled microorganisms, represent a significant fraction of the Earth's biodiversity, yet they remain much less understood than bacteria. One reason for this lack of knowledge is relatively poor genome sampling, which has limited accuracy of the Archaeal phylogenetic tree. In a recent study, researchers approximately doubled the genomic diversity sampled from this domain and reconstructed the first complete genomes for Archaea using cultivation-independent methods resulting in an extensive revision of the Archaeal tree of life. They sequenced DNA in sediment and groundwater samples from a uranium-contaminated aquifer at DOE's Integrated Field Research Challenge site near Rifle, Colorado, a former uranium mill.

The study revealed Archaea in the terrestrial subsurface contribute primarily to carbon and hydrogen cycling, suggesting these organisms may be involved in processing the sizeable reservoir of buried organic carbon. This finding can be immediately implemented within genome-resolved ecosystem models to more accurately reflect the key role played by Archaea in the global carbon cycle.

Castelle CJ, KC Wrighton, BC Thomas, LA Hug, CT Brown, MJ Wilkins, KR Frischkorn, SG Tringe, A Singh, LM Markillie, RC Taylor, KH Williams, and JF Banfield. 2015. "Genomic Expansion of Domain Archaea Highlights Roles for Organisms from New Phyla in Anaerobic Carbon Cycling." *Current Biology* 25(6):690-701. DOI:10.1016/j.cub.2015.01.014.

Sponsor: DOE Office of Science, Office of Biological and Environmental Research



New Models Closer to Nature

Uranium oxide is the most economically important uranium mineral and most common nuclear fuel in reactors. It contains the less soluble and immobile form of uranium in nature, and as a result is the common desired end product of bioremediation strategies.

Researchers from the University of Chicago, PNNL and three user facilities examined the surface structure and composition of UO_2 after exposure to oxygen gas and water at ambient conditions. They performed density-functional theory computations using supercomputers and used x-ray photoelectron spectroscopy in RadEMSL.

The researchers conclude that oxygen does not penetrate UO_2 in the manner of a typically diffusive process. Instead, an oxidation front advances into the material in discrete steps. Researchers found oxygen atoms occupied every third layer below the surface of UO_2. Moreover, uranium existed in three oxidation states: IV, V and VI. Similar structures formed under oxygen gas and water, suggesting the same corrosion process operates under a wide range of conditions.

The findings have important implications for understanding initial stages of oxidative corrosion in materials at the atomic scale.This conceptual framework may be relevant to a wide class of redox-active materials and minerals.

Stubbs JE, AM Chaka, ES Ilton, CA Biwer, MH Engelhard, JR Bargar, and PJ Eng. 2015. "UO_2 Oxidative Corrosion by Nonclassical Diffusion." *Physical Review Letters* 114:246103. DOI:10.1103/PhysRevLett.114.246103.

User Facility: EMSL
Sponsors: DOE Office of Science, Offices of Biological and Environmental Research and Basic Energy Sciences, National Science Foundation

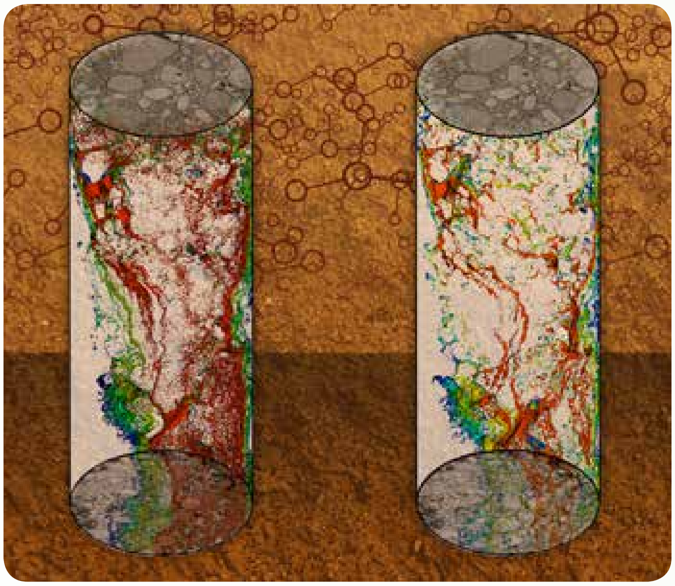
Expanding the Impact of Pore-Scale Simulations

Pore-scale models are useful for studying relationships between fundamental processes at the scale of tens to hundreds of microns—the size of solid soil grains and pore spaces—and phenomena at larger scales that are relevant to real-world applications. However, conventional simulations of the flow of water and chemicals through soils at large scales typically neglect details of pore geometry due to computational demands associated with characterizing large 3D volumes with pore-scale spatial resolution. This study introduces a method for overcoming this challenge and presents the first simulations of pore-scale flow and transport over a large, decimeter-scale volume. The multiscale simulation approach will have a significant impact on the ability to transfer knowledge of small-scale physical processes to larger-scale phenomena and will dramatically improve the capability of numerical models to accurately predict behavior of complex natural systems.

Understanding how water and chemicals flow in soils is important for many practical problems, such as assessing risk of groundwater contamination, developing effective ways to clean up contaminated soils and aquifers, and designing subsurface repositories for waste materials. By bridging the gap between small and large spatial scales, the simulation method could shed light on the effect pore-scale processes have on these field-scale phenomena, paving the way for more accurate assessments of risk of groundwater contamination and development of more effective remediation strategies.

Scheibe TD, WA Perkins, MC Richmond, MI McKinley, PDJ Romero-Gomez, M Oostrom, TW Wietsma, JA Serkowski, and JM Zachara. 2015. "Pore-scale and multiscale numerical simulation of flow and transport in a laboratory-scale column." *Water Resources Research* 51:1023-1035. DOI:10.1002/2014WR015959.

Sponsor: DOE Office of Science, Office of Biological and Environmental Research



By bridging the gap between small and large spatial scales, the simulation method could pave the way for more accurate assessments of the risk of groundwater contamination and the development of more effective remediation strategies. Figure shows a comparison of solute transport simulations using binary segmentation (left image) and ternary segmentation (right image).

Each ARM site launches balloon-borne sounding systems, or weather balloons. The measurements they provide—temperature, pressure, humidity, and wind speed—are the backbone of many atmospheric-related research efforts.

Land, Sea, and Air: ACAPEX Targets Atmospheric Rivers

The ARM Climate Research Facility launched and completed the largest study focused on capturing data from atmospheric rivers during the ARM Cloud Precipitation Experiment (ACAPEX). These rivers are narrow bands of enhanced water vapor associated with the warm sector of tropical cyclones over the Pacific and Atlantic oceans, accounting for 30 to 50 percent of the annual precipitation in California. The team, led by PNNL, chased and sampled four atmospheric rivers that made landfall in northern California during ACAPEX and collected data from instrument ground stations throughout the state.

"During the one really big atmospheric river storm, I was on the G-1 aircraft participating in the data collection across five different research flights. I could look down below the clouds and see the ship directly below the atmospheric river. It was then that I knew we were collecting some good stuff. It was very exciting."

—Dr. Ruby Leung, PNNL Laboratory Fellow

They learned that there are many aerosol types that mix during these atmospheric rivers. All of these particles were mixing like a batch of soup made from scratch. Just as an ingredient changes a soup's flavor, each of these aerosol particles have different effects on clouds. These data could help better prepare for droughts and floods.

Sponsor: DOE Office of Science, Office of Biological and Environmental Research

Greenhouse Effect at Earth's Surface Confirmed Using ARM Data

From 2000 to the end of 2010, 3300 measurements were obtained at ARM's North Slope of Alaska site for the study.

For the first time, scientists observed an increase in carbon dioxide's greenhouse effect at the Earth's surface. Research conducted using data and data products from the ARM Climate Research Facility was reported in *Nature*. The data were used by scientists who were able to measure atmospheric carbon dioxide's increasing capacity to absorb thermal radiation emitted from the Earth's surface over an 11-year period at ARM research sites in Oklahoma and Alaska. Researchers attributed this upward trend to rising carbon dioxide levels from fossil fuel emissions. Study results agree with theoretical predictions of the greenhouse effect due to human activity, which had not been experimentally confirmed outside of a laboratory. The research also provides further confirmation that the calculations used in today's climate models are on track when it comes to representing the impact of carbon dioxide.

Feldman, DR, WD Collins, PJ Gero, MS Torn, EJ Mlawer, and TR Shippert. 2015. "Observational Determination of Surface Radiative Forcing by CO_2 from 2000 to 2010." *Nature* 519: 339-343. DOI:10.1038/nature14240.

Sponsor: DOE Office of Science, Office of Biological and Environmental Research

Tall Clouds from Tiny Raindrops Grow

As rain drops descend to the surface, they can evaporate and cool the air. Cold air then spreads horizontally and forms pools at the surface that displace surrounding warm air. The dynamics of cold pools are an important mechanism of organizing convection. Research led by scientists at PNNL investigated how precipitation-driven cold pools over the warm tropical Indian Ocean cause convective clouds to "self-organize." The research used data gathered during the Atmospheric Radiation Measurement (ARM) Madden-Julian Oscillation (MJO) Investigation Experiment/Dynamics of the MJO (AMIE/DYNAMO) field campaign. Using a high-resolution regional model, the team simulated clouds and precipitation during the transition from suppressed to active phases to find that the simulated cold pool lifetimes, spatial extent, and thermodynamic properties agree well with the radar and ship-borne observations from the field campaign. Current climate model resolution is too coarse to resolve individual convective clouds and must rely on parameterizations. These findings represent a new approach to show the effects of cold pools on deep convective clouds.

"Our study highlights the utility of using observations to evaluate how well the next generation of climate models can directly capture the behavior of clouds. While these newer models cannot completely overcome some challenges, they do represent cloud size-depth relationships fairly well."

—Dr. Samson Hagos, PNNL atmospheric scientist

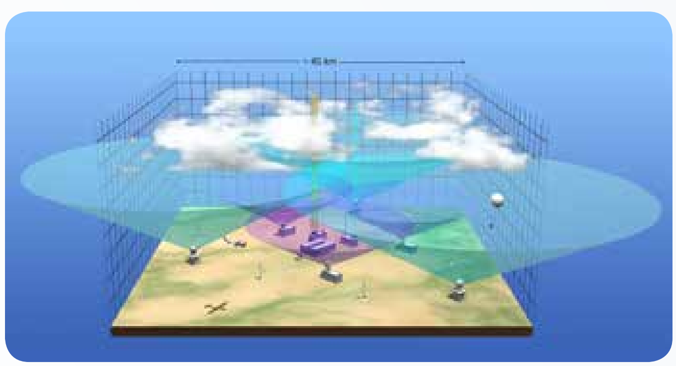
Hagos S, Z Feng, CD Burleyson, KS Lim, CN Long, D Wu, and T Greg. 2014. "Evaluation of convection-permitting model simulations of cloud populations associated with the Madden-Julian Oscillation using data collected during the AMIE/DYNAMO field campaign." *Journal of Geophysical Research – Atmospheres,* 119 (21). DOI:10.1002/2014jd022143.

Sponsor: DOE Office of Science, Office of Biological and Environmental Research

Megasites Accept Mega Challenge: New Directions Take Formation

The ARM Climate Research Facility was the first climate research program to deploy a comprehensive suite of cutting-edge instrumentation to continually measure cloud and aerosol properties and their impacts on Earth's energy balance. This strategy revolutionized scientists' ability to collect long-term statistics of detailed cloud properties and now serves as a model for programs around the world.

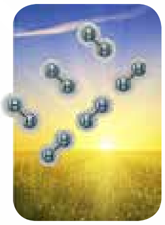
To create a powerful new capability for furthering ARM's mission, ARM is undergoing a reconfiguration that will provide more complete data sets in support of process studies and model development. Combined observational and modeling elements will enable a new level of scientific inquiry. To achieve this vision, a series of workshops were held to focus on key scientific needs, gaps, and priorities needed to develop two "megasites" at ARM's North Slope of Alaska (NSA) and Southern Great Plains (SGP) facilities that will result in more comprehensive scientific data and the processes and tools for scientists to more easily integrate them into climate models. The first of three workshops focused on the SGP megasite, the second for the NSA megasite, and the third, and final, focused on the ARM Aerial Facility. As suggested by the SGP workshop, a team of scientists, led by PNNL, is developing processes to use data from the expanded measurement capabilities being implemented at the megasite to constrain a Large-Eddy Simulation model, a mathematical model for turbulence used to simulate atmospheric air currents and cloud processes. High resolution model simulations will be run on a routine basis, and combined with the detailed ARM observations will enable a new level of scientific analysis by connecting processes and context to observations and providing needed statistics for details that cannot yet be measured.



The ARM Climate Research Facility is undergoing a reconfiguration to better support the linking of ARM measurements with process-oriented models. This illustration depicts the new SGP megasite, incorporating a network of instruments to support model development and evaluation.

HYDROGEN CATALYSIS TEAM

Wins Prestigious National Lectureship



The PNNL team earned the lectureship award for research that has revolutionized understanding of the role of proton movement in the electrocatalytic interconversion of electricity and hydrogen fuel. This work has had a profound impact on catalysis as a whole. The members are **Morris Bullock, Daniel DuBois, Monte Helm, Michel Dupuis, Simone Raugei, Jenny Yang, John Roberts, Molly O'Hagan, Wendy Shaw, Aaron Appel,** and **Eric Wiedner** at PNNL, and Sharon Hammes-Schiffer at University of Illinois.

DICK SMITH

Featured in Special Journal Issue

Battelle Fellow **Dick Smith** was featured in the December 2014 issue of *Journal of the American Society for Mass Spectrometry*. He was the focus of the issue on his contributions to "Advancing High Performance Mass Spectrometry." Smith also had his 1000th peer-reviewed paper published in January.

YU, ZHU

Technology Transfer Award

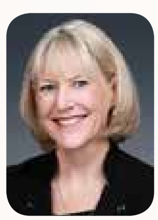
Xiao-Ying Yu

Zihua Zhu

Xiao-Ying Yu, chemical imaging and atmospheric chemistry scientist, and EMSL scientist **Zihua Zhu** were among members of a research team that received a 2015 Excellence in Technology Transfer Award from the Federal Laboratory Consortium for Technology Transfer. The PNNL and EMSL team won for development of the System for Analysis at the Liquid Vacuum Interface, or SALVI, which allows instruments such as mass spectrometers and scanning electron microscopes to image liquid samples in real time and space.

JANET JANSSON

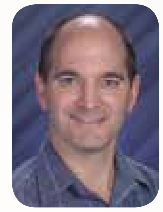
Invited to White House Microbiome Roundtable



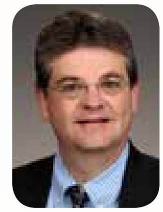
Chief Scientist for Biology, Earth and Biological Sciences **Janet Jansson** was among 15 national experts in the fields of microbiology, genomics, and microbial ecology who participated in a Microbiome Roundtable held by the White House Office of Science and Technology Policy (OSTP) in December 2014. The OSTP invited participants to share their views and identify research areas and approaches that can inform strategies for developing a roadmap to accelerate discovery within the field.

FLYNN, SCHMID

Receive NASA Group Achievement Award



Connor Flynn



Beat Schmid

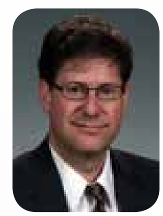
Connor Flynn and **Beat Schmid** received the prestigious 2015 National Aeronautics and Space Administration (NASA) Group Achievement Award as part of a collaborative team. The honor was awarded for the NASA field campaign Studies of Emissions and Atmospheric Composition, Clouds, and Climate Coupling by Regional Surveys. Flynn, physicist and atmospheric scientist, has participated in nearly two dozen field missions from land, sea, and air. Schmid, technical director of DOE's ARM Aerial Facility, has been involved as a participant or leader in nearly 20 multi-agency aircraft campaigns and has authored more than 80 peer-reviewed journal publications.

ASNER, BAER, MUNDY

Elected APS Fellows

David Asner

Don Baer



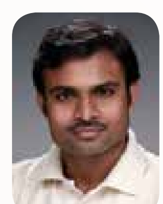
Chris Mundy

Laboratory Fellow and Particle Physics lead **David Asner**, Laboratory Fellow and EMSL Science Theme lead **Don Baer**, and scientist **Chris Mundy** were elected to the rank of fellow in the American Physical Society in recognition of their exceptional contribution to research and capability development. APS is the nation's leading voice for physics.

HALAPPANAVAR, TIPIREDDY

Best Paper Honors by IEEE HST

Mahantesh Halappanavar



Ramakrishna Tipireddy

As part of IEEE Symposium on Technologies for Homeland Security (HST '15), scientists from PNNL and Virginia Tech were honored for their work, employing game theory to mathematically address cyber-system security and resilience challenges in the context of added uncertainties. The team included data scientist **Mahantesh Halappanavar** and computational scientist **Ramakrishna Tipireddy**. Their work presents new ideas for development of a probabilistic framework to reason about attacker payoff uncertainties and uncertainty quantification methods to address sources of uncertainties in the attacker payoffs.

LI, HELDEBRANT, VANDEVENDER

Receive DOE Early Career Research Program Awards


Dongsheng Li

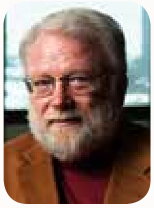

David Heldebrant


Brent VanDevender

Dongsheng Li, materials scientist, **David Heldebrant**, organic chemist, and **Brent VanDevender**, nuclear physicist, were selected to receive 2015 Early Career Research Program Awards. They are three of just 44 recipients nation-wide–including 17 at national laboratories–to receive the annual research awards, and were selected from more than 600 applications. Under the program, they will receive five-year research grants that fund work designed to create new materials for energy storage, reduce carbon emissions, and examine the smallest building blocks of the universe.

THOM DUNNING

Elected New Member of International Academy of Quantum Molecular Science



Battelle Fellow **Thom Dunning**, currently with the Northwest Institute for Advanced Computing, a collaborative center founded by PNNL and the University of Washington, was elected one of six new members to the International Academy of Quantum Molecular Science (IAQMS). IAQMS membership is composed of scientists who have distinguished themselves through their scientific work, pioneering efforts, or leadership in the applications of quantum mechanics to the study of molecules and macromolecules.

GALYA ORR

Inspiring Women in STEM

EMSL scientist and capability lead **Galya Orr** was the recipient of a 100 Inspiring Women in STEM Award from *INSIGHT Into Diversity* magazine, the oldest and largest diversity magazine and website in higher education. She was nominated with three female colleagues at the National Science Foundation-funded Center for Sustainable Nanotechnology, where they are co-principal investigators working and mentoring a diverse group of students.

BEN KRAVITZ

Receives IUGG Early Career Scientist Award

Ben Kravitz, atmospheric scientist, was awarded the Union of Geodesy and Geophysics Early Career Scientist Award. The award is given every four years to 10 outstanding early career researchers worldwide. Kravitz is one of two recipients in the United States recognized for his outstanding scientific contributions in the fields of earth and space science and international research cooperation.

JUSTIN TEEGUARDEN

Appointed to National Academies Committee on Chemical Risk

Justin Teeguarden, toxicologist, was appointed to a National Academies panel that will provide recommendations on integrating new scientific approaches into risk-based evaluations. Teeguarden leads research related to chemical risk assessment and health effects, most notably that relate to the use of Bisphenol A (BPA) in plastics.

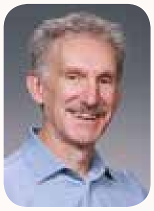
KATE CALVIN

Appointed to NRC Study Team

Kate Calvin, research economist, was selected to serve on a National Research Council committee studying models for understanding complex adaptive systems. Commissioned by the National Geospatial-Intelligence Agency, the charge is to identify and evaluate modeling tools that could aid the intelligence community.

RASCH, GUENTHER

Elected AGU Fellows

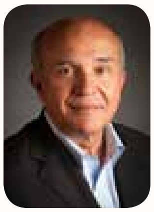

Phil Rasch


Alex Guenther

Laboratory Fellows **Phil Rasch** and **Alex Guenther** attained the elite rank of scientists elected as fellows of the American Geophysical Union (AGU). The honor is bestowed for "exceptional scientific contributions and attained acknowledged eminence in the fields of earth and space science" and is given to no more than one-tenth of one percent of all members of the organization. Rasch and Guenther join two other PNNL researchers as fellows, bringing PNNL's total of AGU fellows to four—the most of any DOE-sponsored national laboratory.

JOHANNES LERCHER

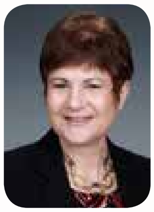
Named Distinguished Chemical Engineering Lecturer



Johannes Lercher, Battelle Fellow and Institute for Integrated Catalysis director, was selected as Yale University's Barnett F. Dodge Lecturer. Lercher spoke about the elementary class of catalyzed transformations for biofuels. He discussed how a detailed knowledge of catalysts leads to new strategies.

CHARLETTE GEFFEN

Elected to UCAR Board of Trustees



Charlette Geffen, director of Research Strategy, Earth and Biological Sciences, was elected to the University Corporation for Atmospheric Research (UCAR) Board of Trustees for a three-year term. She will help determine the corporation's strategic direction.

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 over 4,300 staff, has an annual budget of $1.02 billion, and has been managed by Ohio-based Battelle since the Laboratory's inception in 1965.

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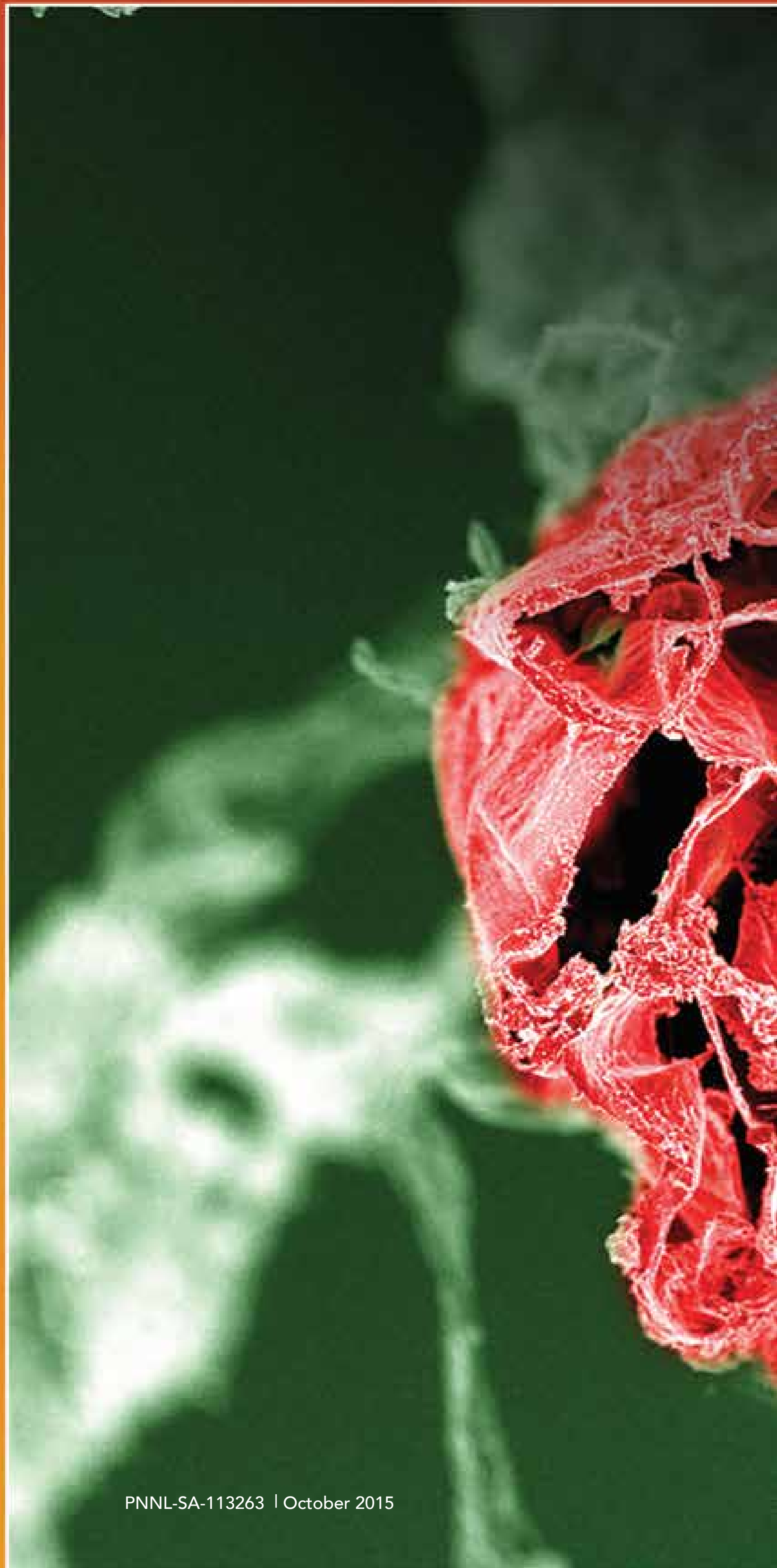

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