



**Subsurface Biogeochemical Research**  
**Contractor-Grantee Workshop**  
**March 29-31, 2010**  
**JW Marriott**  
**Washington, DC**

| Time  | Title   | Room                   |
|---|---|------------------------|
| Monday, March 29, 2010  |   |                        |
| 7:00 AM   | <b>Registration Opens</b>   | Capitol Ballroom Foyer |
| <b>ACCOMPLISHMENTS AND THE ROAD AHEAD</b>   |   |                        |
| 8:30 AM   | <b>David Thomassen</b> , Chief Scientist, Office of Biological and Environmental Research   | Capitol Salons DE      |
| 9:00 AM   | <b>Paul Bayer</b> , Climate and Environmental Sciences Division   | Capitol Salons DE      |
| 9:20 AM   | <b>Complex System Science for Subsurface Fate and Transport</b><br>David Lesmes, Climate and Environmental Sciences Division  | Capitol Salons DE      |
| 9:45 AM   | <b>Advanced Simulation Capability for Environmental Management</b><br>Juan Meza, Lawrence Berkeley National Laboratory (LBNL)   | Capitol Salons DE      |
| 10:15 AM  | <b>BREAK</b>  | Capitol Ballroom Foyer |
| <b>DARCY AND BIRDSALL-DREISS LECTURERS</b>  |   |                        |
| 10:45 AM  | <b>Darcy Lecture</b><br>Timothy Scheibe, Pacific Northwest National Laboratory (PNNL)   | Capitol Salons DE      |
| 11:30 AM  | <b>Birdsall-Dreiss Lecture</b><br>Susan Hubbard, LBNL   | Capitol Salons DE      |
| 12:15 PM  | <b>BUFFET LUNCH (Research Team Meetings)</b>  | Grand Salons III/IV    |
| <b>BREAKOUT SESSIONS:<br/>MICROBIOLOGY, BIOGEOCHEMISTRY, AND TRANSPORT<br/>(See page 4 for details)</b> |   |                        |
| 2:00 PM   | <b>Breakout Session A: Systems Environmental Microbiology: Innovative Approaches to Understand Cellular and Microbial Community Activity and Function</b><br><b>Moderators:</b> Terry Hazen (LBNL) and Paul Bayer (DOE-BER) | Capitol Salons DE      |
| 2:00 PM   | <b>Breakout Session B: Biogeochemical Scale Transitions</b><br><b>Moderators:</b> John Bargar (SLAC-NAL) and Roland Hirsch (DOE-BER)  | Capitol Salon F        |
| 2:00 PM   | <b>Breakout Session C: Modeling and Simulation of Subsurface Systems</b><br><b>Moderators:</b> Carl I. Steefel (LBNL) and David Lesmes (DOE-BER)  | Capitol Salon G        |
| 5:30 PM   | <b>POSTER SESSION I – Hors d'oeuvres and Refreshments (Cash Bar)</b>  | Grand Salons I/II      |



| Time                           | Title   | Room                   |
|--------------------------------|---|------------------------|
| <b>Tuesday, March 30, 2010</b> |   |                        |
| <b>PLENARY SESSION</b>         |   |                        |
| 8:30 AM                        | <b>Anna Palmisano</b> , Associate Director, Office of Biological and Environmental Research   | Capitol Salons DE      |
| 8:45 AM                        | <b>Using Ecological Theory to Evaluate Microbial Community Trajectories During Uranium Bioremediation</b><br>Mary Firestone, University of California, Berkeley                                 | Capitol Salons DE      |
| 9:15 AM                        | <b>Progress in Understanding Mercury Biotransformations: From Molecular Modeling to Microbial Community Dynamics</b><br>Dwayne Elias, Oak Ridge National Laboratory                             | Capitol Salons DE      |
| 9:45 AM                        | <b>Bacterial Nanowires and Extracellular Electron Transfer to Heavy Metals and Radionuclides by Bacterial Isolates from DOE Field Research Centers</b><br>Yuri Gorby, J. Craig Venter Institute | Capitol Salons DE      |
| 10:15 AM                       | <b>BREAK</b>  | Capitol Ballroom Foyer |
| 10:45 AM                       | <b>Microscale Metabolic, Redox and Abiotic Reactions in Hanford 300 Area Subsurface Sediments</b><br>Haluk Beyenal, Washington State University   | Capitol Salons DE      |
| 11:15 AM                       | <b>Release of Aged Contaminants from Weathered Sediments: Effects of Sorbate Speciation on Scaling of Reactive Transport</b><br>Jon Chorover, University of Arizona                             | Capitol Salons DE      |
| 11:45 AM                       | <b>The Influence of Ligands on the Formation of Non-uraninite U(IV) Phases During Biotic and Abiotic U(VI) Reduction</b><br>Max Boyanov, Argonne National Laboratory                            | Capitol Salons DE      |
| 12:15 PM                       | <b>Poster Session II – Box Lunches Provided</b>   | Grand Salons I/II      |
| 3:30 PM                        | <b>BREAK</b>  | Capitol Ballroom Foyer |
| 4:00 PM                        | <b>Science Focus Area: Actinide Transport at Environmental Conditions - Nanoscale and Picomolar Concentrations</b><br>Annie Kersting, Lawrence Livermore National Laboratory                    | Capitol Salons DE      |
| 4:30 PM                        | <b>New Capabilities at the Environmental Molecular Sciences Laboratory (EMSL) – a DOE/BER Scientific User Facility</b><br>Don Baer, Pacific Northwest National Laboratory                       | Capitol Salons DE      |
| 5:30 PM                        | <b>Poster Session III – Hors d'oeuvres and Refreshments (Cash Bar)</b>  | Grand Salons I/ II     |



| Time                             | Title  | Room                   |
|----------------------------------|--|------------------------|
| <b>Wednesday, March 31, 2010</b> |  |                        |
| <b>PLENARY SESSION</b>           |  |                        |
| 8:30 AM                          | <b>Development and Fundamental Understanding of Catalytic DNA Biosensors for On-site and Real-time Detection and Quantification of Radionuclides and Metal Ions</b><br>Yi Lu, University of Illinois at Urbana-Champaign | Capitol Salons DE      |
| 9:00 AM                          | <b>Geophysical Characterization and Monitoring of Groundwater/Surface-Water Interaction in the Hyporheic Corridor at the Hanford 300 Area</b><br>Lee Slater, Rutgers University at Newark                                | Capitol Salons DE      |
| 9:30 AM                          | <b>Advanced Self-potential and Induced Polarization Inversion: Development and Use for Investigating Natural Recharge Processes</b><br>Andre Revil, Colorado School of Mines   | Capitol Salons DE      |
| 10:00 AM                         | <b>BREAK</b>   | Capitol Ballroom Foyer |
| 10:30 AM                         | <b>Tracing Contaminant Transformation, Immobilization, and Transport Using Cr, U, and Hg Isotope Ratios</b><br>Thomas Johnson, University of Illinois at Urbana-Champaign  | Capitol Salons DE      |
| 11:00 AM                         | <b>Carbon Cycling in Terrestrial Ecosystems: Research Challenges and Opportunities</b><br>Margaret Torn, LBNL  | Capitol Salons DE      |
| 12:00 PM                         | <b>Final Comments and Adjourn</b><br>David Lesmes, Climate and Environmental Sciences Division   | Capitol Salons DE      |



**BREAKOUT SESSIONS:  
MICROBIOLOGY, BIOGEOCHEMISTRY, AND TRANSPORT**

|                |   |                          |
|----------------|---|--------------------------|
| <p>2:00 PM</p> | <p><b>Breakout Session A: Systems Environmental Microbiology: Innovative Approaches to Understand Cellular and Microbial Community Activity and Function</b></p> <p><b>Moderators:</b> Terry Hazen (LBNL) and Paul Bayer (DOE-BER)</p> <p><b>Description of Session:</b> Advances in genome-enabled science have enabled an unprecedented opportunity to further the understanding of microbial metabolism and microbial communities in the environment. A continuing challenge is to productively use the enormous amount of information available in a format that aids hypothesis testing and experimentation. This session highlights a few selected projects from the Genomic Sciences program (and external programs) that are representative of new techniques and approaches to utilize genome-enabled information to understand microbial metabolism and function at the single cell and community level. The projects are illustrative of approaches that are or could be adapted more broadly to advance a predictive understanding of microbial processes in the environment. This breakout session is a follow-on to a previous session hosted by SBR program managers and featuring SBR PIs at the Genomic Sciences annual PI meeting in February 2010, in Washington DC and is intended to cross fertilize ideas for environmental microbiology among PIs in both programs.</p> <p>2:00 PM <b>Jennifer Pett-Ridge</b>, Lawrence Livermore National Laboratory (LLNL), Single Cell Environmental Microbiology with Nano Secondary Ion Mass Spectrometry (NanoSIMS)</p> <p>2:30 PM <b>Jennie Reed</b>, University of Wisconsin, Weaving Experimental Data into Genome-Scale Models Provides Insights into Cellular Environments and Behaviors</p> <p>3:00 PM <b>Terry Hazen</b>, LBNL, Ecogenomics with MicrobesOnline and KnowledgeBase</p> <p>3:30 PM <b>Break</b></p> <p>4:00 PM <b>Ross Carlson</b>, Montana State University, Molecular level in silico approaches to study mass and energy flows in microbial consortia.</p> <p>4:30 PM <b>Jillian Banfield</b>, University of California at Berkeley, Integrated 'omic' approaches to resolve structure and function in model natural microbial communities</p> | <p>Capitol Salons DE</p> |
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**BREAKOUT SESSIONS:  
MICROBIOLOGY, BIOGEOCHEMISTRY, AND TRANSPORT  
(Continued)**

2:00 PM

**Breakout Session B: Biogeochemical Scale Transitions**

**Moderators:** John Bargar (SLAC) and Roland Hirsch (DOE-BER)

**Description of Session:** Subsurface biogeochemical processes that govern the transport /fate of contaminants and CO<sub>2</sub> operate across a range of scales, from molecular to field, with numerous intermediate levels. Transitions of processes across scale boundaries (e.g., molecular to pore) correspond to transitions in complexity of media and process characteristics and challenge our ability to model subsurface characteristics and dynamics.

Knowledge of how such processes occurring at different levels of a hierarchical system link with each other and control higher-level behavior (and vice-versa) is essential to predicting solute behavior in complex subsurface systems. Of particular interest for this breakout session is the ability to understand and quantify the influence of molecular-scale processes on solute behavior at larger length scales or in more complex systems.

This breakout session will highlight scaling of molecular-scale biogeochemical processes to larger spatial scales and across different types/levels of complexity. Talks on this subject area will be followed by discussions to identify overarching issues, field research infrastructure needs, and approaches to understanding the roles and functions of molecular-scale processes at the field scale. The breakout session will produce a 2-page report that summarizes overarching scientific questions, logistics issues, and highlights example questions that penetrate deeply into this subject area.

2:00 PM **Huifang Xu**, University of Wisconsin , Role of nanopores in regulating U(VI) speciation and mobility

2:30 PM **Chongxuan Liu**, PNNL, The role of pore-scale reactive mass transfer in the scale-dependency of geochemical and biogeochemical reaction rates: a uranyl desorption case

3:00 PM **James A. Davis**, US Geological Survey, Upscaling Sorption Processes in Porous Media

3:30 PM **Break**

4:00 PM **Li Li**, Penn State University, Effects of Physical and Geochemical Heterogeneities on Biogeochemical Processes and Implications for Uranium Bioremediation

4:30 PM **Group Discussion**

Capitol Salon F





**BREAKOUT SESSIONS:  
MICROBIOLOGY, BIOGEOCHEMISTRY, AND TRANSPORT  
(Continued)**

2:00 PM

**Breakout Session C: Modeling and Simulation of Subsurface Systems**

**Moderators:** Carl I. Steefel (LBNL) and David Lesmes (BER-DOE)

**Description of Session:** The use of computer models to describe contaminant behavior in subsurface systems has expanded dramatically in recent years. The models are widely used for the purposes of prediction of contaminant migration and attenuation, but also now for the design of remediation schemes and for the interpretation of experimental data. Much of the impetus for the expanded use of models follows from the recognition of the complexity of contaminated subsurface systems, where multiple physical, geochemical, and biological processes interact at a variety of space and time scales. Such complex systems in fact may show emergent behavior that is not readily apparent from the individual processes themselves, however well understood these are. A new generation of mechanistic subsurface reactive transport models offers the possibility of unraveling these complex contaminated subsurface systems by providing an in silico laboratory in which process couplings can be analyzed in their appropriate dynamical context.

While subsurface complexity certainly drives much of the interest in a new generation of models, the application of such models are also enabled in an important way by the dramatic advances in high performance computing over the last 10 years. High performance computing (HPC), which will soon be available even to engineers and scientists working on contaminated sites far from the HPC bastions of the universities and national laboratories, will make it possible to carry out analyses at unprecedented levels of fidelity, both in terms of spatial resolution at a variety of scales, but also in terms of the rigor with which individual processes can be represented. With such advances, however, comes the need to collect, interpret, and integrate an ever-increasing array of data. It could be argued that the transformational effects of HPC may be just as significant in terms of what kind of data and observations are collected as in the analysis of the dynamics of the subsurface systems themselves.

Given the discussion above, we hope to be able to address the following questions in the course of the breakout session:

1. How do we identify the weakest links in our reactive transport models – what processes or parameters limit the predictive ability of the models most?
2. What role can the models have in experimental design, including pre-modeling and post-modeling for interpretation of results?

Capitol Salon G



3. What new theories are needed for HPC model development and application? Examples might include new theories for complex systems, for age dependence of biogeochemical rates, and upscaling and downscaling of parameters and processes.
4. How important is computer science and applied mathematics in terms of improving the predictive capabilities of the models?
5. Are there new kinds of data or characterization that can be incorporated into the models to improve their predictive capabilities? Examples might include isotopes, biomolecular signatures, proteomics, and geophysical signatures.
6. What can we do to optimize the relationship between the required data and the increasing levels of complexity in models (i.e., we need to recognize that much of what future models will be capable of could be data limited; how to minimize model complexity)?
7. Is the training for the next generation of environmental scientists adequate in modeling and complex system analysis?

**2:00 PM Steve Yabusaki**, PNNL, Progress and challenges in field-scale coupled process modeling

**2:20 PM Glenn Hammond**, PNNL, The role of high performance computing in Geosciences: Uranium migration at the Hanford 300 Area

**2:40 PM Gary Curtis**, US Geological Survey, Simulations of U(VI) desorption from contaminated sediments at the Naturita UMTRA site

**3:00 PM Group Discussion**

**3:20 PM Break**

**3:40 PM Nic Spycher**, LBNL, Complex reactive mechanisms: two contrasting examples

**4:00 PM Mavrik Zavarin**, LLNL, Predicting 1000 years of subsurface radionuclide transport at the Nevada Test Site

**4:20 PM Group Discussion**