Subsurface Biogeochemical Research

TES/SBR Joint Investigators Meeting
Potomac, MD

April 28-29, 2015

David Lesmes, CESD
Paul Bayer, CESD, EMSL
Roland Hirsch, BSSD – Structural Biology, GenSci, Synchrotrons
Thank You and Congratulations!
Recent SBR PI Award Recipients (2014-2015)

Walter L. Huber Civil Engineering Prize
M. Ye (U Central Fl) – 2015

Subaru Outstanding Women in Science
A. Riscassi (Univ. Virginia) - 2014

World’s Most Influential Scientific Minds
D. Lovley (Univ. Massachusetts) - 2014

- 181 publications in 2012
- 131 publications in 2013
- 104 publications in 2014
- 35 publications (so far) in 2015

AAAS Fellows
D. Lovley (Univ. Massachusetts) – 2014
M. Mayes (ORNL) - 2014

AGU Fellows
P. Santschi (Texas A&M) - 2014

Excellence in Reviews
B. Gu (ORNL) – 2014
D. Kaplan (SRNL) - 2014
Submit your Highlights!

Keep your SBR Program Manager and Fellow Scientists Informed

- Inform the SBR program.
- Inform fellow scientists.
- Submit:
  - Paragraph
  - Graphic
  - pdf of your pub

Web Page: https://public.ornl.gov/site/submithighlight/
Biological and Environmental Research

Understanding complex biological, climatic, and environmental systems across vast spatial and temporal scales

Genomes to Watersheds and Beyond
SBR Systems Approach: **Iterative, Multi-scale, Interdisciplinary**

Basic understanding of subsurface processes at the intersection of biology, chemistry, and physics. SBR supports interdisciplinary research in an iterative cycle of hypothesis generation, experimentation, and modeling between the laboratory and the field. Historically, the focus has been on elucidating the processes impacting the mobility of contaminant metals and radionuclides found in the subsurface at Department of Energy (DOE) legacy waste sites. Overall, this scientific approach is applicable to a wide range of DOE-relevant energy and environmental challenges.
Environmental System Science (ESS)

Advancing a *robust predictive understanding* of terrestrial ecosystems from “bedrock to atmosphere” and from global to molecular scales using an iterative approach to model-driven experimentation and observation.

**Scales:** Global...Regional...Watershed...Cell...

**Coupled Processes:** Phys+Chem+Bio;
Above ground-below ground interactions;
Terrestrial-Aquatic Interfaces (e.g., gw-sw);
Land-Atmosphere Interactions, etc.

**Models:** ACME...CLM...ED2...RTM...KBase...

**Data Sets:** Heterogeneous and Multiscale

**Computation:** Multiscale-Multiphysics HPC
Inputs to Strategic Directions for SBR

**BER Workshops and Reports**

- **2008**: CESD Integrated Water Cycle
- **2009**: BSSD Carbon Cycle, SBR Complex Systems
- **2010**: CESD Strategic Plan
- **2012**: CESD Integrated Water Cycle, BERAC Virtual Lab
- **2015**: SBR Building Virtual Ecosystems, BER Mol. Sci. Challenges

**Broader Community: BES, ASCR, EM, LM, NSF, USGS**

- **2009**: DOE-SC Scientific Opportunities for GW and Soils
- **20014**: ASCR Software Productivity
- **2009**: LBNL Complex Soil Systems
- **2009**: National CZO Program, Critical Zone Observatories
- **2014**: ISCMEM
- **2014**: CUAHSI

Department of Energy • Office of Science • Biological and Environmental Research
SBR Fundamental Research: **BSSD** ← **SBR** → **CESD**

**Goal:** Advance a robust predictive understanding of the hydrobiogeochemical structure and function of terrestrial environments from genomes to watersheds

**Systems Approach:** Iterative, Multi-scale, Interdisciplinary

*bottom-up*  →  *emergent behaviors*  ←  *top-down*

Mechanistic Formulation  ←  **Theory**  →  Parsimonious Application

**Contributions to CESD, BER and DOE Missions**

- Contaminant Mobility: plumes to watersheds; EM and NE
- Watershed Hydrobiogeochemistry: gw-sw interactions (T/A interface)
- Cycling of Carbon/Critical Elements: microbe-mineral-OM interactions
- Climate Modeling: ESM Grids to Watersheds?
- Land-Atmosphere Interactions?
  - Plant-Soil-Atm. System to Flux Sites to Watersheds
- Water-Energy-Land Nexus + Sustainability of Biofuel Crops?
SBR Restructured

Larger SFAs Research Watersheds
- LBNL SFA Colorado River Rifle to RMBL
- PNNL SFA Columbia River Hanford Site
- ORNL SFA EFP-Creek Oak Ridge Site

Smaller SFAs Fundamental Scales

Facilities, Infrastructure, Capabilities

Synthesis Across Sites and Processes

Computational Modeling & Iterative Exp. and Obs.

BER Computational Ecosystem: Virtual Lab + KBase

EMSL, JGI, Sync AmFlux, ARM, CZOs, E-Crops NGEEs

IDEAS

ESS-WG

SBIR

Univ.

ANL

LLNL

SLAC

E.C.
SBR Science Focus Areas

- **LBNL – Sustainable Systems SFA 2.0 – Genomes to Watersheds**
  - Model-drive enterprise to develop a predictive understanding of multi-scale, complex, and biologically-based terrestrial environments from genomes to the watershed scale.

- **PNNL – Environmental Significance of the Groundwater-Surface Water Interaction Zone**
  - Developing a predictive understanding of the groundwater-surface water interaction zone and its linkages with the water cycle both in terms of seasonal and annual fluctuations.

- **ORNL – Biogeochemical Transformations at Critical Interfaces**
  - Elucidating the mechanisms by which inorganic Hg is transformed into MeHg at the sediment-water interface and the processes that determine net MeHg production.

- **ANL – Fe and S Biogeochemistry in Redox Dynamic Environments**
  - Developing understanding of coupled biotic-abiotic molecular- to core-scale transformations of Fe and S within redox-dynamic environments.

- **LLNL – Subsurface Biogeochemistry of Actinides**
  - Identifying the dominant processes controlling actinide transport in the environment.

- **SLAC – Molecular-Scale Biogeochemical Processes Governing the Speciation, Dynamics and Stability of Uranium**
  - Investigating fundamental biogeochemical redox processes that control the behavior of uranium and critical biogeochemical elements.
### SBR Science Focus Areas

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**Plenary Session III: Radionuclide Biogeochemistry**

**Wednesday 1:30 – 2:30 PM**

**Concurrent Session 7: Multiscale Watersheds**

**Wednesday 2:30 – 4:00 PM**

**Concurrent Session 5: Soil OM – B. Gu**

**Concurrent Session 2: Microbiology – D. Elias**
SCIENCE QUESTIONS
How will climate induced changes in hydrology and vegetation affect subsurface metabolic potential and biogeochemical cycling?

What effect will interactions have on watershed biogeochemical functioning relevant to:
- Carbon cycling
- Contaminant mobility
- Biofuel crop sustainability?

DELIVERABLE
Development of GEWaSC: Genome-Enabled Watershed Simulation Capability
LBNL SFA 2.0 Study Sites

- Sites are located in the most important **western US River Basin - the Colorado River**
- Region **already threatened by global change** that have unexplored consequences to the Co River corridor ecosystem services
- A phased site development approach is in progress

At the data-rich **Rifle floodplain** ‘natural laboratory’, we are investigating O,N and moisture dynamics and genome to floodplain scaling

At the **East River headwaters catchment**, we are investigating meander-through-watershed and bedrock-though-canopy processes relevant to biogeochemical cycles

Photos courtesy of Roy Kaltschmidt, LBNL
Grand Challenge Research to develop multi-scale understanding and models of the terrestrial subsurface/surface water interface to predict contaminant nutrient, and biogenic gas fluxes at the local (10-100 m) and reach scale (50-80 km).

Approach:
- Chemical-hydrologic-microbiologic process interaction studies in the laboratory and field.
- Project team field experiments driven by seasonal/annual river stage variations; reach-scale data synthesis and measurements.
- Multi-scale modeling to link small-scale mechanistic process descriptions to higher system scales contained in ESM.

Key Recent Findings:
- Mixing of groundwater N and riverine (benthic) C creates an active biogeochemical zone at the extended interface.
- Multi-scale models are needed to deal with process complexity and hydrogeologic, geomorphic, and landscape variations.

Impacts: Modeling contaminant discharges to surface waters and biogenic gas emissions from the dynamic active interface.
Overarching objective: Provide scientific understanding of the rates and mechanisms of net MeHg production in contaminated environments.
Local and Global Implications

Foundational data to support cleanup of Hg contamination on ORR.

Key scientific outcome:
Hg, as a model system, serves as a platform for understanding biogeochemical processes that affect fate, toxicity, and fluxes of other trace metals, including radionuclides.

Foundational data to support UNEP’s desire to address Hg contamination globally.
Early Career Scientists – Plenary Session II

- Dan Hayes, ORNL (TES)
  - Geospatial representation of the circumarctic-scale permafrost carbon feedback

- Ming Ye, Florida State University (SBR)
  - Computational Bayesian framework for quantification of predictive uncertainty in environmental modeling

- Joel Rowland, LANL (SBR, NGEE-Arctic, RGCM)
  - Quantifying river dynamics and floodplain exchanges using remotely sensed imagery

- Matt Marshall, PNNL-EMSL (SBR)
  - Multi-system analysis of microbial biofilms

- Heileen Hsu-Kim, Duke University (SBR-PECASE Award)
  - Nanoscale Mercury Sulfide-Organic Matter Interactions and Implications for Solubility and Biomethylation

- Brian Powell, Clemson University (BES HEC-Award)
  - Examination of Actinide Chemistry at Solid-Water Interfaces

- Yongqin Jiao, LLNL (BSSD EC-Award)
  - Systems-level investigation of uranium resistance and regulation by *Caulobacter crescentus*
Building a Computational Infrastructure to Facilitate Cooperation, Competition, and Accelerate Scientific Discovery

➢ Challenges
   ➢ Complexity
   ➢ Fragmentation
   ➢ Disruptive hardware

➢ Scope
   ➢ Develop design requirements and a phased approach for a community model of terrestrial environments:
     ➢ Plants to Plots to Watersheds
     ➢ Mechanistic, multiscale and multiphysics
     ➢ Principles for governance

➢ Leads/Coordinator
   ➢ David Moulton (LANL)
   ➢ Tim Scheibe (PNNL)
   ➢ Carl Steefel (LBNL)
   ➢ David Lesmes (DOE/CESD)

Also posted on the SBR web page:  http://doesbr.org/
Building Virtual Ecosystems:
Virtual Plant-Soil System ↔ Virtual Plot ↔ Virtual Watershed
Building Virtual Ecosystems:
Virtual Plant-Soil System ↔ Virtual Plot ↔ Virtual Watershed

- Watershed-scale processes
- Catchment-scale hydrology and biogeochemistry
- Root interactions with soil and the microbiome
- Plot-scale hydrology and vegetation
Interoperable Design of Extreme-scale Application Software (IDEAS)

Motivation
Enable *increased scientific productivity*, realizing the potential of extreme-scale computing, through a new interdisciplinary and agile approach to the scientific software ecosystem.

Objectives
Address confluence of trends in hardware and increasing demands for predictive multiscale, multiphysics simulations.
Respond to trend of continuous refactoring with efficient agile software engineering methodologies and improved software design.

Impact on Applications & Programs
Terrestrial ecosystem *use cases tie IDEAS to modeling and simulation goals* in two Science Focus Area (SFA) programs and both Next Generation Ecosystem Experiment (NGEE) programs in DOE Biologic and Environmental Research (BER).

Approach
**ASCR/BER partnership** ensures delivery of both crosscutting methodologies and metrics with impact on real application and programs.

**Interdisciplinary multi-lab team** (ANL, LANL, LBNL, LLNL, ORNL, PNNL, SNL)
- ASCR Co-Leads: Mike Heroux (SNL) and Lois Curfman McInnes (ANL)
- BER Lead: David Moulton (LANL)
- Topic Leads: David Bernholdt (ORNL) and Hans Johansen (LBNL)
**Integration and synergistic advances in three communities** deliver scientific productivity; outreach establishes a new holistic perspective for the broader scientific community.

[http://ideas-productivity.org/](http://ideas-productivity.org/)
ESS Working Group: Model-Data Integration
Collectively Building “MODEX” Capabilities in Phases

Use Cases
- Near Term (0-2 yr)
- Intermediate Term (2-5 yr)
- Long Term (5-10 yr)

ESS Working Group Teams
- Software Engineering (SE)
- Model Development (MD)
- Data Management (DM)

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**SBR Fundamental Research:**  \( \text{BSSD} \xleftarrow{SBR} \text{CESD} \)

**Goal:** Advance a robust predictive understanding of the hydrobiogeochemical structure and function of terrestrial environments from genomes to watersheds

**Systems Approach:** Iterative, Multi-scale, Interdisciplinary

- **bottom-up** Mechanistic Formulation
- **emergent behaviors** Theory
- **top-down** Parsimonious Application

**Contributions to CESD, BER and DOE Missions**

- Contaminant Mobility: plumes to watersheds
- Watershed Hydrobiogeochemistry: terrestrial-aquatic interfaces
- Cycling of Carbon/Critical Elements: microbe-mineral-OM interactions
- Climate Modeling: ESM Grids to Watersheds? => **ACME**
- Land-Atmosphere Interactions? => **Session 7, Tuesday 7-8:30PM**
  - Plant-Soil-Atm. System to Flux Sites to Watersheds
- Water-Energy-Land Nexus + Sustainability of Biofuel Crops?
Solicitations

• ESS University Solicitation
  – FY15: Awards Pending
  – FY16: Solicitation Planned
    • SBR component will mainly be smaller projects (~$500k/3yrs)
    • SBR component will be complimentary to SFA’s

• Small Business Innovative Research (SBIR)
  – Technologies for Subsurface Characterization and Monitoring

• BER Early Career Solicitation: Lab and University Awards
  – FY 14: Water-Cycle
  – FY 15: Land-Atmosphere Interactions
  – FY 16: Topic TBD
Questions?

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SBR Website: doesbr.org
Upcoming Workshops

• ESS Workshop on Model-Data Integration
  – April 30 - May 1, 2015

• ASR/ARM/ESS Workshop on Aerial Needs
  – May 13 – 15, 2015

• BES-BER-ASCR Workshop on Basic Research Needs for Environmental Management
  – July, 2015

• CESD Workshop on Data Informatics
  – August, 2015
Integrated Software Ecosystem
Phased Approach to Science-Driven Co-Development

Virtual Watershed
- Watershed Model Components (SSH, SH, LSP, RT)
- vWatershed (SSH, SH, LSP, mgRT, DV)
- vWatershed Multiscale Genomics informed

Virtual Plot
- Plot Model Components (SSH, DV)
- vPlot (SSH, DV, mgRT)
- vPlot Multiscale Genomics informed

Virtual Plant-Soil System
- Plant Model Components (Below-/Aboveground)
- vPS System (ER, M3)
- vPS System Multiscale (ER, M3, MB)

Phase 1
Phase 2
Phase 3

Time
Year 3
Year 5
Year 10
Integrated Software Ecosystem
Phased Approach to Science-Driven Co-Development

Virtual Watershed

Watershed Model Components (SSH, SH, LSP, RT)

vWatershed (SSH, SH, LSP, mgRT, DV)

vWatershed Multiscale Genomics informed

Virtual Plot

Plot Model Components (SSH, DV)

vPlot (SSH, DV, mgRT)

vPlot Multiscale Genomics informed

Virtual Plant-Soil System

Plant Model Components (Below-/Aboveground)

vPS System (ER, M3)

vPS System Multiscale (ER, M3, MB)

Phase 1

Phase 2

Phase 3

Time

Year 3

Year 5

Year 10
Virtual Plant-Soil System: Why and How?

Natural Ecosystems
- Develop more realistic plant-functional-types in ESMs (<20 PFTs in current GCMs)
- Develop mechanistic basis for extrapolating plant structure-function relationships to future climate states using PFTs and trait-based models (e.g., drought, temp., CO₂, etc.)

Sustainable Bioenergy Feedstocks
- Provide integrative framework for understanding plant-soil systems where implications for discovery at smaller scales (e.g., root-microbe interactions) can be examined at whole plant and crop scales => Support hypothesis generation and testing
- Allow the application of optimization algorithms to identify more resource efficient ideotypes to guide breeding of emerging sustainable bioenergy crops: GxE

Phased Approach to Development: Design, Build, Test, Learn
- Integrate isolated models of plant components and processes to develop a framework to mechanistically capture the structure and function of whole plant-soil systems
- Start with biophysical models of 1 to 2 herbaceous bioenergy crop monocultures (“model organisms”) with robust aboveground and belowground plant components coupled to reactive transport models of soil (including microbiome genomics)
- Compelling science questions drive an iterative cycle of co-development and testing to increase model fidelity and range of species
- Incorporate plant and microbial genomic information
Integrated Software Ecosystem

Multiscale-Multiphysics Framework: Modular, interoperable, extensible, agile and easy to use across platforms (HPC to PC)

Computer Science:
- Software Eng.
- Applied Math
- Libraries
- Couplers
- Etc…

Domain Science:
- Systems:
  - Plants
  - Crops
  - Watersheds
  - River Basins
  - iH₂O Cycle
  - Etc…

Processes:
- Phy ⇔ Chm ⇔ Bio
Integrated Software Ecosystem
Building Virtual Ecosystems: Plants to Plots to Watersheds and Beyond...

Computational Science:
- Software Engineering
- Applied Mathematics
- Algorithms
- Computer Science
- Numerical Libraries
- Process Coupling
- Frameworks/Toolkits
- Performance
- Portability

Domain Science:
- Processes
  - Biological
  - Geochemical
  - Physical ...
- Systems
  - Plants, Plant-Soil
  - Crops
  - Watersheds
  - River Basins
  - Water Cycle ...

Interdisciplinary Community Development
Workshop Outcomes

- Workshop report on BER website
  http://doesbr.org/VirtualEcosystems/
- IDEAS Productivity project, supported by ASCR and BER
  https://ideas-productivity.org/
- Environmental System Science (ESS) Working Group being developed on Model-Data Integration
  - Modeling Frameworks + Data Management and Workflows + Software Engineering
- Two publications from the workshop discussions
  - “Plants in Silico”, Long, Zhu, Stitt, Millar, Lynch and LeBauer, Plant, Cell & Environment (PCE), accepted
  - “Virtual Watersheds,” in preparation
Subsurface Biogeochemistry of Actinides

- **Justification:** Advance our understanding of actinide behavior to enable actinide remediation, long-term stewardship, & safe storage

- **Mission:** Identify the dominant biogeochemical processes and mechanisms controlling actinide transport (Pu and Np) to reliably predict and control cycling and mobility of actinides in the subsurface

- **Approach:** Integrate molecular-scale mechanistic investigations and field studies. Advance research capabilities to achieve our scientific goals.
Argonne SBR SFA: Fe and S Biogeochemistry in Redox Dynamic Environments

Understanding coupled biotic-abiotic molecular to core-scale transformations of Fe and S within redox-dynamic environments and the effects of Fe and S biogeochemistry on the transformation and mobility of major/minor elements and contaminants.