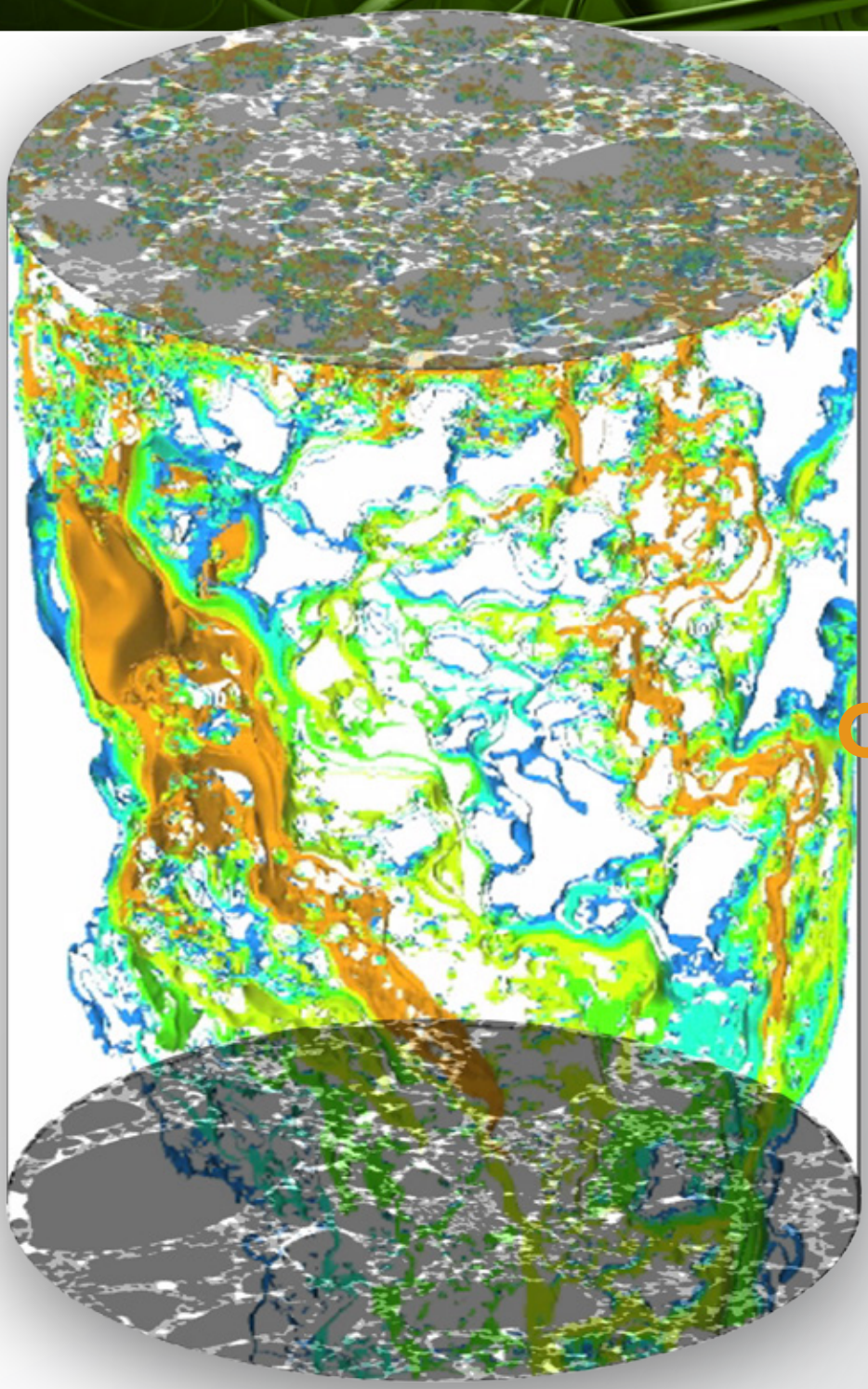
EMSL

THE MOLECULAR BOND

SCIENTIFIC INNOVATION THROUGH INTEGRATION

OCTOBER 2014



FAST COMPANY

Also inside this issue:

NWChem 6.5 Released

Improving Biofuels Production

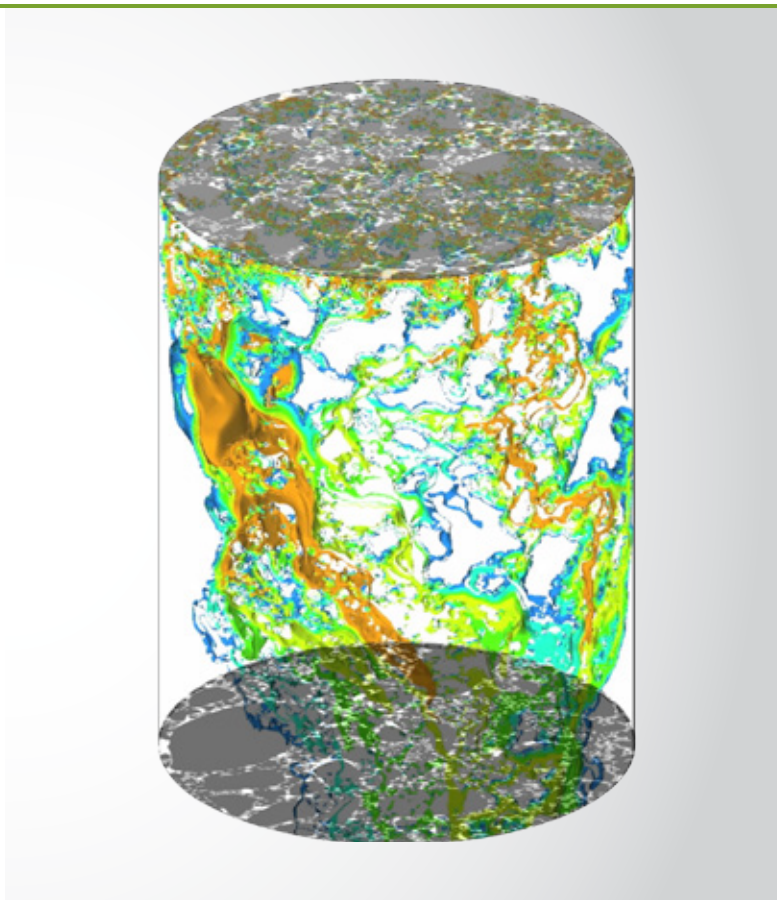
Postdoc Fellowship Open

Wiley Joins Editorial Board

Key Accomplishments Report Available

About the Cover

Researchers from the Pacific Northwest National Laboratory Subsurface Biogeochemistry Research Scientific Focus Area project combined flow and transport experiments with X-ray tomographic characterization and high-performance computing to study fluid flow and contaminant transport in complex natural porous media.



About *The Molecular Bond:*

The Molecular Bond is EMSL's bimonthly newsletter for users, potential users and other interested individuals. EMSL Communications oversees the production of *The Molecular Bond*.

EMSL, the Environmental Molecular Sciences Laboratory, is a national scientific user facility sponsored by the Department of Energy's Office of Biological and Environmental Research in the Office of Science. Located at Pacific Northwest National Laboratory in Richland, Wash., EMSL offers an open, collaborative environment for scientific discovery to researchers around the world. Its integrated computational and experimental resources enable researchers to realize important scientific insights and create new technologies. More information about EMSL is available at: www.emsl.pnnl.gov

To request additional copies or to subscribe, contact: EMSL Communications at email: emslcom@pnnl.gov

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EMSL's supercomputer Cascade is designed to run computationally intensive biology, climate, chemistry and materials science simulations aligned with the mission of the DOE's Office of Biological and Environmental Research. EMSL IT engineers James Czebotar (center) and Ian Smith check one of Cascade's data storage units. (EMSL file photo)

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EMSL

FROM THE DIRECTOR

Allison Campbell

EMSL helps scientists understand fundamental processes in biological, climate, environmental and energy systems through its impressive group of experts, advanced instrumentation and state-of-the-art facilities. In this issue, we explore the impact of integrating experiment and theory – and how advancing both parts of the equation can accelerate scientific impact. I'm pleased to share with you details on EMSL's new supercomputer, called Cascade, that we brought online last winter and how it and our computational chemistry code, NWChem, have enabled our users to make significant strides in studies related to biofuels and renewable energy. And we look at how we're continuing to evolve NWChem to be even more relevant for biological studies.

Integrating experimental and computational resources allows us to better understand and predict the behavior of complex systems such as climate and environmental systems. We encourage our users to consider how they can work with EMSL through both theory and experiment – let us know how this type of integration could benefit your research.

—Allison

Crystalline films are used in scientific and technological fields, including electronics, magnetics, magneto-optics, photonics, thermal- and photo-catalysis, and geochemistry. The molecular beam epitaxy deposition system at EMSL allows researchers to deposit and characterize oxide films with a high degree of specificity in both composition and structure. EMSL Scientist Yingge Du used the system for the research highlighted in the article "Angling Chromium to let Oxygen Through." (PNNL file photo)

NEWS & KUDOS

EMSL's Website has a new Look

EMSL's redesigned website highlights the research being done at the national scientific user facility.

You may have noticed EMSL's website has been redesigned. The fresh look better highlights the science being done at EMSL. The site also offers improved functionality, such as enhanced search capabilities, expanded drop-down menus and easier navigation to make the information you are looking for more accessible. Check it out at **http://www.emsl.pnnl.gov/emslweb** and let us know what you think of our new look.

2014 Key Accomplishments Report now Available

The Pacific Northwest National Laboratory 2014 Key Accomplishments: Fundamental & Computational Sciences report is now available as a downloadable PDF. The 32-page full-color brochure highlights some of the year's most noteworthy achievements at PNNL addressing global challenges in the areas of energy, security and environmental sustainability.

The report includes a section featuring EMSL's science highlights. As a national scientific user facility, EMSL's contributions to research discoveries are noted throughout the document.

(continued on page 4)

The brochure also features sections on advanced computing, biological systems science, chemical imaging, chemistry and geochemistry, climate and Earth systems science, materials sciences, and nuclear and particle physics. Selected staff awards and achievements also are recognized.

Download the 2014 Key Accomplishments report at **http://www.pnnl.gov/science/pdf/2014accomplishments.pdf**

2015 Wiley Postdoc Fellowship Position Open

Dr. William R. Wiley

EMSL is accepting applications for its 2015 William Wiley Distinguished Postdoctoral Fellowship through Nov. 7.

Starting in 2010, EMSL established the fellowship to attract high-performing newly graduated, junior Ph.D. scientists who have the potential to become full-time scientific staff at EMSL.

Candidates must display superb ability in scientific research and must show promise of becoming outstanding leaders in their research areas. In addition to a current curriculum vitae and unofficial transcripts, all candidates must submit a statement of research interest aligning with one or more of EMSL's Science Themes.

More information is available online at **http://www.emsl.pnnl.gov/emslweb/wiley-distinguished-postdoctoral-fellowship**.

The fellowship is named after a former Pacific Northwest National Laboratory director and the visionary leader of EMSL, Dr. William R. Wiley.

NWChem Version 6.5 Released

EMSL has released version 6.5 of NWChem, its premier open-source computational chemistry software.

NWChem allows researchers to tackle large complex and challenging molecular-scale scientific problems in the areas of catalysis, materials, geochemistry, atmospheric chemistry and biochemistry on highly scalable, parallel computing platforms to obtain the fastest time-to-solution. NWChem is being continuously updated and developed to include new theoretical methodologies and new parallel algorithms.

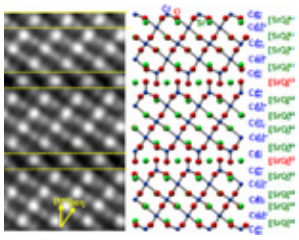
"The 6.5 version of NWChem provides users with several novel capabilities to model molecular systems and processes on existing and emerging hybrid computer architectures," said Karol Kowalski, acting technical lead and senior research scientist at EMSL.

Some of the new capabilities of latest release include:

- Analytical TDDFT gradients
- Analytical COSMO gradients
- Accurate calculation of Electron Affinities (EA) and Ionization Potentials (IP) with equation-of-motion coupled-cluster theory (IP/EA-EOMCCSD)
- Intel MIC port for the TCE CCSD(T) module
- Complete list of exchange-correlation functionals within planewave DFT
- Temperature accelerated molecular dynamics (TAMD).

Developed at EMSL, NWChem is one of the U.S. Department of Energy's premier computational chemistry tools. Highly scalable and portable, NWChem runs on a wide range of platforms from supercomputers, such as EMSL's Cascade and DOE's leadership class computing facilities, to desktop computers. NWChem is widely used at universities, other national laboratories and computer centers around the world. Since becoming open source at the end of 2010, the software has been downloaded more than 50,000 times.

Angling Chromium to let Oxygen Through



Scanning transmission electron micrograph (left) and structural model (right) for an ordered, nanostructured, rhombohedral phase, $SrCrO_{2.8}$ showing oxygen-deficient SrO_2 planes, which enable facile oxygen anion diffusion at low temperature. Brighter spheres are strontium ions; less-bright spheres are chromium ions. Oxygen anions are barely visible, and oxygen vacancies appear as black.

Scientists at EMSL and Pacific Northwest National Laboratory have generated a material that allows oxygen to efficiently move through it at relatively low temperatures. The team's attempts to make metallic $SrCrO_3$ led to the formation of semiconducting $SrCrO_{2.8}$. Oxygen can easily diffuse through this material's oxygen-deficient planes. The results represent an important scientific advancement that could lead to an increase in the efficiency of solid oxide fuel cells, which require oxides capable of absorbing and transmitting oxygen anions at low temperature. The findings were reported in *Nature Communications*.

(continued on page 5)

The team used a combination of experimental and theoretical methods. The scientists grew ultra-pure crystalline films with EMSL's molecular beam epitaxy deposition system, or MBE, and characterized the films using other EMSL resources. They used first-principles modeling to determine the structural transformations and oxygen anion diffusion kinetics.

Reference: Zhang H, Y Du, PV Sushko, ME Bowden, RJ Colby, and SA Chambers. 2014. "Reversible Nano-Structuring of $SrCrO_{3-\delta}$ Through Oxidization and Reduction at Low Temperatures." *Nature Communications 5*, Article number 4669. DOI: 10.1038/ncomms5669.

Wiley on *BMC Biology* Editorial Board

H. Steven Wiley

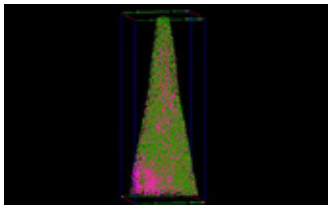
H. Steven Wiley, a PNNL Laboratory Fellow and EMSL scientist, has been appointed to the editorial board of *BMC Biology*, a peer-reviewed biology journal.

"*BMC Biology's* editorial board comprises an illustrious, international group of scientists in the field of biology, including several Nobel laureates," said Wiley. "I'm honored to have been asked to join this editorial board."

Some of the board's notable scientists include George Church with the Harvard Medical School and Michael Eisen with Lawrence Berkeley National Laboratory.

BMC Biology is the flagship biology journal of the BMC series, publishing peer-reviewed research and methodology articles in the area of biology.

EMSL Scientists Featured in *C&EN*



Atom probe tomography results from $Li_{1.2}Ni_{0.2}Mn_{1.6}O_2$ nanoparticle was one of several videos Devaraj provided for the *C&EN* "Microscopy Method Goes Deep" cover story.

The Oct. 13 issue of *Chemical & Engineering News*, or *C&EN*, highlights work by EMSL scientists Arun Devaraj and Daniel Perea. The cover story, entitled "Microscopy Method Goes Deep," explores developing the technique of atom probe tomography, or APT, for the analysis of energy, environmental and biological materials.

The *C&EN* article describes Devaraj's catalysis study recently published in the *Journal of Physical Chemistry Letters*. The *C&EN* article also features several videos and science images Devaraj produced using EMSL's APT and other capabilities.

In addition, the *C&EN* article explains Perea's efforts to use APT to analyze soft biomaterials by freezing them to cryogenic temperatures.

Water Gunks up Biofuels Production

Bio-oil is an alternate route to make transportation fuels currently derived from petroleum.

While trying to understand the chemistry that turns plant material into biofuel, researchers discovered water in the conversion process forms an impurity that slows down key chemical reactions. The findings reported online at the *Journal of the American Chemical Society* can help improve the processes to produce biofuels from plants.

The scientists from Pacific Northwest National Laboratory examined the conversion of bio-oil produced from biomass into transportation fuels. The researchers performed simulations using resources in EMSL to explore what happens to a common bio-oil byproduct. They found water turns the byproduct into an impurity that disrupts and blocks the reactions that create biofuels. The results apply not only to water but to related liquids in bio-oil such as alcohols and certain acids.

Reference: Yoon Y, R Rousseau, R Weber, D Mei and J Lercher. 2014. "First-principles Study of Phenol Hydrogenation on Pt and Ni Catalysts in Aqueous Phase." *Journal of the American Chemical Society*. DOI: 10.1021/ja501592y.

Watch EMSL's iDirector on YouTube

EMSL Director Allison Campbell interviews EMSL Lead Scientist Tim Scheibe about multiscale modeling and high-performance computing. Campbell talked with Scheibe as part of her monthly iDirector interview series available on EMSL's YouTube channel at **www.youtube.com/user/EMSLatPNNL**.

FAST COMPANY

High performance computing accelerates scientific advances

Computational speed is essential for scientists wanting to model or verify experimental systems in biology, climate and chemistry. The newest supercomputer at the Environmental Molecular Sciences Laboratory packs 20 times the processing power of its predecessor. But speed alone isn't enough to tackle the complex computational problems. Scientists are developing methods for fine tuning computing power to better parse chemical and biological reactions at the atomic level. Researchers can then apply that information, with more accuracy and predictability, to bigger scientific challenges.

"This is a critical issue," said Tim Scheibe, lead scientist for multi-scale modeling and high performance computing at EMSL. "While fundamental molecular science is our focus, we need to increase the impact of that science by making it relevant to large-scale questions about things like climate change, energy production and storage, or contaminated soil remediation."

"... we give you the ability to integrate physical experiments with computational modeling to enhance research results."

To increase the impact, supercomputers can help scientists narrow the gap between theoretical predictions and experimental results. If computations with EMSL's new machine, called Cascade, can provide more accurate details about chemical and biological reactions – calculating precisely when, where and how electrons, atoms and molecules move around – then the information can improve experimental design and efficiency, pushing the pace of the scientific process.

"One of the unique things about EMSL is we don't just give you one instrument to work with, we give you the ability to integrate physical experiments with computational modeling to enhance research results," Scheibe said.

The Need for Speed

Cascade is rated among the top 20 fastest computers in the world, with a 3.4 petaFLOPS rating. Each "FLOPS" (Floating-point Operations Per Second) is one math operation per second, and a "peta" is a quadrillion, Scheibe explained. So, the computer can perform more than one million, billion math operations every single second.

"Speed is an enabling thing," Scheibe said. For example, to optimize an organism for biofuel production, researchers could change one gene at a time and run 1,000 experiments, or run 1,000 simulations on the computer to get 10-15 best candidates for the actual experiment.

◀ **EMSL's Cascade supercomputer is rated among the top 20 fastest computers in the world.**

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Computers with that kind of speed need a radically different design.

"Engineering has hit a wall," said Karol Kowalski, computational chemistry expert at EMSL. "They can't make faster chips, so they add more. But instead of stacking more chips on each other, they use nodes with accelerator cards attached."

> ***"We need to combine the experimental with computation to really get at the reaction mechanism at the molecular level."***

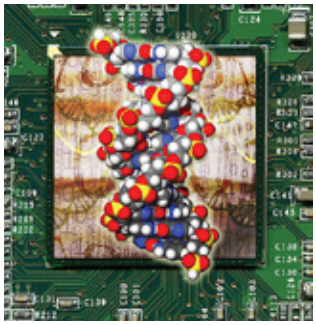
This new architecture can't support the same old software. So, EMSL's scientists developed new implementations in NWChem, a computational chemistry software code that gives researchers a suite of tools to help simulate molecular processes at the atomic level. To keep up with Cascade, the NWChem team, in collaboration with Intel, just issued NWChem 6.5. This new release enables users to take advantage of accelerators available on the new machine. (Read about the release of NWChem 6.5 on page 4.)

Boosting Biomass

Harnessing the speed of computers to refine experimental results has been a career-long approach for David Dixon, the Robert Ramsay Chair of chemistry at The University of Alabama.

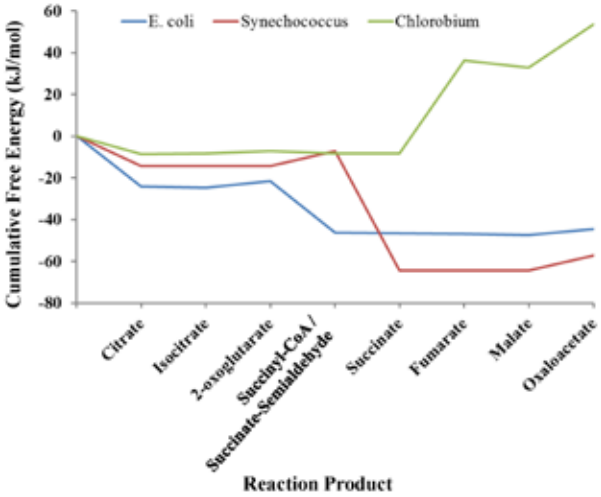
Decades ago, when mainframe computers took up entire buildings, he convinced DuPont computer modeling could save the company millions of dollars by predicting the properties of chemical compounds to minimize the costs of experiments. Now, the former associate director of theory, modeling and simulation of EMSL, leads a Department of Energy-funded effort on biofuels and industrial chemical intermediates. This research uses one of the largest time allocations on Cascade and has already produced nearly 20 publications.

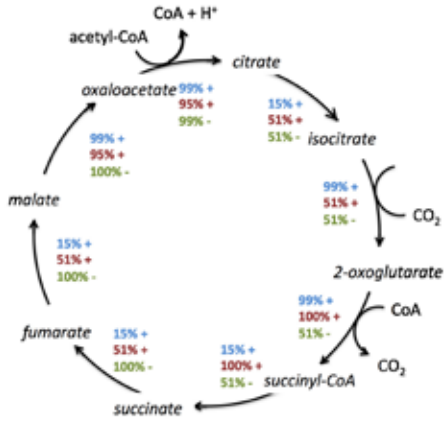
"Our team is trying to come up with new materials to catalyze chemical reactions with more control and less byproduct formation. This is a broad, long-term project to understand how biomass can most efficiently be converted to biofuel and valuable chemical intermediates," Dixon said.



EMSL's NWChem software is being used for applications in biology such as modeling metabolic pathways.

One quest for catalysis researchers is to find cheap, abundant elements to use – manganese or nickel – instead of expensive materials like platinum. To effectively use these "first row" transition metals, so called for their location in the periodic table, Dixon wants to understand precisely how atoms are bonding in specific reactions, and how much energy is needed to do so. With this knowledge, he can modify catalytic processes in the computer to model faster reaction times and avoid unwanted byproducts.





Using data from NWChem, statistical simulations determine thermodynamic energy profiles for metabolic pathways. (Top) In this case, the same pathway from three microbes were compared, and the resulting thermodynamic profiles reflect the ecological niche that the organisms are found in. (Bottom) The tricarboxylic acid cycle pathway showing the percent efficiency that each reaction that contributes to the net flux of material through the pathway.

With the computational resources at EMSL, Dixon and his team have worked out one part of the puzzle: how to convert alcohols into more useful products. By understanding alcohol conversions, eventually they can more efficiently convert sugars. Sugars are the building blocks of cellulose, a key biomass feedstock for biofuels.

"The goal is to understand the mechanism and find the governing chemical descriptors," said Dixon. "We can't get it just from experiments. We need to combine the

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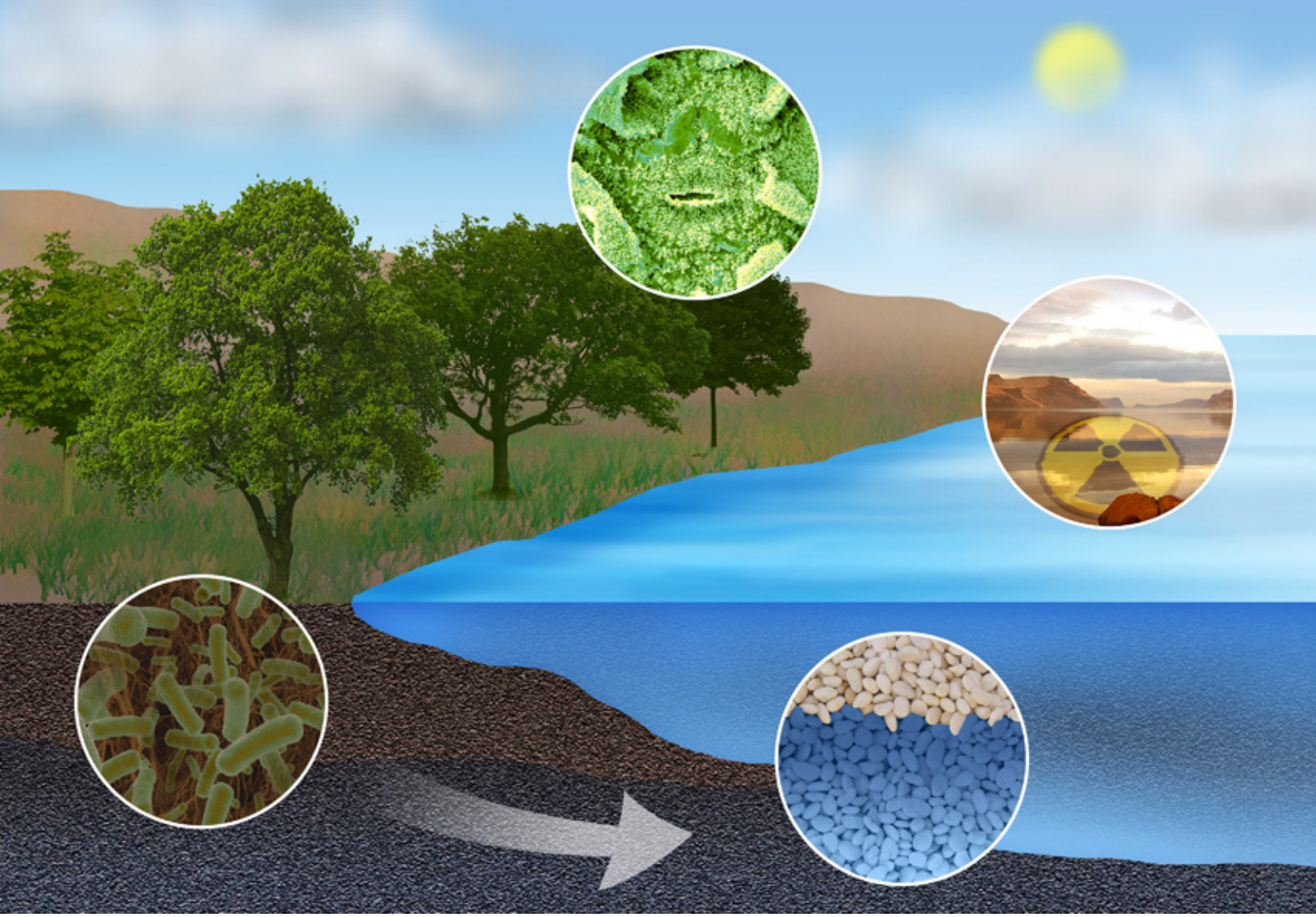

The integration of experiment and multi-scale computation improves the predictive power of models to better understand the relationship of the carbon cycle, microbial activity, and pore-scale flow and transport to help address diverse and critical global challenges including climate change and contaminated soil remediation.

experimental with computation to really get at the reaction mechanism at the molecular level. The experiments are critical as they benchmark our calculations and provide key constraints on the mechanisms."

The calculations are so large it takes the speed of Cascade, and NWChem software, to get the high level of accuracy needed to make reliable predictions of those mechanisms.

Chemical Computation

While some accuracy is derived from speed, some of it also comes from improvements in the way information is processed and calculations are performed. Even supercomputers are only as good as the slowest computational step.

"Sometimes people have the impression only the computers are getting faster. But algorithms and methods are getting better too," said Don Truhlar, a theoretical and computational chemist at the University of Minnesota.

One of the complex problems Truhlar's group tackled is the computational treatment of charge transfer and charge transport in photoactivated systems. In the same way Dixon tracks molecular bonding, Truhlar wants to account for electron movement in light-activated systems; information fundamental to understanding, and then manipulating, solar energy and other photoactivated catalytic processes.

In order to treat charge transport and charge balance, Truhlar needs to know where the charge is to begin with, and then how it moves. Although conventional simulation methods can predict charge movement in systems with only a few electrons, these methods breaks down in more complex systems where electrons and charged functional groups can exist in multiple excited states.

Truhlar and his group are creating methods to account for more complex electronic behaviors – such as multiple possible orbits and "tunneling" through boundaries – that exceed the accuracy of existing practical computational methods.

By "bootstrapping," Truhlar benchmarks the accuracy of new treatments against smaller systems, and then applies them to bigger systems. The NWChem software is an

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Cascade, EMSL's 3.4 petaFLOPS supercomputer was designed to run computationally intensive biological, climate and chemistry simulations aligned with the mission of the DOE's Office of Biological and Environmental Research.

important part of this research because it has modules to do the required accurate, high-level benchmarking calculations on Cascade. As new methods and algorithms are validated, Truhlar and his group are working with EMSL Scientist Niri Govind to integrate them into NWChem software.

Biology Blitz

While Truhlar is focused on developing tools for chemical computation, Bill Cannon, a senior scientist at Pacific Northwest National Laboratory, is modifying NWChem codes for applications in biology.

With a background in statistical thermodynamics and enzymology, Cannon recognized the mathematics he used to simulate protein metabolism could also be applied to modeling metabolic pathways. With more accurate thermodynamic models of these pathways, he ultimately wants to simulate the whole system of metabolic reactions – the mass action kinetics – in a single organism, and then scale it up.

"Only one group has ever been able to do that, and even then it was with tremendous effort and approximations," Cannon said. Right now, most models are based on conservation of mass; balancing amounts of "ingredients" against the end products in a particular reaction. But without accounting for energy and kinetics, the models are missing key statistical descriptions that affect whether reactions are even possible.

The conventional approach to simulating dynamics and predicting metabolite levels relies on having reaction rate constants, a difficult parameter to determine that varies tremendously with each enzyme-catalyzed reaction. But Cannon is "turning the usual approach to kinetics on its head." He sets metabolite levels and then lets the supercomputer find the rates, which makes the entire process faster. His group has already successfully simulated small pathways, such as the tricarboxylic acid cycle, a common metabolic route many organisms use to generate energy.

With more accurate modeling, researchers could simulate things such as: what happens when a vitamin gets added to growth medium for bacteria, or whether microbes still grow after one gene gets knocked out.

"There's a lot of unintended consequences from engineering microbes. We need something that will better predict what happens before an actual experiment," Cannon said. He estimates they're a year away from getting a large scale model of an organism, and maybe five years from mapping out a complex microbial community.

"Everybody asks how this will impact applications such as engineering for biofuels," Cannon said. "But the biggest breakthrough will be the capability to run dynamic simulations without using rate constants. That's much more fundamental."

Fast Forward

Although Cascade has been operational for users less than a year, EMSL is already planning a more integrated approach to bringing the next supercomputer on campus. In the past, when older computers were dismantled to make way for the new, scientists inevitably wanted to keep parts of the more familiar instrument. To smooth out transitions between machines, when Cascade came in, EMSL factored in ways to overlap with a new system every two years.

"We need something that will better predict what happens before an actual experiment."

"This new approach will also give us a chance to try different things. It's not always about speed," Scheibe said. "Sometimes there's greater efficiency in building more memory or disk space. Sometimes different computer architectures suit one kind of science more than another."

Those kinds of differences were discussed at a workshop Scheibe recently co-organized for connecting computational models across scales and science disciplines. In the future, supercomputers could be linked together; perhaps connecting a machine good for fast mathematical computations (Cascade) to an instrument better suited to sorting large data sets. Running these machines simultaneously could get answers faster and avoid time-consuming data transfer.

As scientific imaging becomes increasingly sophisticated, this parallel data processing will become more important. For instance, when EMSL's new dynamic transmission electron microscope comes online, it will generate terabytes of data every second. If information can be processed in real time, then the storage crisis could be avoided.

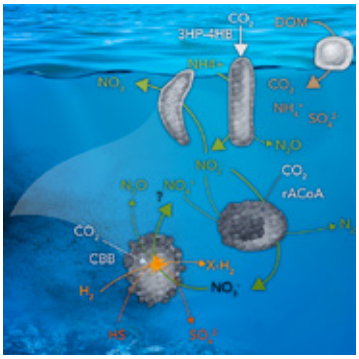
With each generation of supercomputers, EMSL users get another opportunity to rev up molecular research with innovations to help answer larger scientific questions. ■

Elizabeth Devitt is a science journalist and freelance writer.

SCIENCE HIGHLIGHTS

Marine Microbes Key Players in Study

How climate change will affect marine microbes



Oxygen-minimum zones, or OMZs, are widespread and naturally occurring oceanographic features. These zones are caused by microbial respiratory oxygen demand during 'remineralization' (transformation) of organic matter in poorly ventilated waters. Climate change is expected to cause OMZs to expand and intensify due to increased stratification and changes in ocean circulation patterns. The potential effects of OMZ expansion on microbial community structure and function are uncertain. This is the first metaproteomic study to examine microbial community responses to OMZ expansion across a range of water column redox states.

The findings reveal how OMZ expansion will affect coupled metabolic processes linking marine carbon, nitrogen and sulfur cycles. This has important implications for understanding the long-term ecological and biogeochemical impact of OMZ expansion on greenhouse gas production and nutrient availability in the ocean. At the same time, these findings directly inform the development of predictive models based on metaproteomic data.

Funding: This research was supported by the Department of Energy Joint Genome Institute and EMSL, the Tula Foundation funded Centre for Microbial Diversity and Evolution, the Natural Sciences and Engineering Research Council of Canada, Canada Foundation for Innovation and the Canadian Institute for Advanced Research through grants awarded to S.J.H.

Publication: Hawley A, H Brewer, A Norbeck, L Pasa-Tolic and S Hallam. 2014. "Metaproteomics Reveals Differential Modes of Metabolic Coupling among Ubiquitous Oxygen Minimum Zone Microbes." *PNAS* 111(31), 11395-400 (2014). DOI: 10.1073/pnas.1322132111

Participating Organizations: Hallam Lab at University of British Columbia, EMSL and DOE Joint Genome Institute.

How Atmosphere Ice Forms

New insights into atmospheric ice formation could improve climate models

The formation of ice crystals in the atmosphere strongly affects cloud dynamics, cloud radiative properties and the water vapor budget, and thus plays an important role in climate. To gain new insights into this poorly understood process, researchers used state-of-the-art micro-spectroscopy and chemical imaging methods to characterize the physical and chemical properties of ice-nucleating particles sampled from ambient air.

The study reveals the abundance of a given type of particle in the atmosphere can play a stronger role in ice formation than the particle-specific ice-nucleation propensity determined by the specific chemical and physical particle properties. These findings significantly advance our understanding of the underlying mechanisms that lead to ice formation in the atmosphere and could improve the accuracy of predictive cloud and climate models.

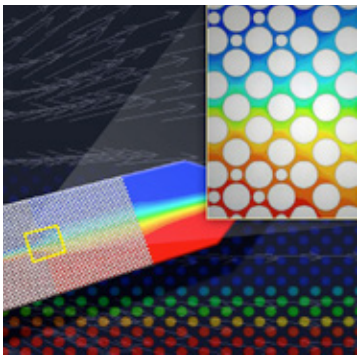
Funding: The Atmospheric Radiation Measurement Program sponsored by Department of Enegy's Office of Science's Office of Biological and Environmental Research, Climate and Environmental Sciences Division provided funding for sample collection. DOE's Atmospheric System Research Program, OBER, CESD provided funding for data analysis. PNNL provided Laboratory Directed Research and Development funds.

Publication: Knopf D, P Alpert, B Wang, R O'Brien, S Kelly, A Laskin, M Gilles and R Moffet. 2014. "Micro-Spectroscopic Imaging and Characterization of Individually Identified Ice Nucleating Particles from a Case Field Study." *Journal of Geophysical Research – Atmospheres*. DOI: 10.1002/2014JD021866

Participating Organizations: Stony Brook University, EMSL, Lawrence Berkeley National Laboratory and University of the Pacific.

How Chemicals Spread in Soils

Better bimetallic catalysts for fuel and chemical industries



Understanding how water and chemicals flow in soils is important for practical problems such as assessing the risk of groundwater contamination, developing effective ways to clean up contaminated soils and aquifers, and designing subsurface repositories for waste materials. A variety of pore-scale models use different computational approaches to capture important physical processes such as flow at the scale of microns – the size of soil grains and pores. This study tests pore-scale models by comparing computational results to carefully designed and replicated experimental data sets.

By highlighting the relative strengths of each computational approach, the study will accelerate progress in the field and lead to a better understanding of important pore-scale processes. This information could be used to accurately assess the risk of groundwater contamination and develop effective remediation strategies.

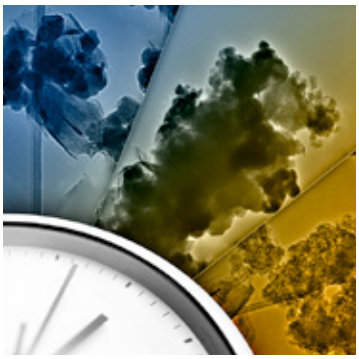
Funding: The experiments were conducted in 2011 at EMSL as part of the Pore-scale Modeling Research Campaign. The Sandia National Laboratory co-authors were supported as part of the Center for Frontiers of Subsurface Energy Security, an Energy Frontier Research Center funded by Department of Energy, Office of Science, Office of Basic Energy Sciences. Support from Los Alamos National Laboratory's Laboratory Directed Research and Development Program and Institutional Computing Center is acknowledged. Support for the University of Illinois' team was provided by the DOE's Subsurface Biogeochemical Research Program. The University of Texas' contribution was partly supported by the Center for Frontiers of Subsurface Energy Security, an Energy Frontier Research Center funded by DOE, Office of Science, and Office of Basic Energy Sciences. The Computational Fluid Dynamics simulations were performed using PNNL's Institutional Computing Center.

Publication: Oostrom M, et al. 2014, "Pore-Scale and Continuum Simulations of Solute Transport Micromodel Benchmark Experiments." *Computational Geosciences*. DOI 10.1007/s10596-014-9424-0

Participating Organizations: EMSL; PNNL; Los Alamos National Laboratory; Sandia National Laboratory; University of Illinois at Urbana-Champaign; University of Texas, Austin; University of Strathclyde, Glasgow; and Shell Global Solutions, Rijswijk.

Sequestration of Technetium

Promising remediation strategy



Technetium-99 is a common radioactive contaminant in groundwater at nuclear waste reprocessing sites and a top priority for remediation. After reacting with ferrous iron, technetium poses a lower risk of groundwater contamination. However, the long-term benefit of technetium sequestration as an oxide is uncertain because technetium oxide is highly susceptible to chemical conversion back to a soluble form. This study examines an alternative remediation strategy involving the sequestration of technetium as sulfide by sulfide-transformed nano zero-valent iron.

The findings suggest nano zero-valent iron can be used to promote sulfidic conditions and the subsequent formation of technetium sulfide, which is more resistant to oxidation than technetium oxide. Further study and careful evaluation of nano zero-valent iron with high sulfate concentration could represent a promising remediation strategy to improve the long-term stability of this heavy metal contaminant.

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Participating Organizations: Oregon Health and Science University, Stanford University and EMSL.

"Science is competitive, aggressive, demanding. It is also imaginative, inspiring, uplifting."

– Vera Rubin

About this Art

There is a growing realization that the physiology of higher organisms is strongly impacted by the associated microflora. This is also true of plants where microbes aid in nutrient acquisition and environmental tolerance. A multi-institutional group of scientists is studying the role and impact of microbial communities in the rhizosphere using multiple capabilities. This work is specifically focused on understanding how carbon allocation to the root environment impacts the diversity and size of the rhizosphere community. As is the case for most environmental microbial communities many of the organisms present are unculturable but new genomic methods allow their identification. This soil bacterium, shown attached to the plant root surface, was imaged using the Helios Nanolab dual-beam focused ion beam/scanning electron microscopy, or FIB/SEM, microscope at EMSL.

The project team included Ljiljana Paša-Tolic, Alice Dohnalkova, Joshua Aldrich, David Hoyt, Heather Brewer, Angela Norbeck and Galya Orr, all from EMSL; Kevin Minard, Charles Ansong, Will Chrisler and Meng Markillie, all from Pacific Northwest National Laboratory; Gary Stacey and Yaya Ciu, both from University of Missouri-Columbia; Susannah Green Tringe from DOE Joint Genome Institute; Michael Sadowsky and Chan Lan Chun, both from University of Minnesota; and Richard Ferrieri and Lihui Song, both from Brookhaven National Laboratory. *(Image colorized)*