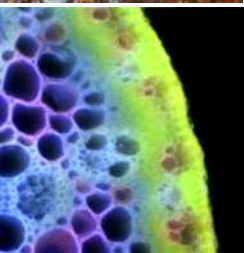


Subsurface Biogeochemical Research



SBR/TES Joint Investigators Meeting
Potomac, MD

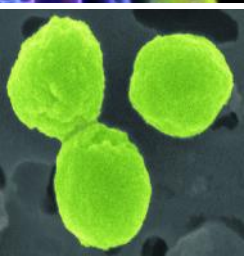
April 25-26, 2017



Paul Bayer, CESD

David Lesmes, CESD

Roland Hirsch, BSSD



U.S. DEPARTMENT OF
ENERGY

Office
of Science

Office of Biological
and Environmental Research

PI Awards and Publications (2016-2017)

Congratulations and Thank You!



Inaugural Editor-in-Chief
ACS Earth and Space
Chemistry Journal
J. Blum (U. Michigan) – 2016



AAAS Fellows
B. Gu (ORNL) – 2016
P. Sobecky (Alabama) – 2016

- 114 publications in 2014
- 112 publications in 2015
- 113 publications in 2016
- 34 publications (so far) in 2017



AGU Fellows
M. Firestone (UC Berkeley) – 2016
A. Revil (CSM) - 2016



SOCIETY OF EXPLORATION
— GEOPHYSICISTS —

Harold Mooney Award
S. Hubbard (LBNL) - 2016



AAM Fellows
F. Loeffler (ORNL/UT) - 2016



Berkeley Lab Director's
Early Career Scientific Achievement Award
H. Wainwright (LBNL) – 2016



E4D-RT: Real-Time
Four-Dimensional
Subsurface Imaging
Software
T. Johnson (PNNL)

Subsurface Biogeochemical Research (SBR) Program

Goal: The SBR program seeks to understand complex hydrobiogeochemical interactions from genome to watershed scales to enable new environmental and clean energy solutions.

Approach: SBR supports a wide range of research activities to advance the development of fully coupled models of subsurface environmental processes. These models incorporate:

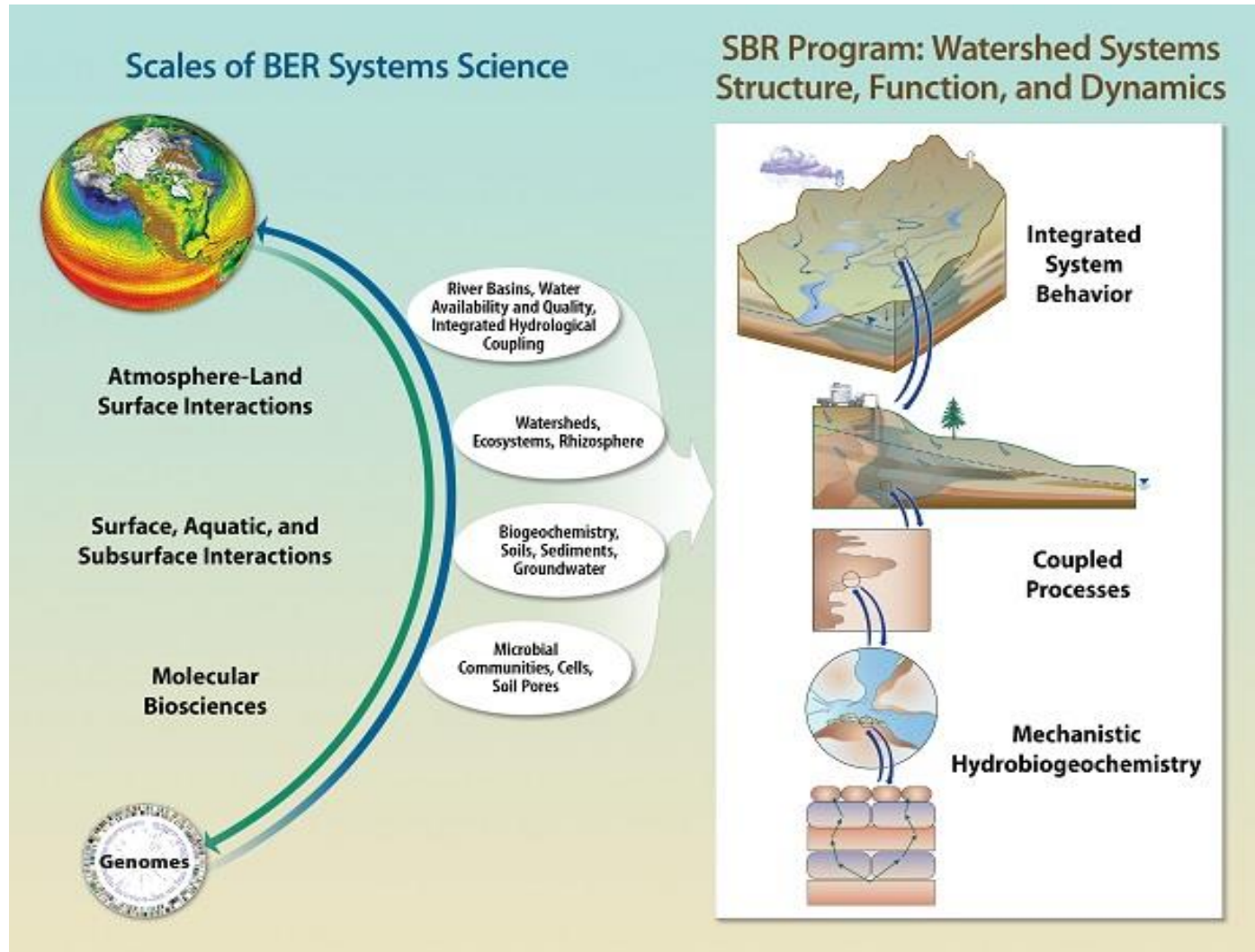
- Metabolic modeling of microbial processes;
- Molecular-scale understanding of geochemical stability, speciation, and biogeochemical reaction kinetics; and
- Diagnostic signatures of the system response at varying spatial and temporal scales.

Collaborative interactions as an Environmental Systems Science group with the Terrestrial Ecosystem Science (TES) Program.



Subsurface Biogeochemical Research (SBR) Program

Predictive understanding of integrated subsurface-watershed system behavior and response to perturbations



SBR Program Structure

Biology-Environment-Climate/ESM

DOE Energy &
Environmental Mission
*Disturbed and Managed
Watershed Systems*

Predictive
Understanding

**Larger SFAs:
*Integrated -
Watershed
Function***

LBNL SFA
Colorado River
Rifle to RMBL

PNNL SFA
Columbia River
Hanford Site

ORNL SFA
EFPCreek
Oak Ridge Site

**Smaller SFAs:
*Mechanistic
Hydro-BGC***

*Synthesis Across
Sites and Processes*

SLAC

LLNL

ANL

E.C.

EMSL, JGI, Synch
ESSDA, AmFlux,
NGEEs, CZOs

Univ.

IDEAS

SBIR

ESS-WG

*Computational Modeling &
Iterative Exp. and Obs.*

BER Computational Ecosystem: Virtual Lab

SBR Science Focus Areas

➤ **LBNL: Watershed Function**

- Biogeochemical dynamics from genome to watershed scales.

➤ **PNNL: Hydrobiogeochemical Process Dynamics in the Groundwater-Surface Water Interaction Zone***

- Developing a predictive understanding of the groundwater-surface water interaction zone and its linkages with the water cycle.

➤ **ORNL: Biogeochemical Transformations at Critical Interfaces**

- Determining the coupled hydro-biogeochemical processes controlling mercury fate and transformation in low-order freshwater stream systems.

➤ **ANL: Fe and S Biogeochemistry in Redox Dynamic Environments**

- Understanding the interplay among microbial metabolic activities, solution chemistry, and mineralogy that contribute to element and contaminant transformations.

➤ **LLNL: Subsurface Biogeochemistry of Actinides**

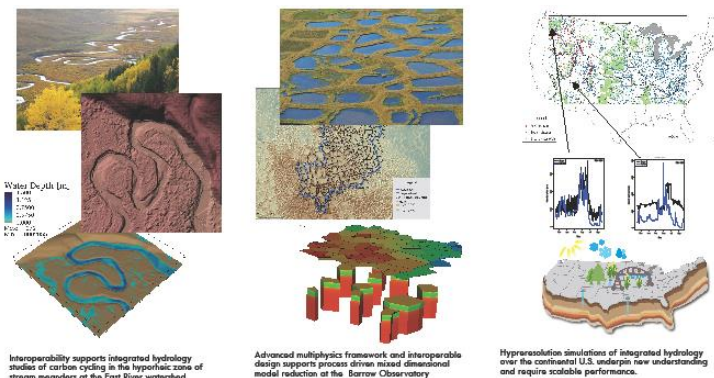
- Identifying biogeochemical processes that control actinide mobility in the environment.

➤ **SLAC: Coupled Cycling of Organic Matter, Uranium and Biogeochemical Critical Elements***

- Advancing predictive understanding of uranium subsurface biogeochemistry, fate, and transport.

ESS Scientific Goal

Improve software productivity and sustainability through ESS Use Cases.



Significance and Impact:

- Foundation for a Scientific Software Ecosystem (code and capabilities that are version controlled, open source, documented, tested)
- An interoperable system of codes could be used to explore scientific questions and predictive understanding in a variety of ways.

Domain Package Ecosystem:

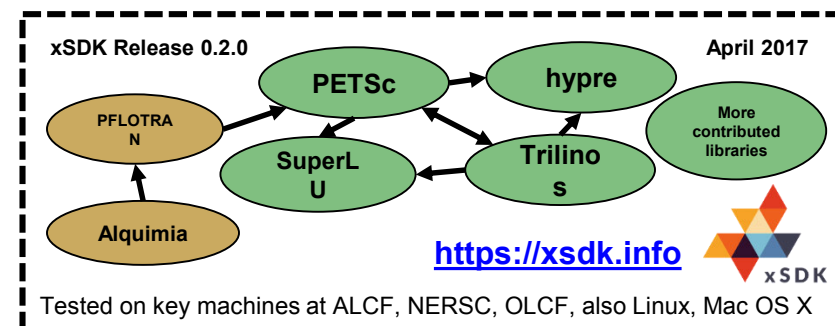
Alquimia, Amanzi, ATS, CrunchFlow, ParFlow, and PFLOTRAN

ASCR

xSDK: Extreme-scale Scientific Software Development Kit

- Numerical libraries: hypre, PETSc, SuperLU, Trilinos
- Domain components: Alquimia, PFLOTRAN

Improve software interoperability, quality, sustainability.



xSDK4ECP: Extend xSDK as needed by ECP applications

- Coordinated use of on-node resources
- Community policies and interoperability layers
- Integrated execution

IDEAS-ECP: Collaborate with ECP app teams to understand productivity bottlenecks and improve practices

- Productivity and Sustainability Improvement Planning Tools
- Coming summer 2017: New web-based hub for scientific software improvement exchange

<https://github.com/betterscientificsoftware/PSIP-Tools>



SBR Solicitations

- **ESS/SBR University Solicitations**

- FY17 SBR FOA 1724: SBR anticipates making ~10 awards.
 - CONUS and complementary to SFAs
- FY16 ESS FOA 1437: SBR made 12 awards.
 - Five 3-year awards and seven 1-year awards
- FY15: ESS FOA 1172: SBR made 4 awards.
 - CONUS and complimentary to SFA's

- **BER Early Career Solicitation: Lab and University Awards**

- Previous SBR Awardees: Matt Marshall (PNNL), Helen Hsu-Kim (Duke), Ming Ye (FSU); Joel Rowland (LANL), Jonathan Raff (Indiana U.)

- **Small Business Innovative Research (SBIR)**

- Technologies for Subsurface Characterization and Monitoring

SC Graduate Student Research (SCGSR) Program

<http://science.energy.gov/wdts/scgsr/>

2017 Solicitation 1: Due May 16, 2017

Supplemental Awards. 3 to 12 months conducting part of their doctoral thesis/dissertation research at a DOE lab. Collaborate with a DOE laboratory scientist.

Environmental System Science

FY16, Round 1 (SBR)

- K. Georgiou, UC-Berkeley (B. Riley, LBNL) – Mineral and Microbial Mechanisms Controlling Soil Carbon Cycling and Storage
- M. Nelson, UC-Irvine (J. Dunbar, LANL) – Trait-Based Approach to Microbial Comm. Charac.
- A. Ortiz, UTEP (E. Sonnenthal, LBNL) – Field, Exper. and Modeling to Understand Impacts of Flood Irrigation on Pedogenic CaCO_3 and CO_2 Dynamics in Drylands
- J. Rungee, UC-Merced (S. Hubbard, LBNL) – Hydrological Response to Multi-Year Dry Periods in the U.S. Mountain West

FY16, Round 2 (SBR)

- M.K. Hoffman, U Cincinnati (R. Kipps, LLNL) – Physiochemical Characterization of Ca-Rich Soil Samples from Marshall Islands
- L. Foster, CSM (K. Williams, LBNL) – Alpine Sensitivity to Climate Feedbacks

SBR Web Site & SC Highlights

<http://doesbr.org/>

Content and Graphics Updated

➤ Highlights:

<https://public.ornl.gov/site/submithighlight/newhl.cfm?seeform=yesfull>

➤ Videos: <http://doesbr.org/videos.shtml>

➤ Research Progress Timeline:

<http://doesbr.org/program/timeline.shtml>

➤ External Recognition:

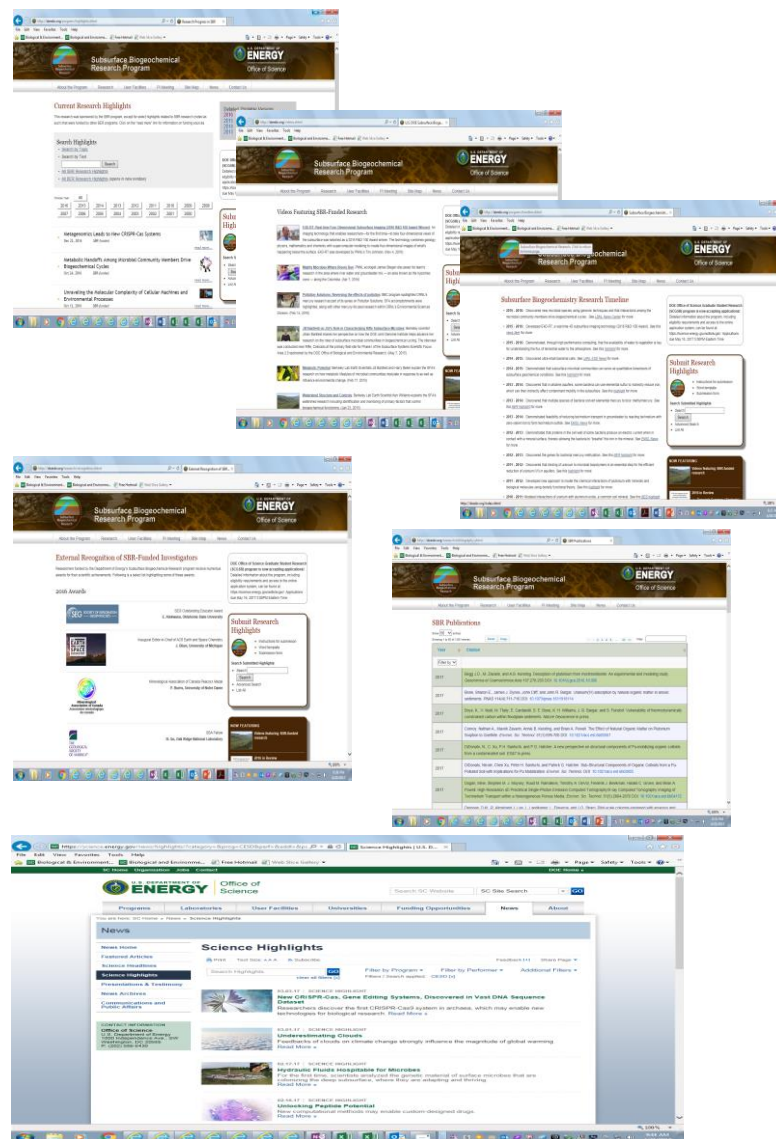
<http://doesbr.org/research/recognition.shtml>

➤ Bibliography:

<http://doesbr.org/research/bibliography.shtml>

Office of Science Highlights

➤ <https://science.energy.gov/news/highlights/>



SBR/TES in CESD Strategic Planning

Vision: Improve a systems level understanding and predictability of the earth system in support of DOE's mission, through integrative theory, modeling, and experiment, over a variety of spatial and temporal scales.

5-Year Scope: Integration of atmospheric, oceanic, terrestrial, ecological, hydrological, and human components, and inclusion of system-level uncertainty quantification.

High-Level Grand Challenges:

- System forcers – drivers of the coupled Earth-energy-human system.
 - High latitude – process feedbacks and interdependencies with the global system.
 - Biogeochemistry – biogeochemical processes and cycles across multiple scales.
 - Integrated water cycle – scale-aware and response to short and long-term perturbations.
-
- Data-model integration: interconnected capabilities and facilities that support the integration and management of models, experiments, and data across a hierarchy of scales and complexity.

Programmatic coordination with the BER Scientific User Facilities (ARM, EMSL, JGI and Synchrotrons) **Tues Lunch session; Wed. Breakfast session**

SBR Town Hall

Tuesday Evening (6:30 - 8:00 pm, Ben Franklin Hall)

- 6:30 pm SBR overview and expectations for Town Hall and Breakouts (D. Lesmes)
- 6:40 pm SBR Science: Bridging Scales and Disciplines to Advance Understanding and Enable Solutions to DOE's Energy and Environmental Challenges (S. Hubbard, T. Scheibe)
- 6:55 pm Overview of Watershed Systems Breakout (K. Williams)
- 7:05 pm Overview of Hydro-Biogeochemical (HBGC) Processes Breakout (J. Bargar)
- 7:15 pm Guided Discussion (S. Hubbard, T. Scheibe)
- 8:00 pm Adjourn

Wednesday Morning (8:30 am – 12:00 pm, Room 4 and Room 17A/B)

"Watershed Systems" Breakout (Room 4)

Hydro-Biogeochemical Processes Breakout (Room 17A/B)

Wednesday Afternoon (4:55 - 5:20 pm, Ben Franklin Hall)

Outbriefs from the SBR Town Hall

SBR Town Hall

Wednesday Morning (8:30 am – 12:00pm)

"Watershed Systems" Breakout Agenda (K. Williams, X. Chen, S. Painter, Room 4)

- 8:30 am "Watershed Systems" Supporting Research Questions and Sub-Questions (K.W., X.C., S.P.)
- 8:45 am DOE Cleanup and Stewardship Challenges: The Importance of Understanding Watershed Function Across Scales (E. Pierce)
- 9:00 am Developing Energy-Water-Nexus Test Beds and Modeling Frameworks (B. Vallario)
- 9:15 am National Water Model Developments and Future Needs (M. Smith)
- 9:30 am SBR Watershed Scale Test Beds: Predictive Understanding of Watershed System Structure, Function, and Dynamics pertinent to DOE missions in Energy & Environment (K.W., X.C., S.P.)
- 10:00 am BREAK
- 10:15 am University and Early Career Pop Up Presentations (2-min per pop-up)

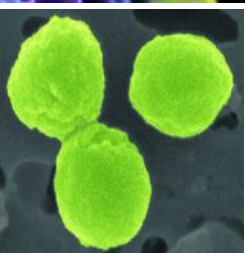
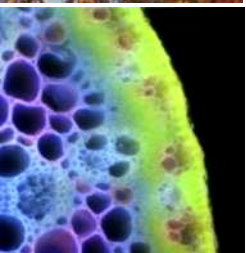
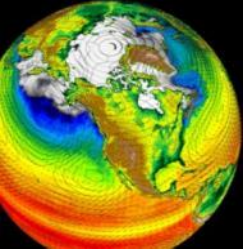
F.D. Lewis; L. Li; K. Maher; R. Maxwell; J. Rowland; J. Sharp; R. Wanty; M. Wilkins, M. Ye, J. Demers
- 10:35 am Hydrologic models across scales: From catchment to watershed to CONUS with focus on National Water Model development (R. Maxwell)
- 10:50 am Guided Discussion on Crosscutting Capabilities, Needs and Opportunities:
- 11:40 pm Community Building: Improving productive connections between projects, programs, agencies, and consortia (short, medium and long term)
- 12:00 pm Adjourn

SBR Town Hall

Wednesday Morning (8:30 am – 12:00pm)

**“Hydro-Biogeochemical Processes” Breakout Agenda (J. Bargar, K. Kemner,
M. Zavarin, Room 17A/B)**

- 8:30 am Coupled Hydrological and Biogeochemical Processes Controlling Iron and Arsenic Cycling within Asian Megadeltas (S. Fendorf)
- 8:50 am Mechanistic Modeling of Hydro-BGC Processes across Time and Spatial Scales (T. Scheibe)
- 9:00 am Modeling Microbial Community Diversity and Function (E. Brodie)
- 9:10 am DOE Cleanup and Stewardship Challenges (E. Pierce)
- 9:20 am University Pop Up Presentations (2-min per pop-up)
 - Yu Yang (University of Nevada, Reno)
 - Brian Powell (Clemson University)
 - Mike Wilkins (Ohio State)
 - Jeremy Smith (ORNL)
 - Jonathan Raff (Indiana University, Bloomington)
 - Marco Keiluweit (UMass, Amherst)
- 9:45 am Updated Scientific Grand Challenge and Supporting Science Questions (J.B., K.K., M.Z.)
- 9:55 am Guided Discussion: Supporting Science Questions
- 10:15 am Break
- 10:30 am Moderated Discussion to Develop Supporting Science Questions (Break into 3-4 subgroups)
- 11:15 am Report-outs from each Subgroup
- 11:30 am Identify Cross-Cutting Themes and Capability Needs
- 12:00 pm Adjourn



Questions?

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SBR Website: doesbr.org



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ESS PI Meeting - Memory Stick

➤ PI Meeting Agenda and Abstract Book

➤ Programmatic Documents

➤ BER

➤ BERAC

➤ Research Programs

- BSSD, CESD
- SBR, TES (New)

➤ User Facilities

- Overview Brochure
- EMSL, JGI, ARM



EMSL Integration/Multi-Omics for Microbiomes Conference

- August 1-3, 2017, Richland, WA
- <http://bit.ly/2eZOJzN>